ASD-TDR-62-858

A Computer Program for the Matano Analysis of Binary Diffusion Data

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TECHNICAL DOCUMENTARY REPORT NO. ASD-TDR-62-858

November 1962

Directorate of Materials and Processes
Aeronautical Systems Division
Air Force Systems Command
Wright-Patterson Air Force Base, Ohio

Project 7351, Task 735101

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FOREWORD

This report was prepared by Mr. Craig S. Hartley of the High Temperature Metals Section, Metals and Ceramics Laboratory, Directorate of Materials and Processes, and by Mr. Kenneth Hubbard of the Programming Branch, Digital Computation Division, Directorate of Systems Dynamic Analysis. The work was initiated under Project No. 7351, "Metallic Materials," Task 735101, "Refractory Metals," by the Directorate of Materials and Processes, Aeronautical Systems Division, Wright-Patterson AFB, Ohio.

The authors would like to express their appreciation to Dr. E. J. Rapperport of Nuclear Metals, Inc., for permission to use unpublished data.

ABSTRACT

A computer program for the Boltzmann-Matano solution to Fick's second law in semi-infinite binary diffusion couples is presented. The program is written in FORTRAN for the IBM 7090 digital computer. An error function curve fit is used to interpolate between and smooth experimental data, and the calculations performed on the regenerated data.

Examples are given of application of the program to incremental couples with no intermediate phases and to pure metal couples with and without intermediate phases. Phase boundaries in couples with intermediate phases can also be obtained with a high degree of accuracy. By substituting lattice spacings for ordinary distance units, a correction for molal volume change due to composition differences can be programmed.

This technical documentary report has been reviewed and is approved.

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TABLE OF CONTENTS

	Page
INTRODUCTION	1
THE COMPUTER PROGRAM	4
Definition of Symbols	4
Outline of Program Operations	6
Discussion of Operation	6
Input Preparation	9
Error Messages and Stops	10
Output	10
Limitations	10
DISCUSSION OF RESULTS	11
CONCLUSIONS	12
LIST OF REFERENCES	13
FIGURES	14-25
APPENDIX A: PROGRAM LISTING	27
APPENDIX B: SAMPLE OUTPUT AND INPUT	49

LIST OF ILLUSTRATIONS

Figure		Page
1.	Schematic Concentration-Penetration Curve for a Semi-Infinite Diffusion Couple	14
2.	Probability Plot for the System Cu-Ni for 362 Hrs. at 947°C	15
3.	Probability Plot for the System Cu-Ni for 312 Hrs. at 1054°C	16
4.	Probability Plot for the System W-Ru for 168 Hrs. at 1800°C	17
5.	Concentration-Penetration Curve for the System Cu-Ni for 312 Hrs. at 1054°C	18
6.	Interdiffusion Coefficient versus Concentration for the System Cu-Ni for 312 Hrs. at 1054°C	19
7.	Diffusivities in the System Cu-Ni at 1054°C	20
8.	Probability Plot for Cu-Alpha Brass Couple for 507 Hrs. at 837°C	21
9.	Concentration-Penetration Curve for Cu-Brass Couple for 507 Hrs. at 837°C	22
10.	Diffusivity versus Concentration for Cu-Brass for 507 Hrs. at 837°C	23
11.	Concentration-Penetration Curve for W-Ru Couple for 168 Hrs. at 1800°C	24
12.	Diffusivity versus Concentration for W-Ru for 168 Hrs. at 1800°C	25

INTRODUCTION

Diffusion is the transport of matter by atomic motion. The driving force for the process is a difference in free energy from one region of a specimen to another; this may be due to a gradient in composition, temperature, electrical potential, pressure, or any other Hamiltonian variable. That aspect of diffusion which is of particular interest to the metallurgist and which has been most extensively investigated in metals is mass flow due to composition differences.

The phenomenological laws which govern diffusion were first formulated by Fick (ref 1) by analogy with Fourier's Laws of heat conduction. Stated in its most general form, Fick's First Law for an isotropic substance may be written:

$$\vec{J} = -B \ \mathrm{grad}\ \mu \tag{1}$$

where $\vec{J}$ is the vector of the diffusion current, i.e., mass motion, B is the mobility or diffusion current for unit driving force, and μ is the chemical potential. The surface of reference is usually chosen perpendicular to $\vec{J}$. Although metals are not isotropic substances, they are usually considered so for diffusion analyses.

For the case of diffusion due to a concentration gradient along one direction only, equation 1 may be written:

$$\vec{J} = -D \frac{dc}{dx} \tag{2}$$

where $D = B \frac{d\mu}{dc}$ is called the chemical diffusivity or diffusion coefficient. In using equation 2 to determine D we must find an experimental arrangement which enables us to measure both dc/dx and $\vec{J}$; this is not generally feasible in cases where one metal is diffusing through another. The usual method of evaluation involves a measurement of the change in concentration with time due to diffusion. Considering a volume element with unit cross-sectional area and infinitesimal thickness, dx, we may express the concentration change with time as:

$$\frac{dc}{dt} = \frac{d}{dx}\left(D \frac{dc}{dx}\right) \tag{3}$$

The above expression implies that D is a function of concentration as is usually observed in metal systems.

A common experimental arrangement for the evaluation of D in binary metal systems is the semi-infinite diffusion couple. In this experiment two slabs of metal whose thicknesses are very large with respect to the distance over which diffusion will occur are brought into intimate contact under time and temperature conditions sufficient to establish a measureable concentration gradient in regions near the original interface. The variation of concentration along the diffusion distance is measured and the diffusivity calculated using a solution of equation 3 with appropriate boundary conditions.

Manuscript released by the authors 17 September 1962 for publication as an ASD Technical Documentary Report.

Although the foregoing discussion implies that diffusion in metals is a mutual phenomenon, i.e., the current of atoms of one type through the lattice of the other metal is equal to its complementary effect, sophisticated analyses show that this is not the case. To account for all experimental observations, it is necessary to hypothesize the existence of a third diffusing entity, vacancies, or empty lattice sites, into which the diffusing atoms move. This complicates the mathematical analysis somewhat and introduces two more diffusion coefficients, which are somewhat more difficult to measure with the usual experimental arrangements. Since the observed effects are usually small with respect to those resulting from the process as a whole, their exclusion from the analysis of diffusion does not vitiate the more "macroscopic" description developed above (ref 2).

The boundary conditions for the semi-infinite diffusion couple may be stated:

$$c = c_o; \quad x<0; \quad t = 0 \qquad c = c_o; \quad x = -\infty; \quad t \neq 0$$

$$c = c_f; \quad x>0; \quad t = 0 \qquad c = c_f; \quad x = +\infty; \quad t \neq 0$$

where c is the concentration of substance A at some point in the diffusion zone. The solution of equation 3 for the above boundary conditions is given by Boltzmann (ref 3) and was first applied to metal systems by Matano (ref 4). Introducing the parameter $y = xt^{-1/2}$, equation 3 becomes:

$$\frac{d}{dy}\left(D\frac{dc}{dy}\right) = -\frac{y}{2}\left(\frac{dc}{dy}\right) \tag{4a}$$

and upon integration:

$$D = -\frac{1}{2}\left(\frac{dy}{dc}\right)\int_{cf}^{c} y\,dc \tag{4b}$$

Substituting for y we obtain:

$$D = -\frac{1}{2t}\left(\frac{dx}{dc}\right)\int_{cf}^{c} x\,dc \tag{4c}$$

In the above expression x = 0 is defined by the condition that:

$$\int_{c_f}^{c_o} x\,dc = 0 \tag{4d}$$

The quantities dc/dx and that expressed in the left side of equation 4d, hereafter called A*, are obtained by differentiation and integration of an experimentally determined plot of c versus x as shown in figure 1; t is simply the time interval during which diffusion has occurred. Jost (ref 5) has pointed out that equation 4c is valid even when the plot of c versus x has discontinuities, i.e., when intermediate phases are formed during the diffusion process.

It is also instructive to examine the solution of equation 3 for the case of constant D and semi-infinite boundary conditions. In this case:

$$\frac{c - c_f}{c_0 - c_f} = \frac{1}{2}\left[1 - \text{erf}(u)\right] \tag{5}$$

where

$$u = \frac{1}{2} x (Dt)^{-\frac{1}{2}}$$

and

$$\text{erf}(u) = \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2} dt$$

The left side of equation 5 is called the concentration function or the normalized concentration and is denoted c_i. It can also be shown that:

$$\frac{c - c_f}{c_0 - c_f} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} e^{-\frac{t^2}{2}} dt \tag{6}$$

where $z = - u\sqrt{2}$. Equation 6 is the cumulative normal distribution with argument z. In both cases a graph of u or z versus x will be linear and will have a slope related to the diffusion coefficient.

It has been pointed out by Hall (ref 6) that the concentration-penetration curves in certain systems can be approximated with a very high degree of accuracy by a series of linear segments on a probability plot, i.e., one in which the ordinate is linear in z and the abscissa, linear in x. For cases where the experimentally determined curves have no discontinuities, two linear segments may be necessary to describe the curve. This implies that under certain conditions a diffusion couple can be treated as two or more systems in each of which the diffusivity is a constant and different from that in the others. The necessary conditions for this treatment are not well defined but appear to be associated with the width of the diffusion zone.

Baroody (ref 7) has suggested that a polynomial of low degree, i.e., second or third, may be used to fit segments of the probability plot where straight lines are not obtained. By solving for the coefficients of such a polynomial a concentration-penetration curve may be reconstructed on cartesian coordinates. The principal advantage of this device is that it has been observed empirically that the relationship of z or u to x is usually a simpler one than that of c to x.

Figure 2 (ref 8) illustrates a probability plot of a concentration-penetration curve typical of a system which forms a continuous series of solid solutions at the diffusion temperature. Intuitive reasoning concerning physical behavior leads us to believe that the two straight lines should not be extended to the point of intersection (because this would require a discontinuity in the diffusion coefficient, hence, in the structure of the alloy) but both should gradually deviate from linearity and join so that the slope is well defined and single-valued at all points in the region of intersection. For relatively short diffusion distances the resolution of most analytical techniques is frequently insufficient to illustrate this deviation. However, for longer zones, such as that in figure 3 (ref 8), the deviation is readily apparent, and for a sufficiently wide zone a linear plot cannot be obtained. However, the graph shown in figure 3 can be approximated by two linear segments joined by a parabola or cubic. Similar effects occur in multi-phase diffusion couples such as the one shown in figure 4 (ref 9).

THE COMPUTER PROGRAM

Definition of Symbols

In the following tabulation, problem variable symbol means the symbol used for a quantity in the text of this report while program symbol refers to the symbol used for that quantity in the computer program.

PROBLEM VARIABLE SYMBOL	PROGRAM SYMBOL	DEFINITION
x_i	TX (I)	Experimentally determined distances from one end of the diffusion zone in units compatible with CVF
$c_i(x_i)$	TY (I)	Experimentally determined concentrations at position x_i
c_i	CA (I)	Normalized concentration
x_i	X (I)	Distances in regenerated data
c	CA (I)	Concentrations in regenerated data
None	NS	Number of segments for curve fitting purposes
N	NP	Total number of input data points
None	N (I)	Number of points in Ith segment
None	ND (I)	Degree curve fit desired for Ith segment
None	DX	Tabulation interval for regenerated data

Definition of Symbols (Cont'd)

t	TME	Diffusion time
None	CVF	A factor for converting the computed diffusivities to desired units
c_o	CMDH	Maximum concentration of component A in the diffusion couple
c_f	CMDL	Minimum concentration of component A in the diffusion couple
None	ID	Hollerith information for output identification
x_m	XM	The Matano interface
c	CAF (I)	Concentration at which diffusivity is calculated
x_f	XF	Computed distance for a given concentration c
D	D	Diffusivity obtained using error-function slope
None	DP	Diffusivity obtained using parabola slope
None	DERF	Slope of the concentration-penetration curve from error function
None	DERP	Slope obtained from a parabola fit through the three tabular points nearest to XF, CAF (I)
None	DTI	Concentration interval at which diffusivities are calculated

Outline of Program Operations

The program performs the following operations in the order listed:

1. Normalizes the input concentrations by the transformation where c_i is equal to the relationship expressed by the left term of equation 6.

2. For the normalized c_i, finds z from the relationship given by the right term of equation 6.

These values result in a table of z_i versus x_i.

3. Fits a least-squares curve of specified degree to z_i, x_i; i.e.,

$$z = \sum_{n=0}^{3} A_n x^n$$

when $n \leq 3$.

4. Using these curve fits, re-tabulates the data at a specified interval of x by computing c_i where c_i is equal to the relationship expressed by the right term of equation 6. The resulting tabulation of c vs. x_i is called the regenerated data.

5. Converts the regenerated data back to original units (un-normalized).

6. Uses Simpsons's Rule integration to find $\int c_i(x)\,dx$ over the range of x.

7. Translates the origin of the regenerated curve to (c_f, x_m).

8. Computes x and the area A* for CAF(I); CAF(1) = CMDH - DTI.

9. Computes DERP, DERF, D, DP, for CAF(I).

10. Tabulates CAF, D, DP, XF, DERP, and DERF.

11. Sets CAF(I + 1) = CAF(I) - DTI and repeats 8, 9, 10, and 11 until CAF(I) = CMDL - DTI.

12. Reads input data for next case or returns control to the FORTRAN Monitor if this is is the last case.

Discussion of Operation

The main purpose of this discussion is to enable the reader to use the program with a reasonable amount of effort. A FORTRAN Language listing is provided in Appendix A and is considered an adequate documentation of the program. A job deck punched from this list can be used to compile and run the program on the IBM 7090 computer, using the standard FORTRAN system. The only requirement is that the system peripheral input tape be Logical Tape No. 2, and the system peripheral output tape be Logical Tape No. 3. If this is not the case simple changes to the input-output statements of the program will eliminate this necessity.

Three quantities must be determined from an experimental curve of concentration versus distance in the diffusion zone. First, the Matano interface, which defines the zero point on the abscissa, must be obtained. Next, a computation of the diffusivity at a specified concentration requires that the slope of the curve and the area, A*, be evaluated at the concentration, c, for which the diffusivity is to be calculated. It is readily apparent that the values of D obtained from such an analysis are very sensitive to the particular curve drawn through the experimental points. In many cases two apparently reasonable freehand curves through the experimental points will yield slopes differing by a factor of two or more at some points. The Matano interface and the area A*, will also be affected but to a lesser degree. Thus, the curve fit used is the crux of the problem in the analysis of diffusion data.

The experimental data are used to construct a concentration-penetration curve by fitting a low order (first, second, or third degree) least-squares polynominal to a plot of z (as defined earlier) versus x, the distance along the diffusion zone. The concentration function is set equal to zero and 1000 at some values of distance chosen to define the width of the diffusion zone. It frequently happens that a straight line is sufficient to describe most of the data. However, in the case where two straight-line segments must be used in a single phase field, a second degree fit may be used in the region of intersection to avoid a discontinuity in the slope. A new concentration-penetration curve, called the regenerated curve, is calculated from the least-squares fit and tabulated at equal distance intervals. The concentration function is then converted back to the original concentration units. The quality of the curve fit thus obtained is checked by comparison with the original data; the fit is considered satisfactory if the original data are reproduced to within the estimated experimental accuracy. An additional check is available for multi-phase couples since the regenerated curve must yield the phase boundary compositions at the x-coordinates of discontinuities.

The Matano interface is found by numerical integration of the entire curve by the following scheme. By referring to figure 1, this interface is defined such that A = A′; the area A can be calculated by subtracting the area $\int_0^{x_m} c\,dx$ from the large rectangle $(c_o - c_f)(x_m - 0)$ where x = 0 in this case is the distance coordinate of the last point where c = 1.000 (reading from left to right). Now the area A′ is obviously $\int_{x_m}^{x_n} c\,dx$, where x_n is the distance coordinate of the first point for c = 0.000. Thus, since A = A′,

$$(c_o - c_f)(x_m) = \int_0^{x_m} c\,dx + \int_{x_m}^{x_n} c\,dx$$

$$= \int_0^{x_n} c\,dx \qquad (7)$$

The integral is simply the area under the concentration-penetration curve in the diffusion zone. If c_f = 0 and c_o = 1, the numerical value of this area is x_m. To perform the remainder of the analysis, the distance axis may now be shifted such that x_m = 0.

The curve which is used to fit the raw data is of the general form:

$$z = A_i + B_i x + D_i x^2 + E_i x^3 \tag{8}$$

For the ith segment:

$$\frac{dc}{dx} = \frac{dz}{dx}\frac{dc}{dz} = \frac{(B_i + 2D_i x + 3E_i x^2)e^{-\frac{z^2}{2}}}{\sqrt{2\pi}} \tag{9}$$

Thus, the slope of the regenerated curve on a cartesian plot can be calculated using the coefficients of the polynomial which fits the data on a probability plot and the derivative of the normal distribution function with respect to z. For a given value of c for which D is to be calculated, the program determines the segment of the probability plot upon which it falls, retrieves the coefficients, B_i, D_i, and E_i, and computes the slope by the above method. Another method (used also as a check) fits a parabola to the three tabular points on the regenerated cartesian plot nearest that for which the slope is to be calculated. If the tabulation interval is small enough, the slope of such a parabola at the point of interest will be very nearly that of the true curve. In fact, for the cases investigated, the difference between these slopes rarely exceeds 10 percent and is frequently much less.

Finally, the area A* is calculated. From figure 1 we note that A* may be divided into three segments. The distance coordinate of the composition for which D is to be calculated is called x_f and the distance coordinate of the nearest tabular point, x_k. The subscript k increases for x_o to x_n as defined above. Four cases occur in the computation of A*; these necessitate different methods of finding S_1, S_2, and S_3.

Case 1: $x_k < x_f < x_m$

$$S_1 = (x_m - x_f)(c_o - c)$$

$$S_2 = (x_f - x_k)(c_o - c) - \frac{1}{2}(x_f - x_k)(c + c_k)$$

$$S_3 = (x_k - 0)(c_o - c) - \int_0^{x_k} c\,dx$$

Case 2: $x_f < x_k < x_m$

$$S_1 = (x_m - x_k)(c_o - c_k)$$

$$S_2 = (x_k - x_f)(c_o - c_f) - \frac{1}{2}(x_k - x_f)(c + c_k)$$

$$S_3 = (x_f - 0)(c_o - c_f) - \int_0^{x_{k-1}} c\,dx - \frac{1}{2}(x_f - x_{k-1})(c + c_{k-1})$$

Case 3: $x_m < x_f < x_k$

$$S_1 = (x_f - x_m)(c - c_f)$$

$$S_2 = \frac{1}{2}(x_k - x_f)(c_k + c)$$

$$S_3 = (x_n - x_k)(c_k - c_f) - \int_{x_k}^{x_n} c\,dx$$

Case 4: $x_m < x_k < x_f$

$$S_1 = (x_f - x_m)(c - c_f)$$

$$S_2 = \frac{1}{2}(x_k - x_f)(c_k + c)$$

$$S_3 = (x_n - x_{k+1})(c_{k+1} - c_f) - \int_{x_{k+1}}^{x_n} c\,dx$$

The diffusivity is the product of $\frac{1}{2t}$, $\frac{dx}{dc}$ and A* as shown in equation 4(c).

Input Preparation

The preparation of data for input to the computer involves some preliminary work to determine the type of curve fit desired. First, the data are normalized as described in equation 5 or 6. Next, they are plotted on probability coordinates versus the distance along the diffusion zone. It is determined from visual observation whether the data may be adequately represented by a straight line, a curve, or by various combinations of the two. The selection of a second or third degree fit for the curved segments is rather arbitrary and, generally, either may be used. However, one or the other occasionally matches more smoothly with the other segments at the points of intersection.

Based on the above considerations, the total curve is divided into segments and the number of experimental points on each segment determined. The x-coordinates of any discontinuities, i.e., phase interfaces, are also recorded.

All symbols used are program symbols as previously defined. The first card of the input deck can contain any combination of legal Hollerith characters. Columns 1 - 72 of this card will be printed with the output for identification purposes. The following quantities are entered with a format of I3, beginning with column 1 of the second card in the order shown: NS, NP, N(1), N(2). . . N(NS), ND(1), ND(2), . . . , ND(NS). All of the above must be right justified in the field. No decimal point is used. Beginning with the third card, the quantities listed below are entered five per card in the order shown, using a format of E 13.7: TX(I), TY(I), DX, TME, CVF, CMDH, CMDL, DTI. Another card is not started if the tabulation of a given variable does not fill the last field of a card. If the input data contains discontinuities, the value of x at which the discontinuity occurs is entered with a corresponding negative concentration. This point is used only to locate discontinuities and is not considered part of any segment. It must, however, be included in the total number of points, NP.

Error Messages and Stops

There are no stops in the program. A stop normally occurs only when the input data is exhausted. Errors in input data can cause the FORTRAN system to terminate the problem. The program writes an error message on the output tape when the following conditions occur:

1. The solution for the intersection between two segments yields no root that falls between the last point on the ith segment and the first point on the (i + 1)th segment. The message printed is: BREAK POINT ERROR. The roots found are printed following the message. The program processes the data as usual but the results obtained are questionable and changes required in curve fit are indicated.

2. When tabulating D versus concentration, the program fails to find a segment on which a given value of concentration falls. The message printed is: PROGRAM FAILED TO LOCATE SEG. FOR CA = C.

3. The value of x_f found for a given concentration does not lie between x_{k-2} and x_{k+2} when x_k is the distance, in the regenerated data, such that the corresponding concentration is nearest the concentration at which D is to be calculated. The message printed is: UNSATISFACTORY XF FOR CA = C.

Output

The first line of output is always the data ID card. This is followed by a tabulation of the input quantities NS, NP, N(1) . . . N(NS), and $c_i(x_i)$ versus x_i in the order listed. All other output is clearly identified and needs no further explanation. A sample output is given in Appendix B.

Limitations

Although the following are limitations of the program as presented, most of them can be removed by simple changes to the program.

1. A maximum of 200 points of input concentration data.

2. A tabulation internal for x must be chosen so that there will be no more than 2000 data points of regenerated data.

3. Least-squares curve fits specified must not exceed 3rd degree.

4. The number of points in any one segment of concentration input data must not be greater than 100.

5. Input concentrations must be non-increasing with increasing x.

DISCUSSION OF RESULTS

A typical curve fit obtained from this program is shown in figure 5. This is the cartesian plot reconstructed from figure 3. The first six and last seven points in figure 3 were fitted with straight lines, while the center segment was fitted with both a second and a third degree polynomial. This was done primarily to obtain the best possible fits at the intersections of the linear segments. It is evident that no difference is detectable on the cartesian plot, but the diffusivity versus concentration relationship for this couple, shown in figure 6, shows noticeable changes at the concentrations corresponding to the intersections. It seemed that the diffusivity calculated using the slope of a parabola fitted to the three tabular points nearest the concentration of interest may exhibit a more continuous behavior in these regions. However, little is gained by this procedure, as illustrated in figure 7. Although it is somewhat difficult to explain the physical basis for these changes, the computed diffusivities are believed to be more accurate than those calculated by manual techniques.

An example of a pure metal/alloy couple which forms no intermediate phases on diffusion, e.g., copper/alpha brass, is given in figures 8, 9, and 10. The probability plot, figure 8, illustrates the linear relationship on one side of the original interface and nonlinear behavior on the other. In this case a second degree fit was used for the latter. The reconstructed concentration-penetration curve is shown in figure 9 along with the experimental points. The corresponding relationship of diffusivity versus concentration is shown in figure 10.

Finally, the case of a pure metal/pure metal couple which forms an intermediate phase on diffusion is shown in figures 11 and 12. A probability plot for this pair is given in figure 4. The values of phase boundaries obtained from the reconstructed data agree extremely well with those obtained by other techniques (ref 10). Again the diffusivity-concentration relationship shows a sharp change at the intersection of the two linear segments on the probability plot. Computing the diffusivity by using the parabola slope does not appreciably affect this behavior. Values of D calculated by a graphical technique are also shown in figure 12. Although agreement is generally good, the graphical technique does not show the sharp change which characterizes the computer values.

An analysis of each step in the calculation of D, comparing graphical integration and differentiation with values obtained by the computer, shows that the only appreciable discrepancy occurs in the computation of the slope of the concentration-penetration curve. The fact that the values obtained by the computer are calculated by two essentially independent methods, yet usually agree to within five percent or better, leads us to believe that these are the more accurate values.

A point which might be raised in connection with the curve fitting technique is the following: if, over some composition range, a linear relationship holds between x and z (or u) in equations 5 and 6, this implies a constant diffusivity in that range (ref 5). This diffusivity, D , may be calculated directly from the slope of the linear segment. However, a constant diffusivity is not obtained by the Matano analysis, as shown in figures 6, 7, 10, and 12. A careful examination of equation 5 (or 6) will show that if only one straight line which passes through an origin defined by choosing the original interface as x = 0 could be used to represent the experimental points, the Matano analysis would yield a constant D that would be the same as D′. It is not obvious, however, that the Matano analysis performed on a composite cartesian curve constructed from two or more linear segments will yield constant diffusivities over the linear regions; in fact, it does not for the cases investigated, although the variation of diffusivity with concentration is frequently quite slight.

CONCLUSIONS

The program described in this report represents a major improvement in accuracy and reduction in time in the analysis of binary diffusion data. Using a binary deck to avoid compilation time, a typical analysis can be completed in thirty seconds. In the case of multiphase couples the output provides useful information on phase boundary compositions in addition to the diffusivity calculations.

Although not an original development of this program, one outstanding advantage of the curve fitting technique is the ability to obtain a maximum of information from a minimum of data. For instance, if a diffusion zone is extremely narrow so that only one data point may be obtained in a particular phase, a linear fit may be made on probability coordinates using this point and the phase boundary composition, which must exist at the interface, as the other (assuming this is known). While the absolute values of the diffusivities calculated in such a region are certainly questionable, at least some curve may be constructed through these points, and, since its contribution to the total area is usually very small, it is possible to calculate reasonably good diffusivities for the other portions of the curve.

Finally, it should be pointed out that while the concentrations and distances used in the examples given are in terms of atomic fraction and centimeters (or inches) respectively, this need not be the case. If the variation of molal volume with composition is known for the system under investigation, the input concentrations may be converted to the units of atoms/unit volume and the distances to lattice spacings. The computed diffusion coefficients will then be corrected for molal volume changes in the diffusion zone, if there is no gross porosity.

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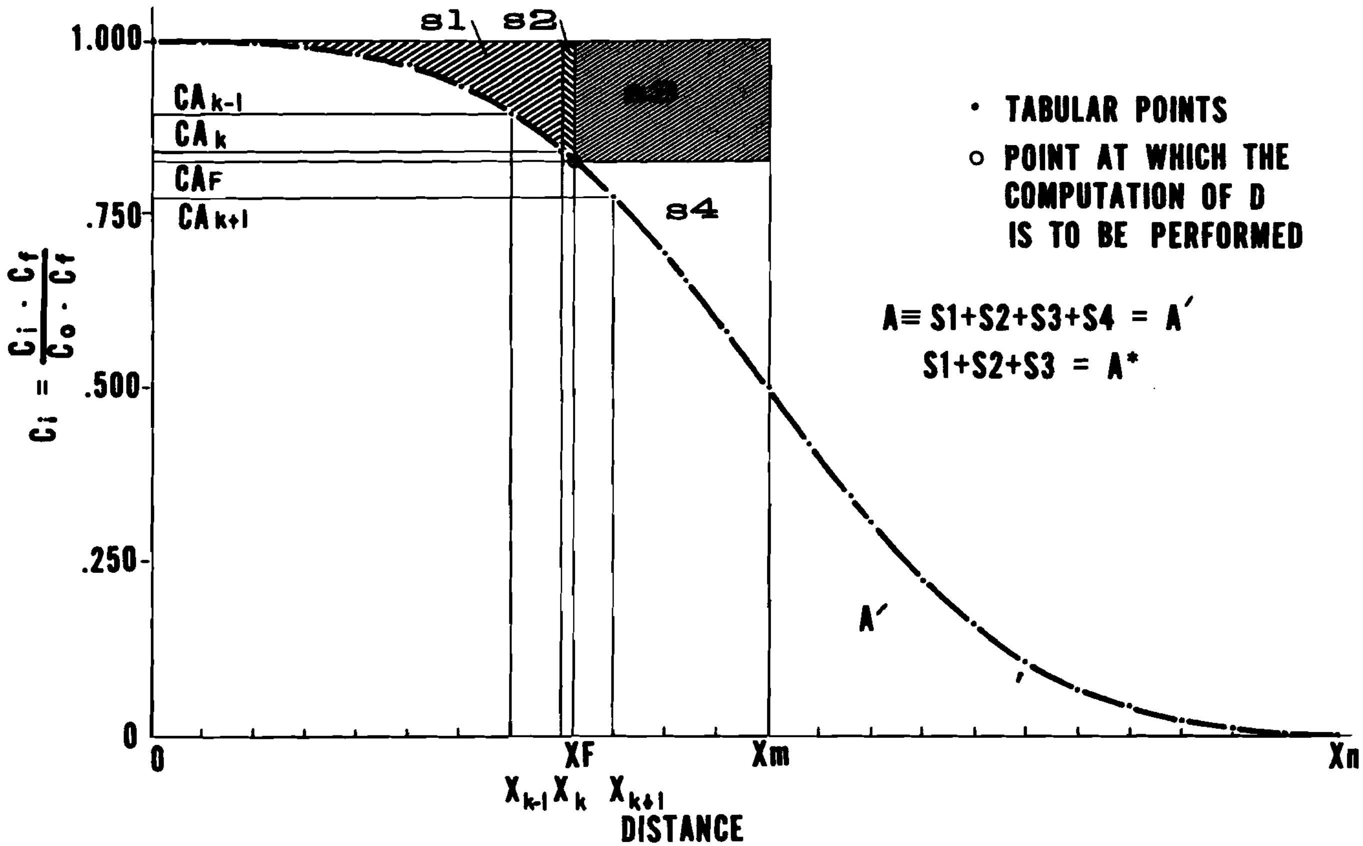

Figure 1. Schematic Concentration-Penetration Curve for a Semi-Infinite Diffusion Couple

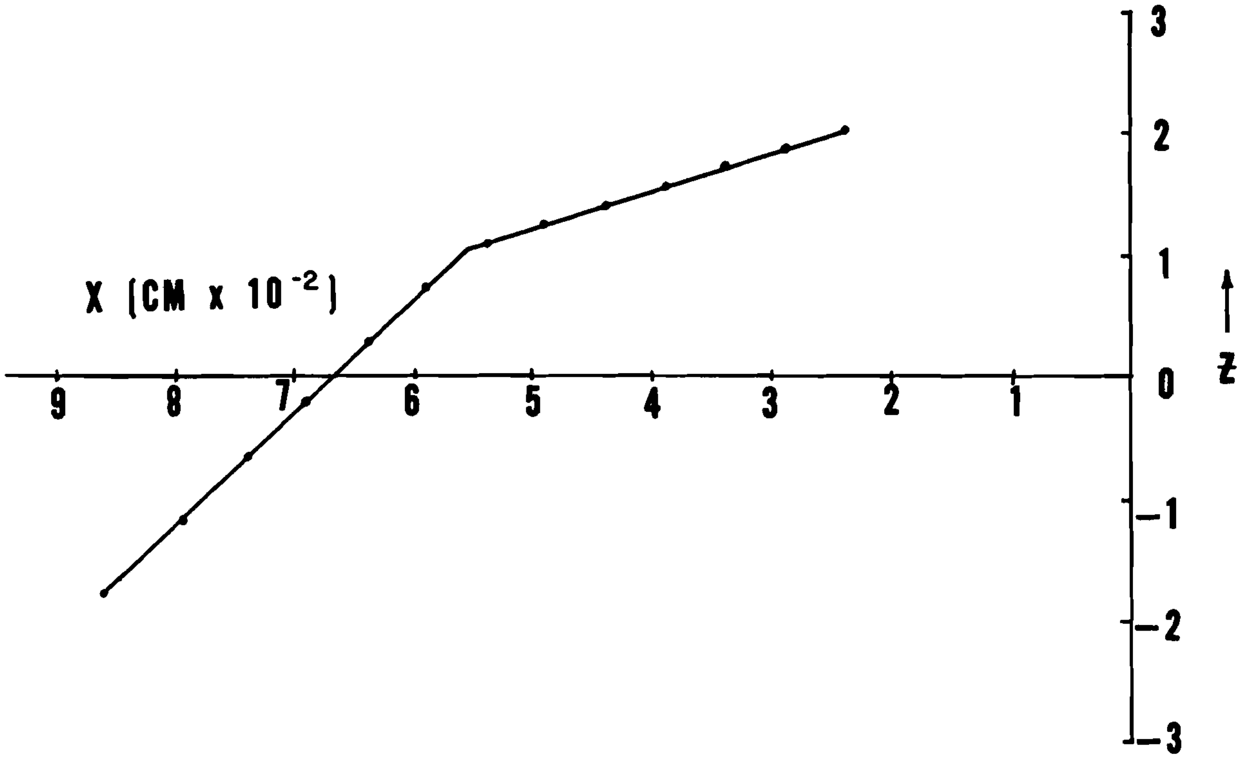

Figure 2. Probability Plot for the System Cu-Ni for 362 Hrs. at 947°C

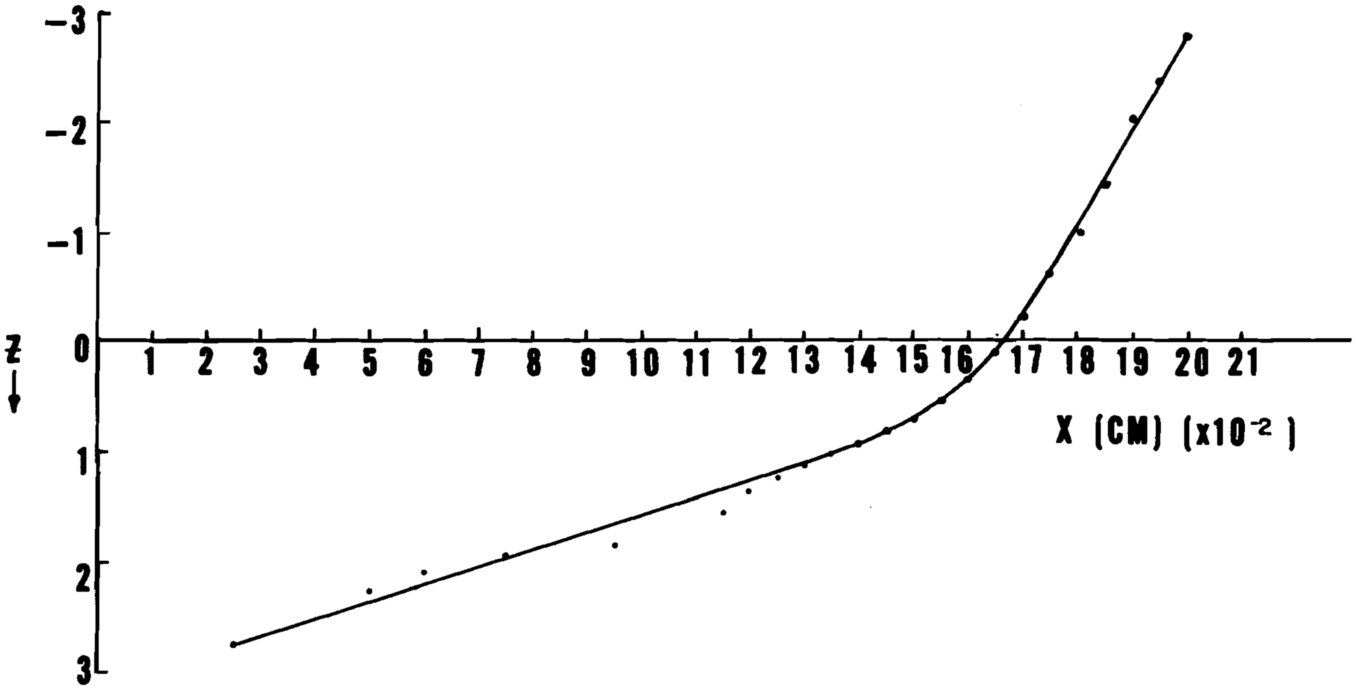

Figure 3. Probability Plot for the System Cu-Ni for 312 Hrs. at 1054°C

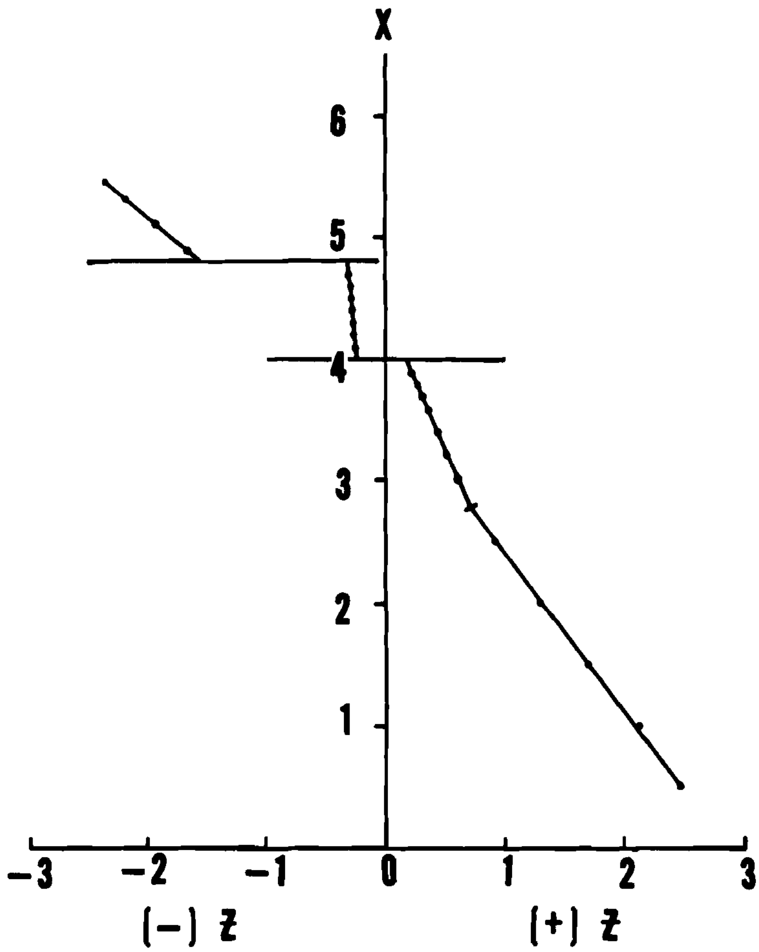

Figure 4. Probability Plot for the System W-Ru for 168 Hrs. at 1800°C

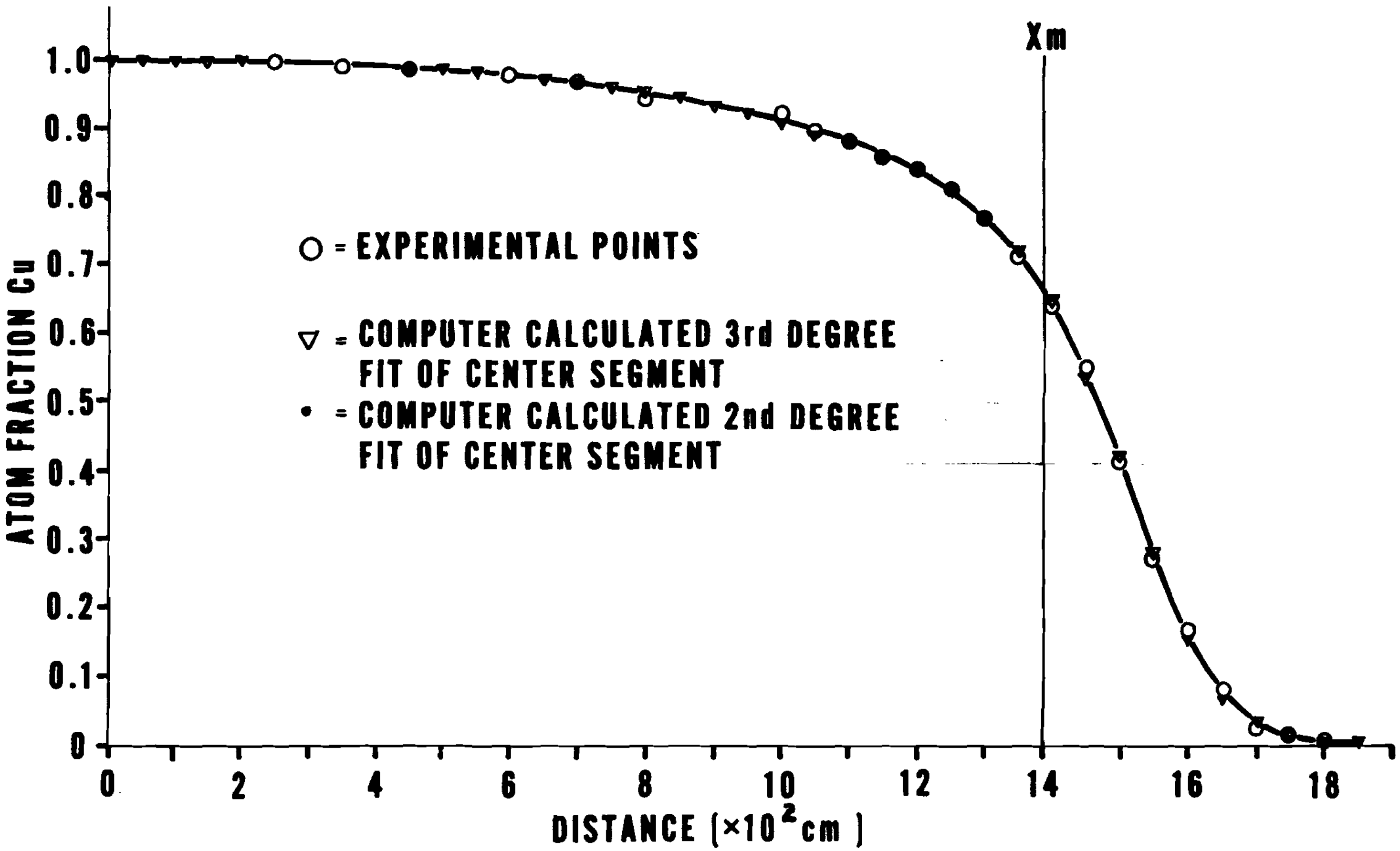

Figure 5. Concentration-Penetration Curve for the System Cu-Ni for 312 Hrs. at 1054°C

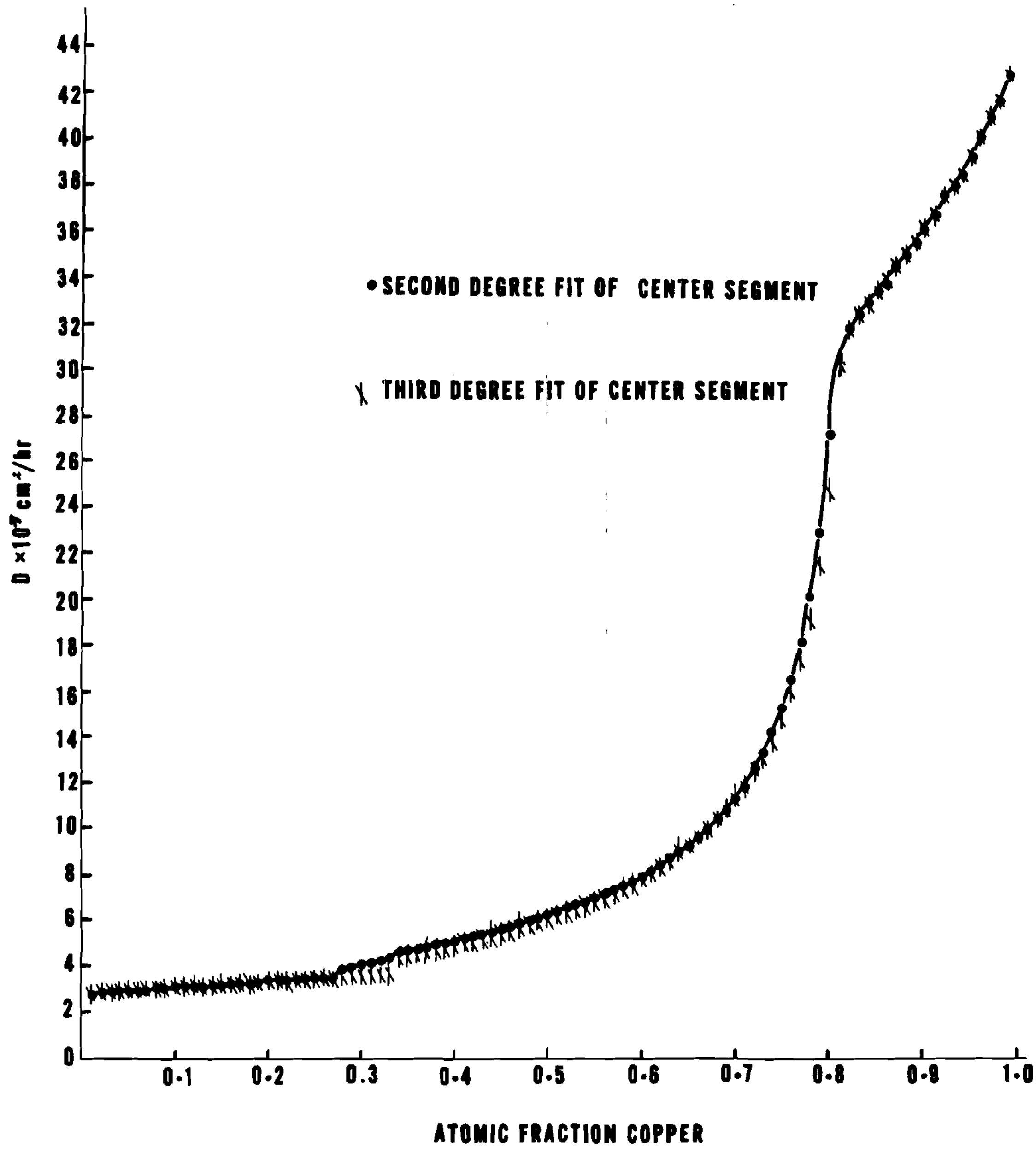

Figure 6. Interdiffusion Coefficient versus Concentration for the System Cu-Ni for 312 Hrs. at 1054°C

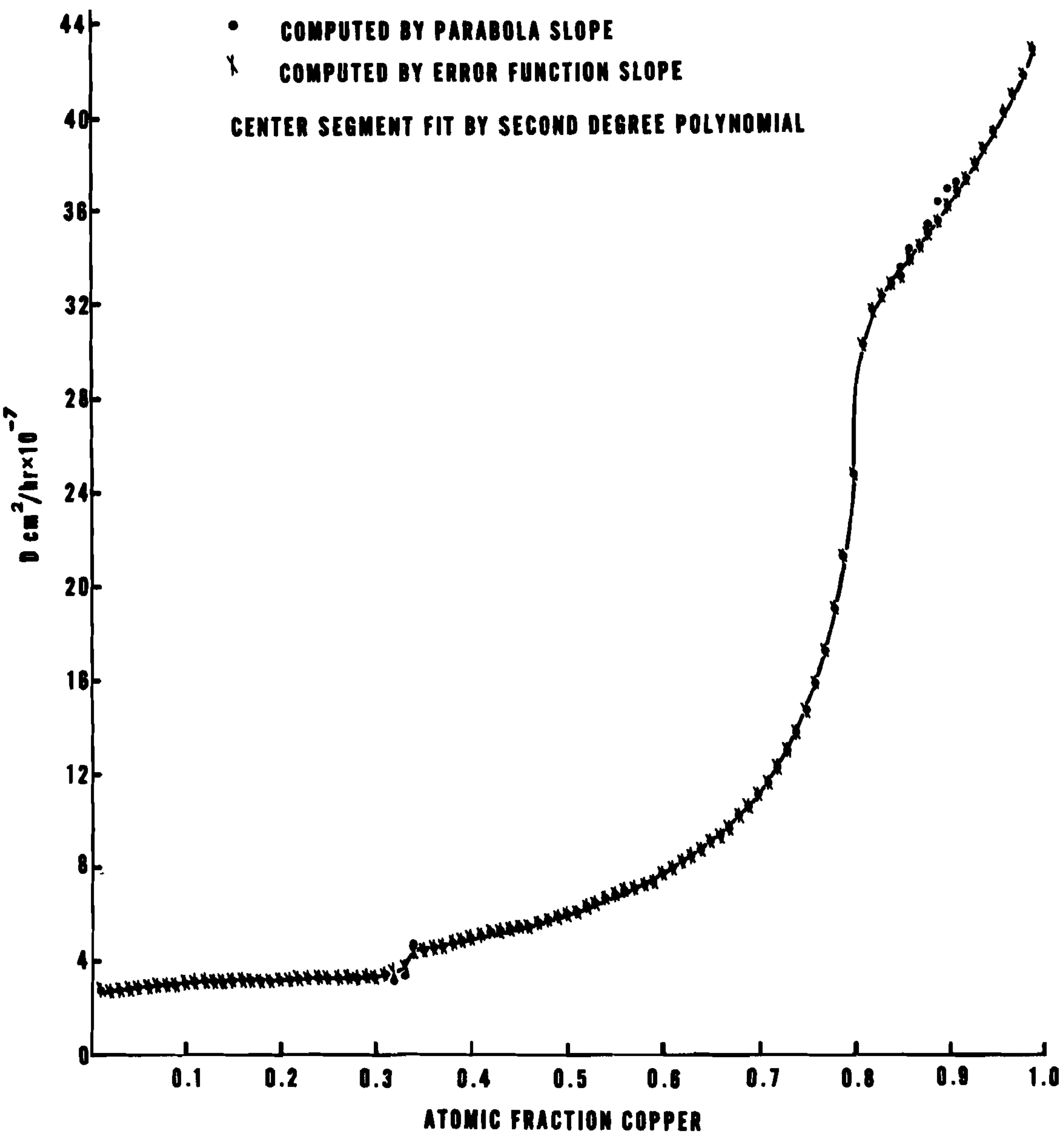

Figure 7. Diffusivities in the System Cu-Ni at 1054°C

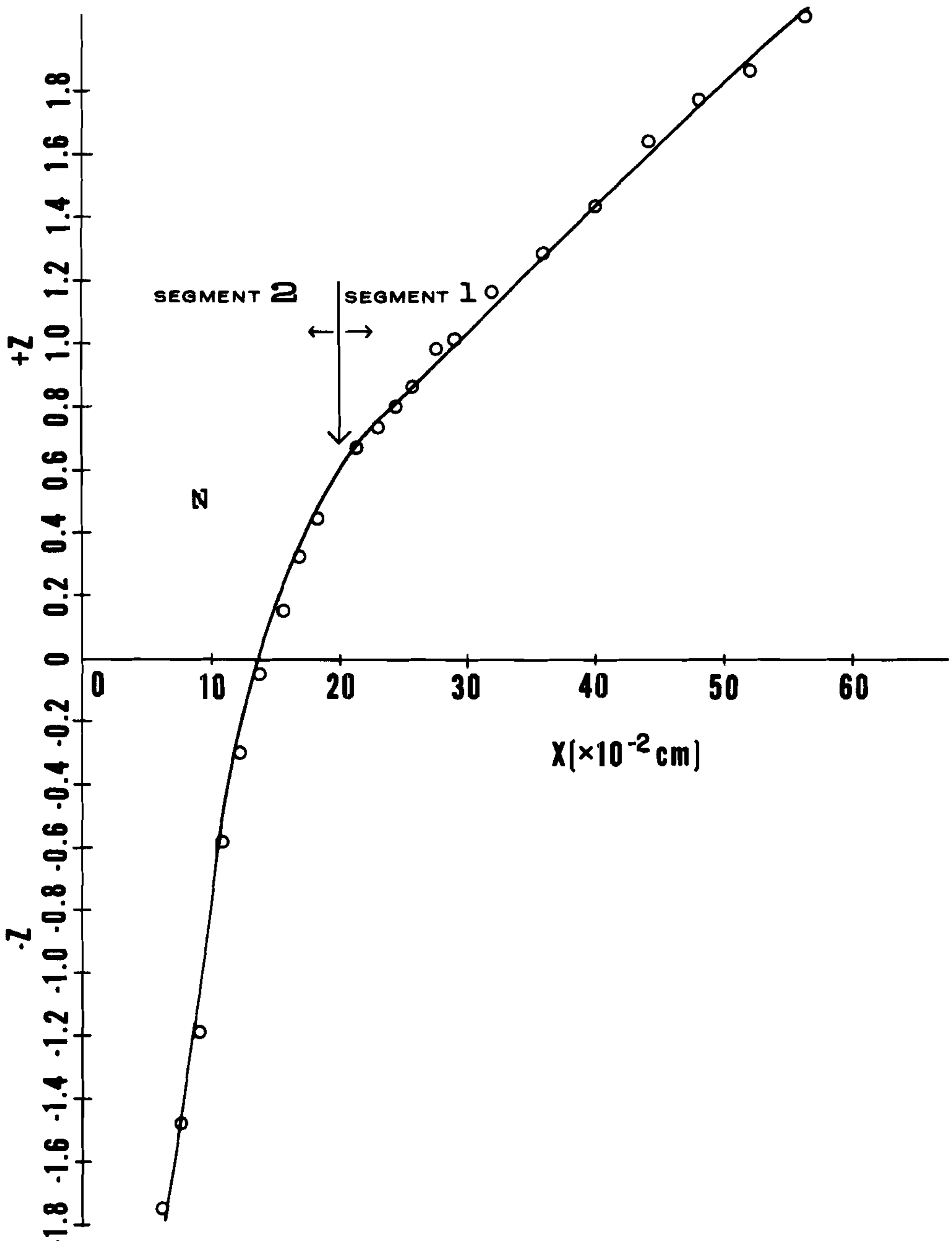

Figure 8. Probability Plot for Cu-Alpha Brass Couple for 507 Hrs. at 837°C

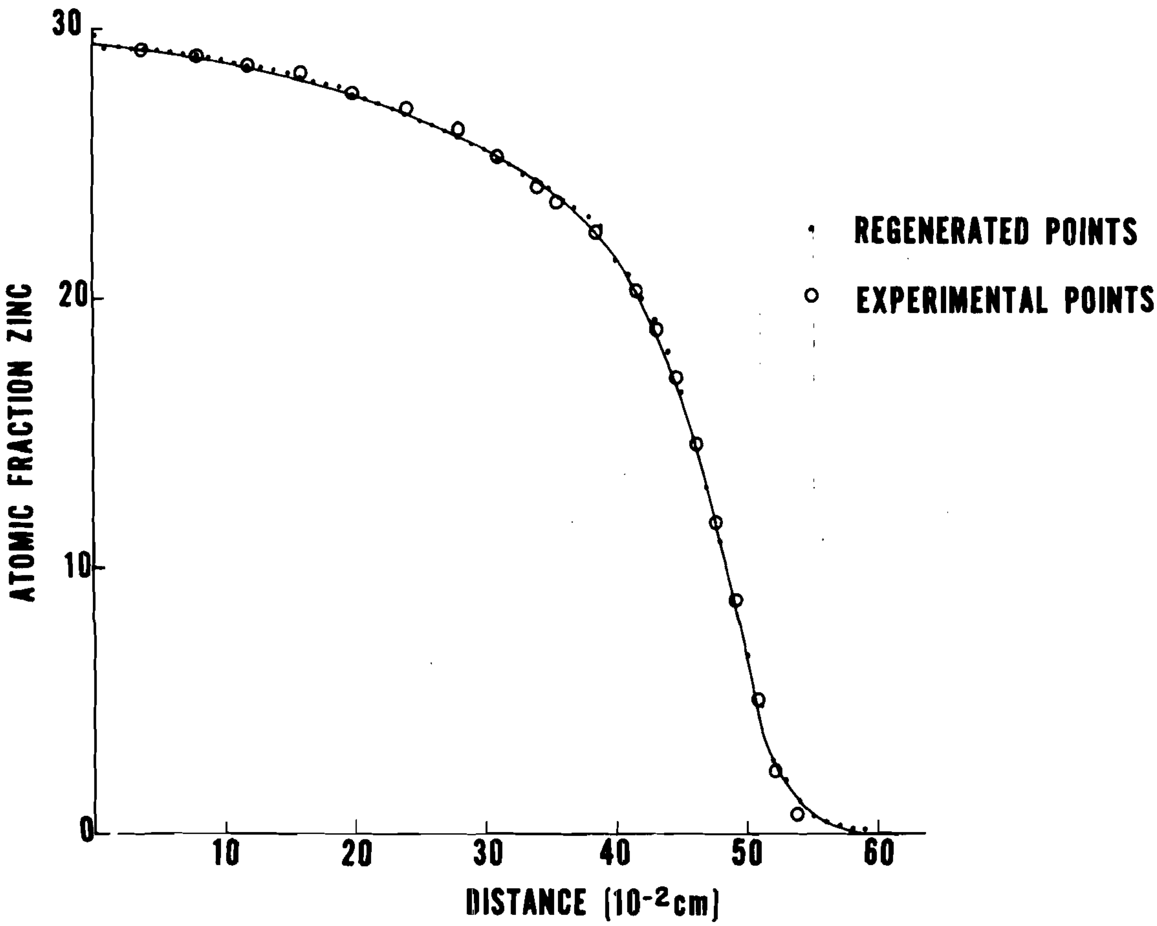

Figure 9. Concentration-Penetration Curve for Cu-Brass Couple for 507 Hrs. at 837°C

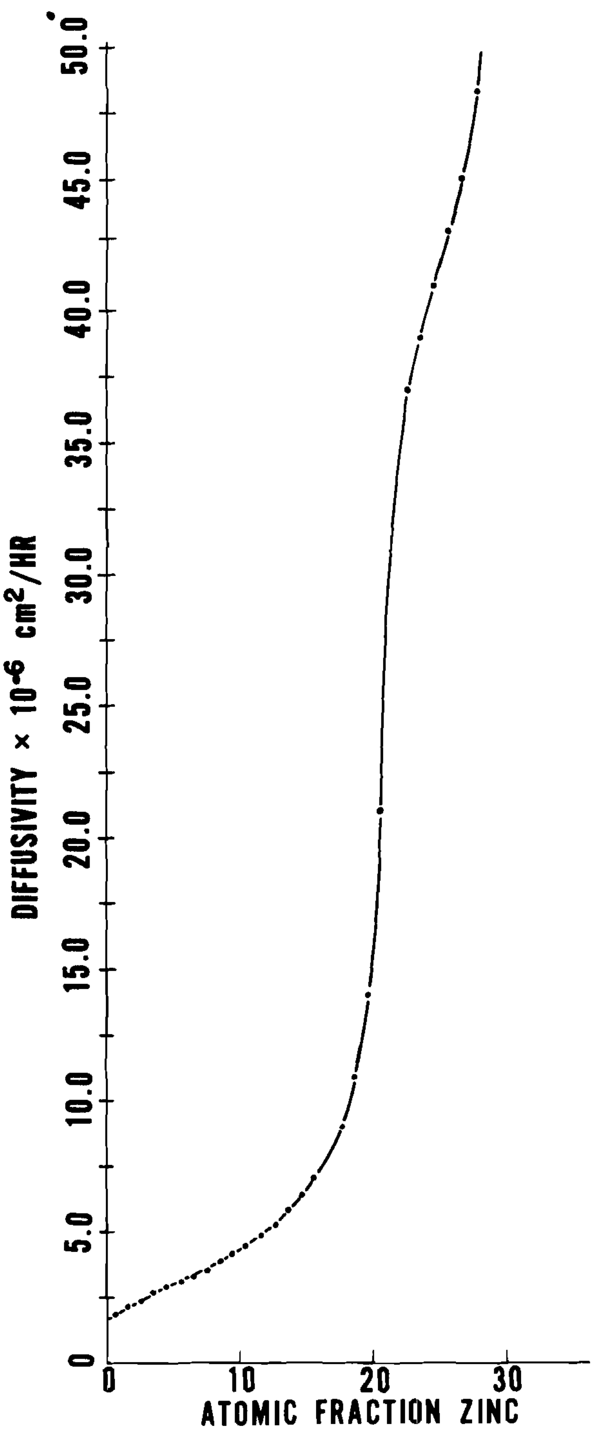

Figure 10. Diffusivity versus Concentration for Cu-Brass for 507 Hrs. at 837°C

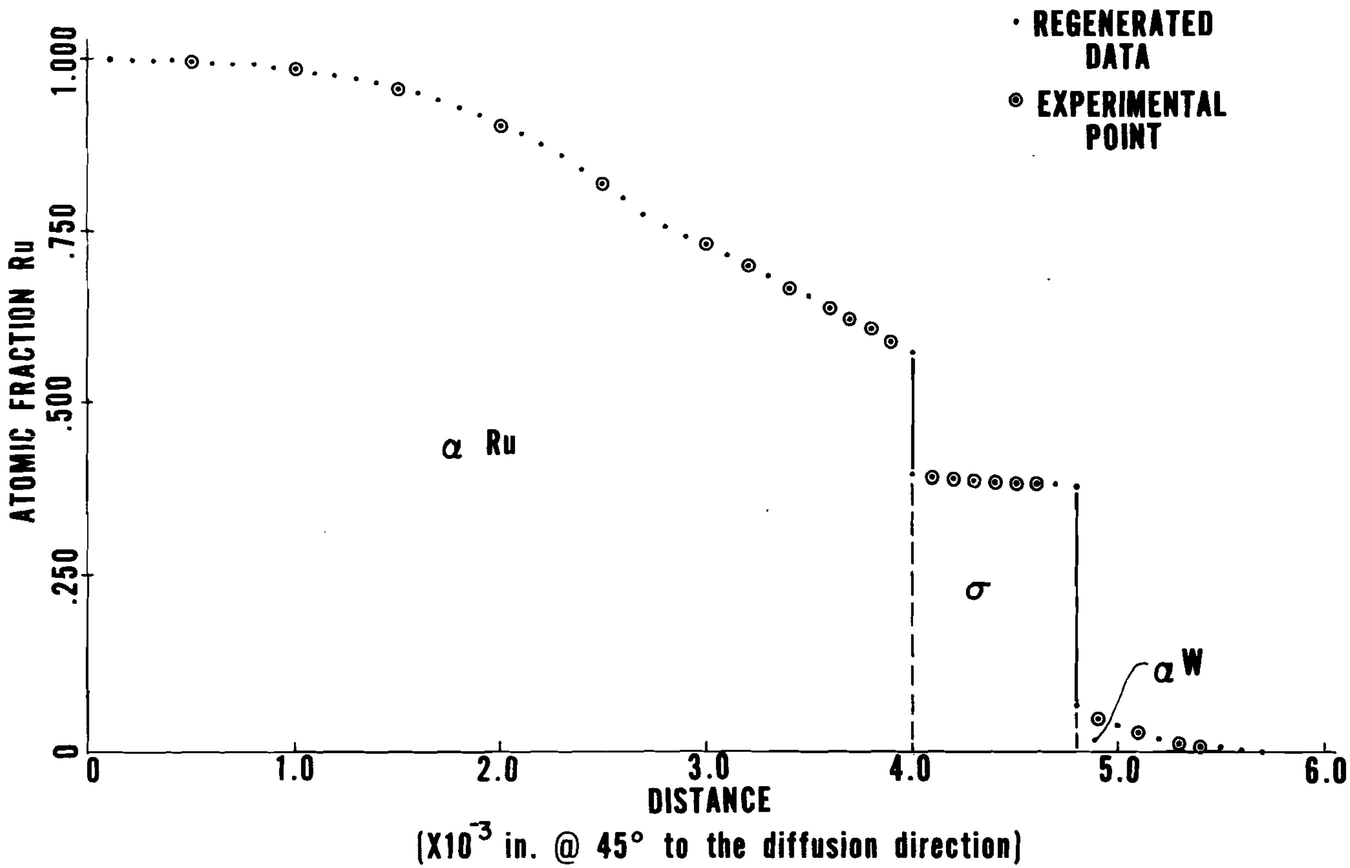

Figure 11. Concentration-Penetration Curve for W-Ru Couple for 168 Hrs. at 1800°C

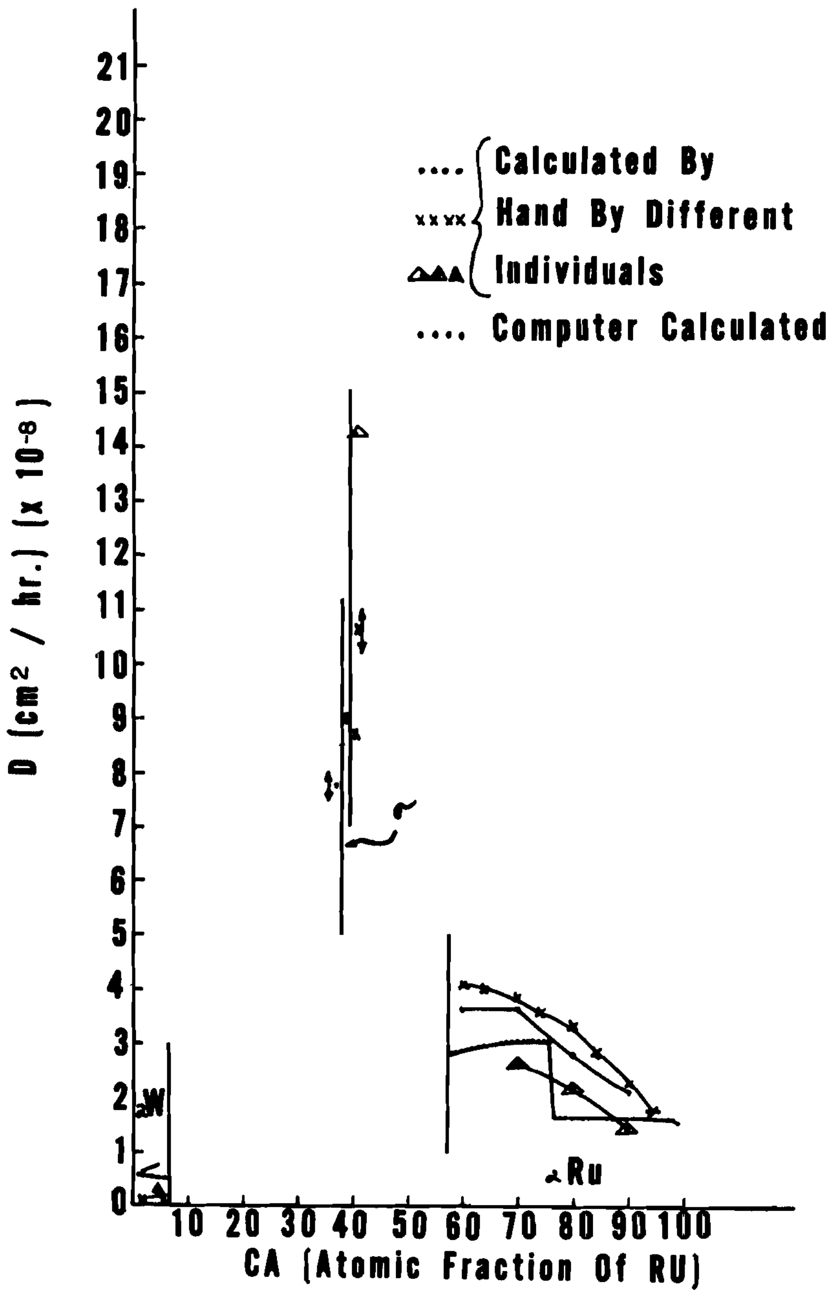

Figure 12. Diffusivity versus Concentration for W-Ru for 168 Hrs. at 1800°C

APPENDIX A

PROGRAM LISTING

```
      DIMENSION C1(32,8),C2(32,8),ERRORS(4,4,2),A(100,5),
     1DUMMY(1332),TX(200),TY(200),X(2000),CA(2000),N(10),SBP(10),
     2SP(10),SQ(10),ID(12),ND(10),SR(10),ST(10),C(51),R(100)
      COMMON DUMMY,A,CA,XB,H,N,X,KB,CAF,D,TME,CAMAX,CAI,CVF,SBP,SP,SQ,
     1KK,DX,XF,NS,CMDH,CMDL,DTI,SR,ST,TPM,ID,ND
3     FORMAT(1H1,24X,12A6////)
4     FORMAT(1H 2(1PE15.7))
8     FORMAT(6X,3HXM=1PE14.7,6X,5HTIME=1PE14.7,6X,4HCVF=1PE14.7////)
6     FORMAT(1H0,5X,4HX(I),12X,5HCA(I),6X,16HAFTER AXIS SHIFT///)
5     CALL SETUP
10    CAF=CMDH-CMDL-DTI
      CAI=CMDL
      H=DX
      N=KK
      DO 9 I=1,N
9     CA(I)=CA(I)-CAI
      CAMAX=CA(1)
      CK=0
      M=N/2
      IF(N-2*M)106,105,106
105   N=N+1
      CK=1234.
      CA(N)=.5*(CA(N-2)-5.*CA(N-1))
      X(N)=X(N-1)+H
106   CALL SRINT(1,N,X,CA,SY)
      XB=SY/(CMDH-CMDL)
      DX=XB
      WRITE OUTPUT TAPE 3,8,XB,TME,CVF
      WRITE OUTPUT TAPE 3,6
      IF(CK)107,108,107
107   N=N-1
108   DO 118 I=1,N
      X(I)=X(I)-XB
118   WRITE OUTPUT TAPE 3,4,X(I),CA(I)
      WRITE OUTPUT TAPE 3,3,ID
120   CALL DINT
      IF(CAF-DTI)5,121,121
121   CAF=CAF-DTI
      GO TO 120
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE DINT

      GO TO 504
503   NDEG=3
      C(1)=ST(M)
      C(2)=SR(M)
      C(3)=SQ(M)
      C(4)=SP(M)-ZF
504   CALL ROOTS (C,R,NDEG,.0001,CK1,CK2,CK3)
      DO 508 J=1,5,2
      IF(R(J)-(X(K-2)+DX))508,506,506
506   IF(R(J)-(X(K+2)+DX))507,507,508
507   XF2=R(J)
      XF=R(J)-DX
      GO TO 510
508   CONTINUE
      CTP=CAF+CMDL
      WRITE OUTPUT TAPE 3,600,CTP,R(1),R(2),R(3),R(4),R(5),R(6)
      RETURN
600   FORMAT(1H 26HUNSATISFACTORY XF FOR CA= F4.3/6E18.7)
510   DERP=2.*XF*P+Q
      DERF=  DPCAF(SQ(M),SR(M),ST(M),XF2,ZF)
      DERF=(CMDH-CMDL)*DERF
180   IF(XF)210,185,185
185   S1=CAF*XF
      IF(XF-X(K))186,186,200
186   S2=ABSF((IPCAF(X(K))-IPCAF(XF)))
      GO TO 201
200   S2=IPCAF(X(K+1))-IPCAF(XF)
201   IF(XF-X(K)) 202,202,204
202   LN=N-K+1
      LM=LN/2
      IF(LN-2*LM) 208,203,208
203   N=N+1
      IND=1
      X(N)=.5*(CA(N-2)-5.*CA(N-1))
208   NL=K
      GO TO 207
204   LN=N-K
      LM=LN/2
      IF(LN-2*LM)206,205,206
205   N=N+1
      IND=1
      X(N)=X(N-1)+H
      CA(N)=.5*(CA(N-2)-5.*CA(N-1))
206   NL=K+1
207   CALL SRINT(NL,N,X,CA,SZ)
      SUM=S1+S2+SZ
      IF(IND) 209,261,209
209   N=N-1
      GO TO 261
210   S1=(CAMAX-CAF)*ABSF(XF)
      IF(ABSF(XF)-ABSF(X(K)))250,215,215
215   S2=ABSF(CAMAX*(XF-X(K-1)))-ABSF(IPCAF(XF)-IPCAF(X(K-1)))
      LM=(K-1)/2
      IF((K-1)-2*LM)218,217,218
217   CA(K)=.5*(CA(K-2)-5.*CA(K-1))
      NL=K
```

```
      SUBROUTINE DINT
      DIMENSION C1(32,8),C2(32,8),ERRORS(4,4,2),A(100,5),
     1DUMMY(1332),TX(200),TY(200),X(2000),CA(2000),N(10),SBP(10),
     2SP(10),SQ(10),ID(12),ND(10),SR(10),ST(10),C(51),R(100)
      COMMON DUMMY,A,CA,XB,H,N,X,KB,CAF,D,TME,CAMAX,CAI,CVF,SBP,SP,SQ,
     1KK,DX,XF,NS,CMDH,CMDL,DTI,SR,ST,TPM,ID,ND
    7 FORMAT(1H0,6X,7HFOR CA=F4.3,5X,2HD=1PE10.3,5X,3HDP=E10.3,5X,
     13HXF=E10.3,5X,5HDERP=E10.3,5X,5HDERF=E10.3,5X,5HSEG  I2/)
      DPCAF(R,S,T,U ,V)=(R+2.*S*U+3.*T*U**2)*((EXPF(-(V**2)/2.))
     1/2.50663)
      IPCAF(T)=(P/3.)*T**3+(Q/2.)*T**2+W*T
      IND=0
C HERE WE FIND INDEX OF TABULAR VALUE OF CA NEAREST CAF
      DO 115 I=1,KK
      IF(CA(I)-CAF) 105,108,115
C     ABOVE STATEMENT ASSUMES CA(I) =CA(I+1)I=1,2,...N
  105 IF(ABSF(CA(I)-CAF)-ABSF(CA(I-1)-CAF)) 106,106,108
  106 K=I
      GO TO 120
  108 K=I-1
      GO TO 120
  115 CONTINUE
  120 SAVE=CA(K)
      DEL=X(K-1)**2*(X(K)-X(K+1))-X(K-1)*(X(K)**2-X(K+1)**2)
     1+(X(K)**2*X(K+1)-X(K+1)**2*X(K))
      DP=CA(K-1)*(X(K)-X(K+1))-X(K-1)*(CA(K)-CA(K+1))
     1+CA(K)*X(K+1)-CA(K+1)*X(K)
      DQ=X(K-1)**2*(CA(K)-CA(K+1))-CA(K-1)*(X(K)**2-X(K+1)**2)
     1+X(K)**2*(CA(K+1))-X(K+1)**2*(CA(K))
      DR=X(K-1)**2*(X(K)*CA(K+1)-X(K+1)*CA(K))-
     1X(K-1)*(X(K)**2*CA(K+1)-X(K+1)**2*CA(K))+
     2CA(K-1)*(X(K)**2*X(K+1)-X(K+1)**2*X(K))
      P=DP/DEL
      Q=DQ/DEL
      W=DR/DEL
  122 ARG=CAF/(CMDH-CMDL)
C 122 CONVERTS CAF TO NORMALIZED SYSTEM. MAKES XF CALCULATION CONSISTENT
      CALL WWERFN(-1.,ARG,ZF)
      DO 130 J=1,NS
  124 M=J
      IF(SBP(J)-CAI-CAF)179,179,130
  130 CONTINUE
      CTP=CAF+CMDL
  175 WRITE OUTPUT TAPE 3,166,CTP
      GO TO 300
  166 FORMAT(1H ,41HPROGRAM FAILED TO LOCATE SEG. FOR FOR CA=F4.3)
  179 JC=ND(M)
      GO TO (501,502,503),JC
  501 NDEG=1
      C(1)=SQ(M)
      C(2)=SP(M)-ZF
      GO TO 504
  502 NDEG=2
      C(1)=SR(M)
      C(2)=SQ(M)
      C(3)=SP(M)-ZF
```

```
      SUBROUTINE DINT

      GO TO 220
218   NL=K-1
220   CALL SRINT(1,NL,X,CA,SZ)
      CA(K)=SAVE
      S3=(CAMAX)*(X(K-1)-X(1))-SZ
      SUM=S1+S2+S3
      GO TO 261
250   SAVE=CA(K+1)
      S2=ABSF(XF-X(K))*CAMAX-ABSF(IPCAF(XF)-IPCAF(X(K)))
      LM=K/2
      IF(K-2*LM)252,251,252
251   CA(K+1)=.5*(CA(K-1)-5.CA(K))
      NL=K+1
      GO TO 253
252   NL=K
253   CALL SRINT(1,NL,X,CA,SZ)
      CA(K+1)=SAVE
      S3=(CAMAX)*(X(K)-X(1))-SZ
      SUM=S1+S2+S3
261   D=-(CVF**2)*(.5/TME)*(1./DERF)*SUM
      DE=-(CVF**2)*(.5/TME)*(1./DERP)*SUM
      CTP=CAF+CMDL
      WRITE OUTPUT TAPE 3,7,CTP,D,DE,XF,DERP,DERF,M
300   RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE SETUP
      DIMENSION C1(32,8),C2(32,8),ERRORS(4,4,2),A(100,5),
     1DUMMY(1332),TX(200),TY(200),X(2000),CA(2000),N(10),SBP(10),
     2SP(10),SQ(10),ID(12),ND(10),SR(10),ST(10),C(51),R(100)
      COMMON DUMMY,A,CA,XB,H,N,X,KB,CAF,D,TME,CAMAX,CAI,CVF,SBP,SP,SQ,
     1KK,DX,XF,NS,CMDH,CMDL,DTI,SR,ST,TPM,ID,ND
 1    FORMAT(24I3)
 2    FORMAT(5E13.7)
 3    FORMAT(1H 2F15.5)
 4    FORMAT(1H 3(1PE14.7))
 5    FORMAT(3XI2)
    6 FORMAT(1H0,11X,16HREGENERATED DATA//,7X,8HDISTANCE,8X,
     113HCONCENTRATION//)
 7    FORMAT(12A6)
 8    FORMAT(1H1,24X,12A6)
      READ INPUT TAPE 2,7,ID
      READ INPUT TAPE 2,1,NS,NP,(N(I),I=1,NS),(ND(I),I=1,NS)
CREAD IN NO SEGMENTS,NO POINTS, AND NO POINTS IN EACH SEGMENT
      READ INPUT TAPE 2,2,(TX(I),I=1,NP),(TY(I),I=1,NP),DX,TME,CVF,
     1CMDH,CMDL,DTI
C READ IN ORIGINAL DATA POINTS
      WRITE OUTPUT TAPE 3,8,ID
      WRITE OUTPUT TAPE 3,5, NS,NP,(N(I),I=1,NS)
      WRITE OUTPUT TAPE 3,3,(TX(I),TY(I),I=1,NP),DX
      DO 9 MM=1,NP
 9    TY(MM)=(TY(MM)-CMDL)/(CMDH-CMDL)
C     ABOVE LOOP CONVERTS DATA TO NORMALIZED SYSTEM
      NDX=1
      XBP=0
      PXBP=0
      K=1
      KK=1
      L=0
      ASSIGN 60 TO LK
      DO 100 I=1,NS
      ASSIGN 93 TO LI
      L=L+N(I)
      GO TO LK,(60,80)
 60   MK=0
      DO 10 J=K,L
      MK=MK+1
      A(MK,1)=TX(J)
      CALL WWERFN(-1.,TY(J),RESULT)
 10   A(MK,2)=RESULT
      K=L+1
      C1(3,1)=0
      C1(4,1)=0
      CALL LSCF2(0,ND(I),3,LOOK,C1,C2,ERRORS,N(I),1)
      IF(I-NS)11,94,11
 11   IF(TY(L+1))95,90,90
 80   A1=C1(1,1)
      B1=C1(2,1)
      D1=C1(3,1)
      E1=C1(4,1)
      MK=0
      DO 20 J=K,L
```

```
      SUBROUTINE SETUP
      MK=MK+1
      A(MK,1)=TX(J)
      CALL WWERFN(-1.,TY(J),RESULT)
20    A(MK,2)=RESULT
      K=L+1
      C1(3,1)=0
      C1(4,1)=0
      CALL LSCF2(0,ND(I),3,LOOK,C1,C2,ERRORS,N(I),1)
      A2=C1(1,1)
      B2=C1(2,1)
      D2=C1(3,1)
      E2=C1(4,1)
      C(1)=E1-E2
      C(2)=D1-D2
      C(3)=B1-B2
      C(4)=A1-A2
      IF(C(1))43,40,43
40    C(1)=C(2)
      IF(C(1))42,41,42
41    C(1)=C(3)
      C(2)=C(4)
      NDEG=1
      GO TO 44
42    NDEG=2
      C(2)=C(3)
      C(3)=C(4)
      GO TO 44
43    NDEG=3
44    CALL ROOTS(C,R,NDEG,.CC0001,CK1,CK2,CK3)
30    NLI=L-N(I)
      DO 33 KJ=1,5,2
      IF(R(KJ)-TX(NLI))33,31,31
31    IF(R(KJ)-TX(NLI+1))32,32,33
32    XBP=R(KJ)
      GO TO 35
33    CONTINUE
      XMV= (TX(NLI)+TX(NLI+1))/2.
      P1=ABSF(R(1)-XMV)
      P2=ABSF(R(3)-XMV)
      P3=ABSF(R(5)-XMV)
      IF(P1-MIN1F(P1,P2,P3))46,50,46
46    IF(P2-MIN1F(P1,P2,P3))47,49,47
47    XBP=R(5)
      GO TO 35
49    XBP=R(3)
      GO TO 35
50    XBP=R(1)
      WRITE OUTPUT TAPE 3,34
      WRITE OUTPUT TAPE 3,200,R(1),R(2),R(3),R(4),R(5),R(6)
      GO TO 35
34    FORMAT(1H 17HBREAK POINT ERROR)
200   FORMAT(1H 6E18.7)
35    IF(I-2)27,25,27
27    JJ=L-N(I)-N(I-1)
      IF(TY(JJ))25,26,26
25    PXBP=X(KK-1)
```

```
      SUBROUTINE SETUP

      GO TO 28
  26  PXBP=X(KK-1)+DX
  28  U=PXBP
C FIND  CONCENTRATION AT END OF EACH SEGMENT
C FOR  USE IN FINDING SEG. ON WHICH INPUT CA FALLS
C SEE  STATEMENTS NEAR 124 OF DINT
      IF(I-NS)89,61,89
  61  SBP(NS)=0
      GO TO 63
  89  ARG=A1+B1*XBP+D1*XBP**2+E1*XBP**3
      CALL WWERFN(1.,ARG,SBP(NDX))
  63  SP(NDX)=A1
      SQ(NDX)=B1
      SR(NDX)=D1
      ST(NDX)=E1
C     SAVE AND IDENTIFY COEFFICIENTS AND BREAK POINTS
      NDX=NDX+1
      DO 71 LL=1,2000
      Z=A1+B1*U+D1*U**2+E1*U**3
      CALL WWERFN(1.,Z,RESULT)
      X(KK)=U
      IF(KK-1)66,65,66
  65  CA(KK)=1.
      GO TO 70
  66  IF(RESULT-.0001)67,67,69
  67  CA(KK)=0.
      GO TO 92
  69  CA(KK)=RESULT
  70  U=U+DX
      KK=KK+1
      IF(XBP-U)92,92,71
  71  CONTINUE
  92  GO TO LI,(93,100)
  93  IF(I-NS) 95,94,95
  94  JJ=L-N(I)
      IF(TY(JJ))91,91,96
  91  PXBP=X(KK-1)
      GO TO 97
  96  PXBP=X(KK-1)+DX
  97  ASSIGN 100 TO LI
      XBP=TX(NP)+10.
      A1=C1(1,1)
      B1=C1(2,1)
      D1=C1(3,1)
      E1=C1(4,1)
      GO TO 28
  95  IF(TY(L+1))17,18,18
  17  ASSIGN 60 TO LK
      ASSIGN 100 TO LI
      IF(I-1)21,16,21
  21  JJ=L-N(I)
      IF(TY(JJ))16,16,19
  19  PXBP=X(KK-1)+DX
      GO TO 15
  16  PXBP=X(KK-1)
  15  K=L+2
```

```
      SUBROUTINE SETUP

      L=L+1
      XBP=TX(L)
      A1=C1(1,1)
      B1=C1(2,1)
      D1=C1(3,1)
      E1=C1(4,1)
      GO TO 28
 18   PXBP=X(KK-1)+DX
      GO TO 100
 90   ASSIGN 80 TO LK
 100  CONTINUE
      WRITE OUTPUT TAPE 3,6
      KK=KK-1
      DO 106 MM=1,KK
 106  CA(MM)=CA(MM)*(CMDH-CMDL)+CMDL
C     ABOVE LOOP CONVERTS DATA BACK TO ORIGINAL SYSTEM
      DO 105 M=1,KK
 105  WRITE OUTPUT TAPE 3,3,X(M),CA(M)
      DO 128 J=1,NS
 128  SBP(J)=SBP(J)*(CMDH-CMDL)+CMDL
CABOVE LOOP CONVERTS CONCENTRATION BREAK POINTS TO ORIGINAL SYSTEM
      RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE SRINT(N1,N,X,Y,SY)
      DIMENSION X(2000),Y(2000)
      SY=0
      M=N-2
      H=X(N1+1)-X(N1)
      DO 150 I=N1,M,2
      IF(X(I)-X(I+1))110,120,110
 110  IF(X(I+1)-X(I+2))140,130,140
 120  SY=SY+(H/2.)*(Y(I+1)+Y(I+2))
      GO TO 150
 130  SY=SY+(H/2.)*(Y(I)+Y(I+1))
      GO TO 150
 140  SY=SY+(H/3.)*(Y(I)+4.*Y(I+1)+Y(I+2))
 150  CONTINUE
 111  RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE WWERFN(I,Z,RESULT)
      IF(I)100,200,240
100   AZ=2.515517
      A1=.802853
      A2=.010328
      B1=1.432788
      B2=.189269
      B3=.001308
      IF(Z-.5)110,110,120
110   X=Z
      GO TO 125
120   X=1.-Z
125   P=SQRTF(-2.*LOGF(X))
      Q=P-((AZ+A1*P+A2*P**2)/(1.+B1*P+B2*P**2+B3*P**3))
      IF(Z-.5)130,130,135
130   RESULT=-Q
      GO TO 300
135   RESULT=Q
      GO TO 300
200   IF(Z) 205,210,210
205   U=-Z
      RESULT=-ERF(U)
      GO TO 300
210   RESULT=ERF(U)
      GO TO 300
240   IF(Z)250,260,260
250   U=-Z/1.414142315
      RESULT=.5-.5*ERF(U)
      GO TO 300
260   U=Z/1.414142315
      RESULT=.5+.5*ERF(U)
300   RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      FUNCTION ERF(ARG)
      P=.47047
      C1=.3084284
      C2=-.0849713
      C3=.6627698
      Y=1./(1.+P*ARG)
      R=-ARG*ARG
      EP=(2./SQRTF(3.141592))*EXPF(R)
      ERF=1.-(C1*Y+C2*Y**2+C3*Y**3)*EP
      RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE LSCF2(MTIN,KTH,MTOUT,LOOK,COEFFO,COEFFT,ERRORS,MPTS,NSE
     1TS)
      DIMENSION C1(32,8),C2(32,8),E(4,4,2),A(100,5),YC(100,4,2),
     1XT(100),DIFFER(100,4,2),RELERR(100,4,2),DUMMY(1332),
     2ERRORS(4,4,2),COEFFO(32,8),COEFFT(32,8),CS(502)
      COMMON DUMMY,A
      MT1=MTIN
      MT2=MTOUT
      K=KTH
      M=MPTS
      N=NSETS
      IF(MT1)99,101,100
 99   MT1=2
C     READ M(NO. OF POINTS),N(NO. OF SETS) FROM FIRST CARD
 100  CALL READT(CS,MT1,L)
      IF(L)15,5,15
 5    M=CS(1)+.5
      N=CS(2)+.5
      IF(N-4)6,6,13
 6    K1=0
      LM=(M*(N+1))+2
      GO TO(1,2,3,4),N
 1    DO 7 I=3,LM,2
      K1=K1+1
      A(K1,1)=CS(I)
 7    A(K1,2)=CS(I+1)
      GO TO 102
 2    DO 8 I=3,LM,3
      K1=K1+1
      A(K1,1)=CS(I)
      A(K1,2)=CS(I+1)
 8    A(K1,3)=CS(I+2)
      GO TO 102
 3    DO 9 I=3,LM,4
      K1=K1+1
      A(K1,1)=CS(I)
      A(K1,2)=CS(I+1)
      A(K1,3)=CS(I+2)
 9    A(K1,4)=CS(I+3)
      GO TO 102
 4    DO 10 I=3,LM,5
      K1=K1+1
      A(K1,1)=CS(I)
      A(K1,2)=CS(I+1)
      A(K1,3)=CS(I+2)
      A(K1,4)=CS(I+3)
 10   A(K1,5)=CS(I+4)
      GO TO 102
 101  IF(N-4)102,102,13
C     TURNS DATA OVER TO LSCF1 FOR SOLUTION
 102  CALL LSCF1(A,M,N,K,L,C1,C2,AT,BT)
C     EXAMINE TEST CONDITION CELL FOR NORMAL RETURN
      IF(L)14,103,14
C     PERFORM ERROR ANALYSIS IN ORIGINAL AND TRANSPOSED SYSTEMS
C     COMPUTE YS IN BOTH SYSTEMS
 103  FM=M
```

```
      SUBROUTINE LSCF2(MTIN,KTH,MTOUT,LOOK,COEFFO,COEFFT,ERRORS,MPTS,NSE

      DO 104 IS=1,2
      DO 104 NN=1,N
      E(3,NN,IS)=0
 104  E(4,NN,IS)=0
      DO 116 IS=1,2
      DO 116 NN=1,N
      NNN=NN+1
      SUMD=0
      SUMR=0
      DO 115 I=1,M
      J=K+1
      YC(I,NN,IS)=0
      GO TO (105,106),IS
 105  YC(I,NN,1)=(YC(I,NN,IS))*A(I,1)+C1(J,NN)
      J=J-1
      IF(J)108,108,105
 106  XT=AT*(A(I,1)+BT)
 107  YC(I,NN,2)=YC(I,NN,2)*XT+C2(J,NN)
      J=J-1
      IF(J)108,108,107
C     COMPUTE DIFFERENCE AND RELATIVE ERROR IN BOTH SYSTEMS
 108  DIFFER(I,NN,IS)=A(I,NNN)-YC(I,NN,IS)
      IF(ABSF(DIFFER(I,NN,IS))-E(3,NN,IS))110,109,109
 109  E(3,NN,IS)=ABSF(DIFFER(I,NN,IS))
 110  IF(A(I,NNN))111,112,111
 111  RELERR(I,NN,IS)=DIFFER(I,NN,IS)/A(I,NNN)
      GO TO 1121
 112  RELERR(I,NN,IS)=DIFFER(I,NN,IS)
 1121 IF(ABSF(RELERR(I,NN,IS))-E(4,NN,IS))114,113,113
 113  E(4,NN,IS)=ABSF(RELERR(I,NN,IS))
 114  SUMD=SUMD+((DIFFER(I,NN,IS))**2)
 115  SUMR=SUMR+((RELERR(I,NN,IS))**2)
      E(1,NN,IS)=SQRTF(SUMD/FM)
 116  E(2,NN,IS)=SQRTF(SUMR/FM)
C     PRINT OUTPUT ON MT2,IF ZERO EXIT
      IF(MT2)1161,127,117
 1161 MT2=3
 117  NN=1
      IP=0
 118  J=M
      NNN=NN+1
      IP=IP+1
C     DUMP PAGE
      WRITE OUTPUT TAPE MT2,301,IP
C     DUMP TITLE
      WRITE OUTPUT TAPE MT2,302,K,M,NN
C     DUMP HEADINGS
      WRITE OUTPUT TAPE MT2,303
      IF(J-49)119,122,122
C     DUMP J ANS WITH COEFFICIENTS
 119  IAC=K+1
      WRITE OUTPUT TAPE MT2,304,(I,A(I,1),A(I,NNN),C1(I,NN),YC(I,NN,1),
     1RELERR(I,NN,1),C2(I,NN),YC(I,NN,2),RELERR(I,NN,2),I=1,IAC)
C     DUMP J ANS WITHOUT COEFFICIENTS
      ID=K+2
      IF(ID-M)120,120,121
```

```
      SUBROUTINE LSCF2(MTIN,KTH,MTOUT,LOOK,COEFFO,COEFFT,ERRORS,MPTS,NSE
 120  WRITE OUTPUT TAPE MT2, 305,(I,A(I,1),A(I,NNN),YC(I,NN,1),
     1RELERR(I,NN,1),YC(I,NN,2),RELERR(I,NN,2),I=ID,M)
      IF(J-49)121,123,123
C     DUMP ERROR ANALYSIS ON SAME PAGE
 121  WRITE OUTPUT TAPE MT2,306,E(1,NN,1),E(1,NN,2),E(2,NN,1),E(2,NN,2),
     1AT,E(3,NN,1),E(3,NN,2),E(4,NN,1),E(4,NN,2),BT
      NN=NN+1
      IF(NN-N)118,118,127
 122  IF(J-54)119,124,124
C     DUMP CONTINUE
 123  IP=IP+1
      WRITE OUTPUT TAPE MT2,307,NN,IP
C     DUMP NEW PAGE THEN GO TO ANS AND ERROR ANALYSIS DUMP
      WRITE OUTPUT TAPE MT2,308,NN,IP
C     DUMPS ERROR ANALYSIS ON SEPARATE PAGE
      GO TO 121
C     DUMP 53 ANS
 124  IAC=K+1
      WRITE OUTPUT TAPE MT2,304,(I,A(I,1),A(I,NNN),C1(I,NN),YC(I,NN,1),
     1RELERR(I,NN,1),C2(I,NN),YC(I,NN,2),RELERR(I,NN,2),I=1,IAC)
      ID=K+2
      WRITE OUTPUT TAPE MT2,305,(I,A(I,1),A(I,NNN),YC(I,NN,1),
     1RELERR(I,NN,1),YC(I,NN,2),RELERR(I,NN,2),I=ID,53)
      ID=54
      J=J-53
 125  IP=IP+1
      WRITE OUTPUT TAPE MT2,307,NN,IP
      WRITE OUTPUT TAPE MT2,308,NN,IP
      WRITE OUTPUT TAPE MT2,309
      IF(J-56)120,126,126
C     DUMP 55 ANS
 126  IAC=ID+55
      WRITE OUTPUT TAPE MT2,305,(I,A(I,1),A(I,NNN),YC(I,NN,1),
     1RELERR(I,NN,1),YC(I,NN,2),RELERR(I,NN,2),I=ID,IAC)
      ID=IAC+1
      J=J-55
      GO TO 125
 127  L=0
      K=K+1
      DO 128 I=1,K
      DO 128 J=1,N
      COEFFO(I,J)=C1(I,J)
 128  COEFFT(I,J)=C2(I,J)
      DO 129 I=1,4
      DO 129 NN=1,N
      DO 129 IS=1,2
 129  ERRORS(I,NN,IS)=E(I,NN,IS)
 14   LOOK=L
      RETURN
 13   L=13
 15   PRINT 200
      WRITE OUTPUT TAPE 3,200
      GO TO 14
 200  FORMAT(1X,60HDATA FOR CURVE FITTING ROUTINE HAS BEEN SENSED AS INC
     1ORRECT.,56X,3HJBH)
C     FORMAT STATEMENTS FOR PRINT OUTPUT TAPE MT2
```

```
      SUBROUTINE LSCF2(MTIN,KTH,MTOUT,LCOK,COEFFO,COEFFT,ERRORS,MPTS,NSE

301   FORMAT(1H1,110X,5H PAGE,I3)
302   FORMAT(14X,34HLEAST SQUARES CURVE FIT OF DEGREE ,I2,9X,I3,
     121H OBSERVED DATA POINTS,9X,11HSET NUMBER I2//)
303   FORMAT(12X,1HX,15X,1HY,9X,12HCOEFFICIENTS,5X,10HY COMPUTED,4X,
     17HREL ERR,4X,12HCOEFFICIENTS,5X,10HY COMPUTED,4X,7HREL ERR/8X,
     28HOBSERVED,8X,8HOBSERVED,6X,12HORIGINAL SYS,4X,12HORIGINAL SYS,5X,
     34HORIG,4X,15HTRANSFORMED SYS,1X,15HTRANSFORMED SYS,2X,5HTRANS//)
304   FORMAT(I4,E15.7,3E16.7,E10.2,2E16.7,E10.2)
305   FORMAT(I4,E15.7,E16.7,E32.7,E10.2,E32.7,E10.2)
306   FORMAT(19X,11HDIFFERENCES,29X,15HRELATIVE ERRORS,22X,
     123HTRANSFORMATION Z=A(X-B)/6X,8HRMS ORG.,E9.2,11H  RMS TRANS,
     2E9.2,5X,8HRMS ORG.,E9.2,11H  RMS TRANS,E9.2,10X,9HWHERE A =,E15.7/
     36X,8HMAX ABS.,E9.2,11H  MAX ABS.  ,E9.2,5X,8HMAX ABS.,E9.2,
     411H  MAX ABS.  ,E9.2,10X,9HWHERE B =,E15.7/111X,7HJBH/LBF)
307   FORMAT(40X,16HDATA OF THIS SET,I2,18H CONTINUED ON PAGE,I3)
308   FORMAT(1H1,46X,19HCONTINUATION OF SET,I2,5H DATA,39X,4HPAGE,I3)
309   FORMAT(12X,1HX,15X,1HY,26X,10HY COMPUTED,4X,7HREL ERR,21X,
     110HY COMPUTED,4X,7HREL ERR/8X,8HOBSERVED,8X,8HOBSERVED,22X,
     212HORIGINAL SYS,5X,4HORIG,20X,15HTRANSFORMED SYS,2X,5HTRANS/)
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE LSCF1(A,M,N,K,L,C1,C2,AT,BT)
      DIMENSION Z(32,40),S(49),D(25),A(100,5),C1(32,8),C2(32,8)
C     ASSUMES THAT K LESS THAN 24
C     FORMS TRANSFORMATION CONSTANTS AI AND BT
      AT=2./(A(M,1)-A(1,1))
      BT=(A(M,1)+A(1,1))/2.
C     MAPS X INTO ZT AND FORMS MATRIX VALUES
      JJ=(2*K)+1
      DO 100 J=1,JJ
 100  S(J)=0.
      KK=K+1
      KKK=KK+N
      DO 1001 J=1,KK
      DO 1001 JJ=1,KKK
      Z(J,JJ)=0
 1001 CONTINUE
      DO 103 MM=1,M
      J=1
      KKK=2*K
      DO 103 KK=0,KKK
      ZT=AT*(A(MM,1)+BT)
      S(J)=ZT**KK+S(J)
      IF(KK-K)101,101,103
C     FORM COLUMN VECTORS OF Y
 101  IC=K+2
      IR=KK+1
      NNN=N+1
      DO 102 NN=2,NNN
      Z(IR,IC)=Z(IR,IC)+((ZT**KK)*A(MM,NN))
 102  IC=IC+1
 103  J=J+1
C     SETS UP MATRIX
      MC=K+1
      DO 104 IC=1,MC
      J=IC
      DO 104 IR=1,MC
      Z(IR,IC)=S(J)
 104  J=J+1
C     USE LINEQ FOR SOLUTION OF SYSTEM
      CALL LINEQ(Z,C2,MC,N,L)
      IF(L)111,105,111
C     REVERTING COEFFICIENTS TO ORIGINAL SYSTEM(C2 TO C1)
 105  II=K+1
      DO 110 NN=1,N
C     FORMS COEFFICIENTS FOR SYNTHETIC DIVISION
      DO 106 I=1,II
 106  D(I)=(C2(I,NN))*(AT**(I-1))
C     PERFORM SYNTHETIC DIVISION
      I=1
      JJ=0
 107  C1(I,NN)=0
      J=K+1
 108  C1(I,NN)=D(J)+(C1(I,NN)*(BT))
      D(J)=C1(I,NN)
      J=J-1
      IF(J-JJ)109,109,108
 109  I=I+1
      JJ=JJ+1
      IF(I-K-1)107,107,110
 110  CONTINUE
      L=0
 111  RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      LINEQ-LINEAREQUATIONSSOLVEP

      SUBROUTINELINEQ(A,X,N,K,L)
      DIMENSIONA(32,40),X(32,8),B(32,40),C(40)
      COMMONB,C,NN,KK,NK,TAP,Z,II,IP,I1,I2,I,J,JJ
      NN=N
      KK=K
      NK=NN+KK
      DO10I=1,NN
      DO10J=1,NK
10    B(I,J)=A(I,J)
      DO180I=1,NN
      II=I+1
      TAP=0.
      DO50J=I,NN
      Z=ABSF(B(J,I))
      IF(Z-1.)30,20,30
20    IP=J
      GOTO60
30    IF(Z-TAP)50,40,40
40    IP=J
      TAP=Z
50    CONTINUE
60    Z=B(IP,I)
      IF(Z)80,70,80
C     DETERMINANT=0INDICATEDBYL=1
70    L=1
      RETURN
80    DO90J=II,NK
90    C(J)=B(IP,J)/Z
      I1=NN
      I2=NN
93    IF(I1-IP)95,160,95
95    Z=B(I1,I)
      IF(Z)130,100,130
100   IF(I1-I2)110,150,110
110   DO120J=II,NK
120   B(I2,J)=B(I1,J)
      GOTO150
130   DO140J=II,NK
140   B(I2,J)=B(I1,J)-Z*C(J)
150   I2=I2-1
160   I1=I1-1
      IF(I2-I)170,170,93
170   DO180J=II,NK
180   B(I,J)=C(J)
      I=NN
185   I=I-1
      IF(I)210,210,190
190   DO200JJ=1,KK
      J=NN+JJ
      I1=I+1
      DO200I2=I1,NN
200   B(I,J)=B(I,J)-B(I,I2)*B(I2,J)
      GOTO185
210   DO220J=1,KK
      I1=NN+J
```

```
      LINEQ-LINEAREQUATIONSSOLVER

      DO220I=1,NN
220   X(I,J)=B(I,I1)
      IFACCUMULATOROVERFLOW230,240
C     FLOATINGPOINTOVERFLOWINDICATEDBYL=2
230   L=2
      RETURN
C     SUCCESSFULCOMPUTATIONINDICATEDBYL=0
240   L=0
      RETURN
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE READT(CS,MT1,L)
      DIMENSION CS(502)
      READ INPUT TAPE MT1,100,CS(1),CS(2)
      M=CS(1)+.5
      N=CS(2)+.5
      IF(M-100) 8,8,12
8     IF(N-4) 9,9,13
9     GO TO (1,2,3,4),N
1     DO 10 I=1,M
      J=2*I+1
      K1=J+1
10    READ INPUT TAPE MT1,100,CS(J),CS(K1)
      GO TO 5
2     DO 20 I=1,M
      J=3*I
      K1=J+1
      K2=J+2
20    READ INPUT TAPE MT1,200,CS(J),CS(K1),CS(K2)
      GO TO 5
3     DO 30 I=1,M
      J=4*I-1
      K1=J+1
      K2=J+2
      K3=J+3
30    READ INPUT TAPE MT1,300,CS(J),CS(K1),CS(K2),CS(K3)
      GO TO 5
4     DO 40 I=1,M
      J=5*I-2
      K1=J+1
      K2=J+2
      K3=J+3
      K4=J+4
40    READ INPUT TAPE MT1,400,CS(J),CS(K1),CS(K2),CS(K3),CS(K4)
5     L=0
6     RETURN
12    L=M
      GO TO 6
13    L=N
      GO TO 6
100   FORMAT(2E14.7)
200   FORMAT(3E14.7)
300   FORMAT(4E14.7)
400   FORMAT(5E14.7)
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

```
      SUBROUTINE ROOTS (C, R, N, TOL, CK1, CK2, L)
      DIMENSION C(51),R(100), A(51), B(51)
      COMMON A, B, NN,          LLL, N1,          Z, T, N2, N3, N4,
     1TK1, TK2, LL, P, Q, M, C1, C2, C3, DP, DQ, D,DELP, DELQ,
     2REAL, DISCR, RT
      EQUIVALENCE (KSCALE, FSCALE)
      LLL=0
      NN=N
      IF (C(1)) 20,10,20
C     HI-ORDER COEFFICIENT = 0. INDICATED BY L=1
10    LLL=1
15    L=LLL
      RETURN
20    DO 30 I=1,NN
30    A(I+1)=C(I+1)/C(1)
      A(1)=1.0
C     REMOVE ZERO ROOTS
      N1=NN
      IF (N1) 32,32,35
C     IMPROPER ARGUMENT N INDICATED BY L=2
32    LLL=2
      GO TO 15
35    IF (A(N1+1)) 50,40,50
40    R(2*N1-1)=0.
      R(2*N1)=0.
      N1=N1-1
      GO TO 35
C     RESCALE THE COEFFICIENTS
50    KSCALE=XINTF(2.*LOGF(ABSF(A(N1+1)))/(.69314718*FLOATF(N1)))
      KSCALE=((KSCALE+XSIGNF(1,KSCALE))/2)*512+66304
      Z=FSCALE
      DO 60 I=1,N1
      A(I+1)=A(I+1)/Z
      R(I)=A(I+1)
60    Z=Z*FSCALE
      T=TOL**2
      IF (T) 81,80,81
80    T=25.0E-14
81    N2=N1
      TK1=0.
      TK2=1.0
      B(1)=1.0
      LL=1
      GO TO 190
90    P=0.
      Q=0.
      PP=1.0
      QQ=1.0
      N6=4
100   M=100
105   B(2)=A(2)-P
      C2=1.0
      C1=B(2)-P
      DO 120 I=2,N2
      B(I+1)=A(I+1)-P*B(I)-Q*B(I-1)
      IF (I-N2) 110,120,120
```

```
      SUBROUTINE ROOTS (C, R, N, TOL, CK1, CK2, L)

 110  C3=C2
      C2=C1
      C1=B(I+1)-P*C2-Q*C3
 120  CONTINUE
      C1=-P*C2-Q*C3
      DP=B(N2)*C2-B(N2+1)*C3
      DQ=C2*B(N2+1)-C1*B(N2)
      D=C2*C2-C1*C3
      IF (D) 130,121,130
 121  GO TO (123,160),LL
 123  IF (M-100) 160,125,125
 125  N6=N6-1
      IF (N6) 160,127,127
 127  P=PP
      Q=QQ
      PP=-QQ
      QQ=P
      GO TO 100
 130  DELP=DP/D
      DELQ=DQ/D
      Z=P**2+Q**2
      IF (Z) 140,135,140
 135  Z=1.0
 140  IF ((DELP**2+DELQ**2)/Z-T) 142,142,145
 142  P=P+DELP
      Q=Q+DELQ
      GO TO 160
 145  M=M-1
      IF (M) 160,150,150
 150  P=P+DELP
      Q=Q+DELQ
      GO TO 105
  160 GO TO (170,250),LL
 170  N3=2*N1-N2
      R(N3+1)=P
      R(N3+2)=Q
      DO 180 I=1,N2
 180  A(I+1)=B(I+1)
      N2=N2-2
 190  IF (N2-2) 200,210,90
 200  R(2*N1)=A(2)
      GO TO 220
 210  R(2*N1-1)=A(2)
      R(2*N1)=A(3)
 220  N2=N1
      N5=N2
      LL=2
      DO 230 I=1,N1
 230  A(I+1)=R(I)
      GO TO 280
 240  N3=2*N1-N5
      P=R(N3+1)
      Q=R(N3+2)
      GO TO 100
 250  N4=N1-N5+1
      REAL=-P*FSCALE/2.0
```

```
      SUBROUTINE ROOTS (C, R, N, TOL, CK1, CK2, L)

      DISCR=REAL**2-Q*FSCALE**2
      IF (DISCR) 260,270,270
260   RT=SQRTF(ABSF(DISCR))
      R(2*N4-1)=REAL
      R(2*N4+1)=REAL
      R(2*N4)=RT
      R(2*N4+2)=-RT
      GO TO 275
270   RT=SQRTF(DISCR)
      R(2*N4-1)=REAL+RT
      R(2*N4)=0.
      R(2*N4+1)=REAL-RT
      R(2*N4+2)=0.
275   TK1=-R(2*N4-1)-R(2*N4+1)+TK1
      TK2=(R(2*N4-1)*R(2*N4+1)-R(2*N4)*R(2*N4+2))*TK2
      N5=N5-2
280   IF (N5-1) 300,290,240
290   R(2*N1-1)=-R(2*N1)*FSCALE
      R(2*N1)=0.
      TK1=TK1-R(2*N1-1)
      TK2=-TK2*R(2*N1-1)
300   D=C(2)/C(1)
      IF (D) 320,310,320
310   D=1.0
320   CK1=(C(2)/C(1)-TK1)/D
      CK2=(C(N1+1)/C(1)-TK2)/(C(N1+1)/C(1))
      IF DIVIDE CHECK 330,340
330   LLL=3
340   IF ACCUMULATOR OVERFLOW 330,15
      END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

APPENDIX B

SAMPLE OUTPUT AND INPUT

W-1R 52 HR AT 2110 DEG C
0040550100290060070010010010 01

3.0	+00 3.5	+00 4.0	+00 4.3	+00 4.5	+00
4.6	+00 4.7	+00 4.8	+00 4.9	+00 5.	+00
5.1	+00 5.2	+00 5.3	+00 5.4	+00 5.5	+00
5.6	+00 5.7	+00 5.8	+00 5.9	+00 6.	+00
6.1	+00 6.2	+00 6.3	+00 6.4	+00 6.5	+00
6.6	+00 6.7	+00 6.8	+00 6.9	+00 7.	+00
7.1	+00 7.2	+00 7.3	+00 7.4	+00 7.5	+00
7.6	+00 7.7	+00 7.8	+00 7.9	+00 8.	+00
8.15	+00 8.3	+00 8.4	+00 8.5	+00 8.6	+00
8.7	+00 8.8	+00 8.9	+00 9.0	+00 9.2	+00
9.3	+00 9.4	+00 9.5	+00 9.7	+00 9.9	+00
9.33	-01 9.04	-01 8.72	-01 8.53	-01 8.24	-01
8.23	-01 8.14	-01 8.0	-01 7.96	-01 7.87	-01
-9.99	+03 7.56	-01 7.49	-01 7.29	-01 7.06	-01
6.98	-01 6.91	-01 6.78	-01 6.70	-01 6.67	-01
6.55	-01 6.43	-01 6.31	-01 6.16	-01 6.	01
5.82	-01 5.72	-01 5.61	-01 5.46	-01 5.36	-01
5.25	-01 5.1	-01 5.03	-01 4.95	-01 4.67	-01
4.67	-01 4.6	-01 4.56	-01 4.36	-01 4.24	-01
-9.99	+03 2.4	-01 2.33	-01 2.26	-01 2.23	-01
2.2	-01 2.04	-01 9.99	+03 6.4	-02 4.4	-02
3.4	-02 2.7	-02 2.0	-02 1.3	-02 6.	03
5.0	-02 5.2	+01 1.79578	-03 1.0	+00 0.	
1.0	-02 .	.	.	.	

Note: Each line is one card; the digit at the extreme left is in column 1 of card 2.

W-1R 52 HR AT 2110 DEG C

4
55
10
29
6
7

3.00000	0.93300
3.50000	0.90400
4.00000	0.87200
4.30000	0.85300
4.50000	0.82400
4.60000	0.82300
4.70000	0.81400
4.80000	0.80000
4.90000	0.79600
5.00000	0.78700
5.10000	-9990.00000
5.20000	0.75600
5.30000	0.74900
5.40000	0.72900
5.50000	0.70600
5.60000	0.69800
5.70000	0.69100
5.80000	0.67800
5.90000	0.67000
6.00000	0.66700
6.10000	0.65500
6.20000	0.64300
6.30000	0.63100
6.40000	0.61600
6.50000	0.60000
6.60000	0.58200
6.70000	0.57200
6.80000	0.56100
6.90000	0.54600
7.00000	0.53600
7.10000	0.52500
7.20000	0.51000
7.30000	0.50300
7.40000	0.49500
7.50000	0.46700
7.60000	0.46700
7.70000	0.46000
7.80000	0.45600
7.90000	0.43600
8.00000	0.42400
8.15000	-9990.00000
8.30000	0.24000
8.40000	0.23300
8.50000	0.22600
8.60000	0.22300
8.70000	0.22000
8.80000	0.20400
8.90000	-9990.00000
9.00000	0.06400
9.20000	0.04400
9.30000	0.03400
9.40000	0.02700
9.50000	0.02000
9.70000	0.01300
9.90000	0.00600

LEAST SQUARES CURVE FIT OF DEGREE 1   6 OBSERVED DATA POINTS   SET NUMBER 1

	X OBSERVED	Y OBSERVED	COEFFICIENTS ORIGINAL SYS	Y COMPUTED ORIGINAL SYS	REL ERR ORIG	COEFFICIENTS TRANSFORMED SYS	Y COMPUTED TRANSFORMED SYS	REL ERR TRANS
1	0.8300000E 01	-0.7060265E 00	0.1063935E 01	-0.7046783E 00	0.19E-02	0.2885819E 01	-0.7046783E 00	0.19E-02
2	0.8400000E 01	-0.7287447E 00	-0.2130859E-00	-0.7259869E 00	0.38E-02	-0.5327148E-01	-0.7259869E 00	0.38E-02
3	0.8500000E 01	-0.7518456E C0		-0.7472955E 00	0.61E-02		-0.7472955E 00	0.61E-02
4	0.8600000E 01	-0.7618695E 00		-0.7686041E 00	-0.88E-02		-0.7686041E 00	-0.88E-02
5	0.8700000E 01	-0.7719705E 00		-0.7899127E 00	-0.23E-01		-0.7899127E 00	-0.23E-01
6	0.8800000E 01	-0.8272418E 00		-0.8112213E 00	0.19E-01		-0.8112213E C0	0.19E-01

DIFFERENCES

RMS ORG. 0.10E-01   RMS TRANS 0.10E-01

MAX ABS. 0.18E-01   MAX ABS. 0.18E-01

RELATIVE ERRORS

RMS ORG. 0.13E-01   RMS TRANS 0.13E-01

MAX ABS. 0.23E-01   MAX ABS. 0.23E-01

TRANSFORMATION Z=A(X-B)

WHERE A = 0.4000000E 01

WHERE B = 0.8550000E 01

JBH/LBF

LEAST SQUARES CURVE FIT OF DEGREE 1   29 OBSERVED DATA POINTS   SET NUMBER 1

	X OBSERVED	Y OBSERVED	COEFFICIENTS ORIGINAL SYS	Y COMPUTED ORIGINAL SYS	REL ERR ORIG	COEFFICIENTS TRANSFORMED SYS	Y COMPUTED TRANSFORMED SYS	REL ERR TRANS
1	0.5200000E 01	0.6932073E 00	0.2281929E 01	0.6636574E 00	0.43E-01	0.4335889E 01	0.6636575E 00	0.43E-01
2	0.5300000E 01	0.6710432E 00	-0.3112061E-00	0.6325368E 00	0.57E-01	-0.4356885E-00	0.6325369E 00	0.57E-01
3	0.5400000E 01	0.6094442E 00		0.6014162E 00	0.13E-01		0.6014162E 00	0.13E-01
4	0.5500000E 01	0.5413471E 00		0.5702956E 00	-0.53E-01		0.5702956E 00	-0.53E-01
5	0.5600000E 01	0.5182553E 00		0.5391750E 00	-0.40E-01		0.5391750E 00	-0.40E-01
6	0.5700000E 01	0.4982757E-00		0.5080544E 00	-0.20E-01		0.5080544E 00	-0.20E-01
7	0.5800000E 01	0.4616874E-00		0.4769338E-00	-0.33E-01		0.4769338E-00	-0.33E-01
8	0.5900000E 01	0.4394801E-00		0.4458132E-00	-0.14E-01		0.4458132E-00	-0.14E-01
9	0.6000000E 01	0.4312089E-00		0.4146926E-00	0.38E-01		0.4146926E-00	0.38E-01
10	0.6100000E 01	0.3984132E-00		0.3835720E-00	0.37E-01		0.3835720E-00	0.37E-01
11	0.6200000E 01	0.3660450E-00		0.3524514E-00	0.37E-01		0.3524514E-00	0.37E-01
12	0.6300000E 01	0.3340608E-00		0.3213308E-00	0.38E-01		0.3213308E-00	0.38E-01
13	0.6400000E 01	0.2945590E-00		0.2902101E-00	0.15E-01		0.2902102E-00	0.15E-01
14	0.6500000E 01	0.2529332E-00		0.2590895E-00	-0.24E-01		0.2590896E-00	-0.24E-01
15	0.6600000E 01	0.2066329E-00		0.2279689E-00	-0.10E-00		0.2279690E-00	-0.10E-00
16	0.6700000E 01	0.1811140E-00		0.1968483E-00	-0.87E-01		0.1968483E-00	-0.87E-01
17	0.6800000E 01	0.1531845E-00		0.1657277E-00	-0.82E-01		0.1657278E-00	-0.82E-01
18	0.6900000E 01	0.1152976E-00		0.1346071E-00	-0.17E-00		0.1346071E-00	-0.17E-00
19	0.7000000E 01	0.9014249E-01		0.1034865E-00	-0.15E-00		0.1034865E-00	-0.15E-00
20	0.7100000E 01	0.6254482E-01		0.7236591E-01	-0.16E-00		0.7236588E-01	-0.16E-00
21	0.7200000E 01	0.2499834E-01		0.4124528E-01	-0.65E 00		0.4124528E-01	-0.65E 00
22	0.7300000E 01	0.7497847E-02		0.1012468E-01	-0.35E-00		0.1012468E-01	-0.35E-00
23	0.7400000E 01	-0.1249713E-01		-0.2099591E-01	-0.68E 00		-0.2099591E-01	-0.68E 00
24	0.7500000E 01	-0.8260912E-01		-0.5211654E-01	0.37E-00		-0.5211651E-01	0.37E-00
25	0.7600000E 01	-0.8260912E-01		-0.8323714E-01	-0.76E-02		-0.8323711E-01	-0.76E-02
26	0.7700000E 01	-0.1001960E-00		-0.1143577E-00	-0.14E-00		-0.1143577E-00	-0.14E-00
27	0.7800000E 01	-0.1102607E-00		-0.1454783E-00	-0.32E-00		-0.1454783E-00	-0.32E-00
28	0.7900000E 01	-0.1607882E-00		-0.1765990E-00	-0.98E-01		-0.1765990E-00	-0.98E-01
29	0.8000000E 01	-0.1913059E-00		-0.2077196E-00	-0.86E-01		-0.2077196E-00	-0.86E-01

DIFFERENCES		RELATIVE ERRORS		TRANSFORMATION Z=A(X-B)
RMS ORG. 0.18E-01	RMS TRANS 0.18E-01	RMS ORG. 0.22E-00	RMS TRANS 0.22E-00	WHERE A = 0.7142857E 00
MAX ABS. 0.39E-01	MAX ABS. 0.39E-01	MAX ABS. 0.68E 00	MAX ABS. 0.68F 00	WHERE B = 0.6600000E 01

JBH/LBF

LEAST SQUARES CURVE FIT OF DEGREE 1   6 OBSERVED DATA POINTS   SET NUMBER 1

	X OBSERVED	Y OBSERVED	COEFFICIENTS ORIGINAL SYS	Y COMPUTED ORIGINAL SYS	REL ERR ORIG	COEFFICIENTS TRANSFORMED SYS	Y COMPUTED TRANSFORMED SYS	REL ERR TRANS
1	0.8300000E 01	-0.7060265E 00	0.1063935E 01	-0.7046783E 00	0.19E-02	0.2885819E 01	-0.7046783E 00	0.19E-02
2	0.8400000E 01	-0.7287447E 00	-0.2130859E-00	-0.7259869E 00	0.38E-02	-0.5327148E-01	-0.7259869E 00	0.38E-02
3	0.8500000E 01	-0.7518456E CO		-0.7472955E 00	0.61E-02		-0.7472955E 00	0.61E-02
4	0.8600000E 01	-0.7618695E 00		-0.7686041E 00	-0.88E-02		-0.7686041E 00	-0.88E-02
5	0.8700000E 01	-0.7719705E 00		-0.7899127E 00	-0.23E-01		-0.7899127E 00	-0.23E-01
6	0.8800000E 01	-0.8272418E 00		-0.8112213E 00	0.19E-01		-0.8112213E CO	0.19E-01

DIFFERENCES
RMS ORG. 0.10E-01   RMS TRANS 0.10E-01
MAX ABS. 0.18E-01   MAX ABS. 0.18E-01

RELATIVE ERRORS
RMS ORG. 0.13E-01   RMS TRANS 0.13E-01
MAX ABS. 0.23E-01   MAX ABS. 0.23E-01

TRANSFORMATION Z=A(X-B)
WHERE A = 0.4000000E 01
WHERE B = 0.8550000E 01

JBH/LBF

LEAST SQUARES CURVE FIT OF DEGREE 1   7 OBSERVED DATA POINTS   SET NUMBER 1

	X OBSERVED	Y OBSERVED	COEFFICIENTS ORIGINAL SYS	Y COMPUTED ORIGINAL SYS	REL ERR ORIG	COEFFICIENTS TRANSFORMED SYS	Y COMPUTED TRANSFORMED SYS	REL ERR TRANS
1	0.90000000E 01	-0.1522345E 01	0.8296073E 01	-0.1501294E 01	0.14E-01	0.1858331E 02	-0.1501294E 01	0.14E-01
2	0.92000000E 01	-0.1706421E 01	-0.1088596E 01	-0.1719014E 01	-0.74E-02	-0.4898684E-00	-0.1719014E 01	-0.74E-02
3	0.93000000E 01	-0.1825415E 01		-0.1827873E 01	-0.13E-02		-0.1827873E 01	-0.13E-02
4	0.94000000E 01	-0.1927263E 01		-0.1936733E 01	-0.49E-02		-0.1936733E 01	-0.49E-02
5	0.95000000E 01	-0.2054188E 01		-0.2045593E 01	0.42E-02		-0.2045593E 01	0.42E-02
6	0.97000000E 01	-0.2226654E 01		-0.2263312E 01	-0.16E-01		-0.2263312E 01	-0.16E-01
7	0.99000000E 01	-0.2512561E 01		-0.2481031E 01	0.13E-01		-0.2481031E 01	0.13E-01

DIFFERENCES
RMS ORG. 0.21E-01   RMS TRANS 0.21E-01
MAX ABS. 0.37E-01   MAX ABS. 0.37E-01

RELATIVE ERRORS
RMS ORG. 0.10E-01   RMS TRANS 0.10E-01
MAX ABS. 0.16E-01   MAX ABS. 0.16E-01

TRANSFORMATION Z=A(X-B)
WHERE A = 0.2222222E 01
WHERE B = 0.9450000E 01
JBH/LBF

REGENERATED DATA

DISTANCE	CONCENTRATION
0.	1.00000
0.05000	0.99435
0.10000	0.99406
0.15000	0.99375
0.20000	0.99343
0.25000	0.99310
0.30000	0.99275
0.35000	0.99239
0.40000	0.99201
0.45000	0.99162
0.50000	0.99121
0.55000	0.99078
0.60000	0.99033
0.65000	0.98986
0.70000	0.98938
0.75000	0.98887
0.80000	0.98834
0.85000	0.98779
0.90000	0.98722
0.95000	0.98663
1.00000	0.98601
1.05000	0.98537
1.10000	0.98470
1.15000	0.98400
1.20000	0.98328
1.25000	0.98254
1.30000	0.98176
1.35000	0.98095
1.40000	0.98012
1.45000	0.97925
1.50000	0.97835
1.55000	0.97742
1.60000	0.97646
1.65000	0.97546
1.70000	0.97442
1.75000	0.97335
1.80000	0.97224
1.85000	0.97110
1.90000	0.96991
1.95000	0.96869

2.00000	0.96742	5.10000	0.77281
2.05000	0.96611	5.10000	0.75641
2.10000	0.96476	5.15000	0.75150
2.15000	0.96337	5.20000	0.74655
2.20000	0.96193	5.25000	0.74154
2.25000	0.96044	5.30000	0.73648
2.30000	0.95891	5.35000	0.73138
2.35000	0.95733	5.40000	0.72622
2.40000	0.95570	5.45000	0.72101
2.45000	0.95402	5.50000	0.71576
2.50000	0.95229	5.55000	0.71046
2.55000	0.95051	5.60000	0.70512
2.60000	0.94867	5.65000	0.69973
2.65000	0.94678	5.70000	0.69429
2.70000	0.94484	5.75000	0.68881
2.75000	0.94284	5.80000	0.68329
2.80000	0.94079	5.85000	0.67773
2.85000	0.93867	5.90000	0.67213
2.90000	0.93650	5.95000	0.66649
2.95000	0.93427	6.00000	0.66082
3.00000	0.93198	6.05000	0.65510
3.05000	0.92963	6.10000	0.64935
3.10000	0.92722	6.15000	0.64357
3.15000	0.92474	6.20000	0.63775
3.20000	0.92220	6.25000	0.63190
3.25000	0.91959	6.30000	0.62602
3.30000	0.91692	6.35000	0.62011
3.35000	0.91418	6.40000	0.61418
3.40000	0.91138	6.45000	0.60821
3.45000	0.90851	6.50000	0.60222
3.50000	0.90557	6.55000	0.59621
3.55000	0.90256	6.60000	0.59017
3.60000	0.89948	6.65000	0.58412
3.65000	0.89633	6.70000	0.57804
3.70000	0.89311	6.75000	0.57194
3.75000	0.88982	6.80000	0.56583
3.80000	0.88645	6.85000	0.55970
3.85000	0.88301	6.90000	0.55355
3.90000	0.87950	6.95000	0.54739
3.95000	0.87592	7.00000	0.54122
4.00000	0.87226	7.05000	0.53505
4.05000	0.86853	7.10000	0.52886
4.10000	0.86472	7.15000	0.52266
4.15000	0.86084	7.20000	0.51646
4.20000	0.85688	7.25000	0.51025
4.25000	0.85285	7.30000	0.50404
4.30000	0.84874	7.35000	0.49783
4.35000	0.84456	7.40000	0.49162
4.40000	0.84030	7.45000	0.48541
4.45000	0.83597	7.50000	0.47921
4.50000	0.83155	7.55000	0.47301
4.55000	0.82707	7.60000	0.46682
4.60000	0.82251	7.65000	0.46064
4.65000	0.81787	7.70000	0.45446
4.70000	0.81316	7.75000	0.44830
4.75000	0.80837	7.80000	0.44215
4.80000	0.80351	7.85000	0.43602
4.85000	0.79858	7.90000	0.42990
4.90000	0.79357	7.95000	0.42380
4.95000	0.78849	8.00000	0.41771
5.00000	0.78334	8.05000	0.41165
5.05000	0.77811	8.10000	0.40561

8.15000	0.39959
8.15000	0.25056
8.20000	0.24718
8.25000	0.24383
8.30000	0.24050
8.35000	0.23720
8.39999	0.23392
8.44999	0.23066
8.49999	0.22744
8.54999	0.22423
8.59999	0.22106
8.64999	0.21791
8.69999	0.21478
8.74999	0.21168
8.79999	0.20861
8.84999	0.20556
8.89999	0.20254
8.89999	0.08188
8.94999	0.07395
8.99999	0.06663
9.04999	0.05987
9.09999	0.05367
9.14999	0.04799
9.19999	0.04280
9.24999	0.03807
9.29999	0.03378
9.34999	0.02990
9.39999	0.02639
9.44999	0.02323
9.49999	0.02040
9.54999	0.01787
9.59999	0.01561
9.64999	0.01360
9.69999	0.01182
9.74999	0.01024
9.79999	0.00885
9.84999	0.00763
9.89999	0.00656
9.94999	0.00562
9.99999	0.00481
10.04999	0.00410
10.09999	0.00349
10.14999	0.00296
10.19999	0.00250
10.24999	0.00211
10.29999	0.00178
10.34999	0.00149
10.39999	0.00125
10.44999	0.00104
10.49999	0.00086
10.54999	0.00072
10.59999	0.00059
10.64999	0.00049
10.69999	0.00040
10.74999	0.00033
10.79999	0.00027
10.84999	0.00022
10.89999	0.00018
10.94999	0.00015
10.99999	0.00012

XM= 6.7178153E 00 TIME= 5.1999999E 01 CVF= 1.7957800E-03

X(I)	CA(I) AFTER AXIS SHIFT
-6.7178153E 00	1.0000000E 00
-6.6678153E 00	9.9434743E-01
-6.6178153E 00	9.9405617E-01
-6.5678152E 00	9.9375167E-01
-6.5178152E 00	9.9343343E-01
-6.4678153E 00	9.9310095E-01
-6.4178153E 00	9.9275368E-01
-6.3678153E 00	9.9239109E-01
-6.3178152E 00	9.9201261E-01
-6.2678153E 00	9.9161767E-01
-6.2178153E 00	9.9120568E-01
-6.1678153E 00	9.9077605E-01
-6.1178153E 00	9.9032815E-01
-6.0678153E 00	9.8986136E-01
-6.0178153E 00	9.8937502E-01
-5.9678153E 00	9.8886847E-01
-5.9178153E 00	9.8834107E-01
-5.8678153E 00	9.8779209E-01
-5.8178153E 00	9.8722084E-01
-5.7678153E 00	9.8662660E-01
-5.7178153E 00	9.8600864E-01
-5.6678153E 00	9.8536620E-01
-5.6178153E 00	9.8469855E-01
-5.5678153E 00	9.8400489E-01
-5.5178154E 00	9.8328443E-01
-5.4678153E 00	9.8253638E-01
-5.4178153E 00	9.8175992E-01
-5.3678153E 00	9.8095423E-01
-5.3178154E 00	9.8011845E-01
-5.2678154E 00	9.7925174E-01
-5.2178153E 00	9.7835324E-01
-5.1678153E 00	9.7742207E-01
-5.1178154E 00	9.7645733E-01
-5.0678154E 00	9.7545815E-01
-5.0178154E 00	9.7442359E-01
-4.9678153E 00	9.7335274E-01
-4.9178154E 00	9.7224468E-01
-4.8678154E 00	9.7109848E-01
-4.8178154E 00	9.6991318E-01
-4.7678154E 00	9.6868784E-01
-4.7178154E 00	9.6742151E-01
-4.6678154E 00	9.6611320E-01
-4.6178154E 00	9.6476195E-01
-4.5678154E 00	9.6336679E-01
-4.5178155E 00	9.6192676E-01
-4.4678155E 00	9.6044084E-01
-4.4178155E 00	9.5890808E-01
-4.3678155E 00	9.5732749E-01
-4.3178155E 00	9.5569805E-01
-4.2678155E 00	9.5401883E-01
-4.2178156E 00	9.5228881E-01
-4.1678156E 00	9.5050702E-01
-4.1178156E 00	9.4867249E-01
-4.0678156E 00	9.4678423E-01
-4.0178156E 00	9.4484129E-01
-3.9678157E 00	9.4284270E-01

-3.9178157E 00	9.4078752E-01
-3.8678157E 00	9.3867478E-01
-3.8178157E 00	9.3650359E-01
-3.7678157E 00	9.3427298E-01
-3.7178158E 00	9.3198208E-01
-3.6678158E 00	9.2962996E-01
-3.6178158E 00	9.2721575E-01
-3.5678158E 00	9.2473861E-01
-3.5178158E 00	9.2219765E-01
-3.4678158E 00	9.1959208E-01
-3.4178159E 00	9.1692106E-01
-3.3678159E 00	9.1418381E-01
-3.3178159E 00	9.1137958E-01
-3.2678159E 00	9.0850760E-01
-3.2178159E 00	9.0556718E-01
-3.1678160E 00	9.0255761E-01
-3.1178160E 00	8.9947824E-01
-3.0678160E 00	8.9632843E-01
-3.0178160E 00	8.9310757E-01
-2.9678160E 00	8.8981509E-01
-2.9178160E 00	8.8645047E-01
-2.8678161E 00	8.8301316E-01
-2.8178161E 00	8.7950275E-01
-2.7678161E 00	8.7591875E-01
-2.7178161E 00	8.7226079E-01
-2.6678162E 00	8.6852850E-01
-2.6178162E 00	8.6472157E-01
-2.5678163E 00	8.6083972E-01
-2.5178163E 00	8.5688272E-01
-2.4678164E 00	8.5285037E-01
-2.4178164E 00	8.4874252E-01
-2.3678164E 00	8.4455907E-01
-2.3178165E 00	8.4029996E-01
-2.2678165E 00	8.3596519E-01
-2.2178166E 00	8.3155481E-01
-2.1678166E 00	8.2706887E-01
-2.1178167E 00	8.2250752E-01
-2.0678167E 00	8.1787096E-01
-2.0178168E 00	8.1315942E-01
-1.9678168E 00	8.0837318E-01
-1.9178169E 00	8.0351259E-01
-1.8678169E 00	7.9857803E-01
-1.8178170E 00	7.9356996E-01
-1.7678170E 00	7.8848888E-01
-1.7178171E 00	7.8333532E-01
-1.6678171E 00	7.7810991E-01
-1.6178172E 00	7.7281330E-01
-1.6178172E 00	7.5640727E-01
-1.5678172E 00	7.5150375E-01
-1.5178173E 00	7.4654818E-01
-1.4678173E 00	7.4154121E-01
-1.4178174E 00	7.3648353E-01
-1.3678174E 00	7.3137589E-01
-1.3178174E 00	7.2621905E-01
-1.2678175E 00	7.2101376E-01
-1.2178175E 00	7.1576090E-01
-1.1678176E 00	7.1046128E-01
-1.1178176E 00	7.0511580E-01
-1.0678177E 00	6.9972534E-01
-1.0178177E 00	6.9429088E-01
-9.6781778E-01	6.8881337E-01
-9.1781783E-01	6.8329381E-01

-8.6781788E-01	6.7773323E-01
-8.1781793E-01	6.7213266E-01
-7.6781797E-01	6.6649321E-01
-7.1781802E-01	6.6081597E-01
-6.6781807E-01	6.5510203E-01
-6.1781812E-01	6.4935260E-01
-5.6781816E-01	6.4356884E-01
-5.1781821E-01	6.3775192E-01
-4.6781826E-01	6.3190311E-01
-4.1781831E-01	6.2602359E-01
-3.6781836E-01	6.2011467E-01
-3.1781840E-01	6.1417761E-01
-2.6781845E-01	6.0821370E-01
-2.1781850E-01	6.0222428E-01
-1.6781855E-01	5.9621063E-01
-1.1781859E-01	5.9017414E-01
-6.7818642E-02	5.8411617E-01
-1.7818689E-02	5.7803805E-01
3.2181263E-02	5.7194121E-01
8.2181215E-02	5.6582700E-01
1.3218117E-01	5.5969687E-01
1.8218112E-01	5.5355219E-01
2.3218107E-01	5.4739435E-01
2.8218102E-01	5.4122486E-01
3.3218098E-01	5.3504509E-01
3.8218093E-01	5.2885644E-01
4.3218088E-01	5.2266039E-01
4.8218083E-01	5.1645834E-01
5.3218079E-01	5.1025174E-01
5.8218074E-01	5.0404200E-01
6.3218069E-01	4.9783068E-01
6.8218064E-01	4.9162027E-01
7.3218060E-01	4.8541257E-01
7.8218055E-01	4.7920900E-01
8.3218050E-01	4.7301100E-01
8.8218045E-01	4.6681997E-01
9.3218040E-01	4.6063737E-01
9.8218036E-01	4.5446460E-01
1.0321803E 00	4.4830312E-01
1.0821803E 00	4.4215435E-01
1.1321802E 00	4.3601965E-01
1.1821802E 00	4.2990050E-01
1.2321801E 00	4.2379827E-01
1.2821801E 00	4.1771436E-01
1.3321800E 00	4.1165017E-01
1.3821800E 00	4.0560705E-01
1.4321799E 00	3.9958640E-01
1.4321799E 00	2.5056129E-01
1.4821799E 00	2.4718322E-01
1.5321798E 00	2.4382964E-01
1.5821798E 00	2.4050075E-01
1.6321797E 00	2.3719673E-01
1.6821797E 00	2.3391780E-01
1.7321796E 00	2.3066411E-01
1.7821796E 00	2.2743585E-01
1.8321795E 00	2.2423317E-01
1.8821795E 00	2.2105626E-01
1.9321795E 00	2.1790525E-01
1.9821794E 00	2.1478027E-01
2.0321794E 00	2.1168149E-01
2.0821793E 00	2.0860901E-01
2.1321793E 00	2.0556298E-01

2.1821792E 00	2.0254352E-01
2.1821792E 00	8.1877134E-02
2.2321792E 00	7.3950890E-02
2.2821791E 00	6.6625129E-02
2.3321791E 00	5.9874363E-02
2.3821790E 00	5.3671837E-02
2.4321790E 00	4.7989852E-02
2.4821789E 00	4.2800087E-02
2.5321789E 00	3.8073890E-02
2.5821788E 00	3.3782545E-02
2.6321788E 00	2.9897541E-02
2.6821787E 00	2.6390772E-02
2.7321787E 00	2.3234743E-02
2.7821786E 00	2.0402748E-02
2.8321786E 00	1.7869011E-02
2.8821785E 00	1.5608799E-02
2.9321785E 00	1.3598528E-02
2.9821784E 00	1.1815820E-02
3.0321784E 00	1.0239579E-02
3.0821784E 00	8.8499970E-03
3.1321783E 00	7.6285787E-03
3.1821783E 00	6.5581352E-03
3.2321782E 00	5.6227706E-03
3.2821782E 00	4.8078448E-03
3.3321781E 00	4.0999427E-03
3.3821781E 00	3.4868233E-03
3.4321780E 00	2.9573552E-03
3.4821780E 00	2.5014766E-03
3.5321779E 00	2.1101125E-03
3.5821779E 00	1.7751269E-03
3.6321778E 00	1.4892407E-03
3.6821778E 00	1.2459755E-03
3.7321777E 00	1.0395870E-03
3.7821777E 00	8.6500123E-04
3.8321776E 00	7.1775541E-04
3.8821776E 00	5.9393421E-04
3.9321775E 00	4.9011409E-04
3.9821775E 00	4.0332228E-04
4.0321774E 00	3.3098087E-04
4.0821774E 00	2.7086213E-04
4.1321774E 00	2.2104383E-04
4.1821773E 00	1.7989054E-04
4.2321773E 00	1.4598668E-04
4.2821772E 00	1.1814386E-04

W-IR 52 HR AT 2110 DEG C

FOR CA=.990	D= 2.160E-07	DP= 3.386E-07	XF=-6.083E 00	DERP=-6.005E-03	DERF=-9.414E-03	SEG	1
FOR CA=.980	D= 2.214E-07	DP= 2.211E-07	XF=-5.312E 00	DERP=-1.713E-02	DERF=-1.710E-02	SEG	1
FOR CA=.970	D= 2.230E-07	DP= 2.343E-07	XF=-4.823E 00	DERP=-2.288E-02	DERF=-2.404E-02	SEG	1
FOR CA=.960	D= 2.230E-07	DP= 2.485E-07	XF=-4.455E 00	DERP=-2.732E-02	DERF=-3.045E-02	SEG	1
FOR CA=.950	D= 2.229E-07	DP= 2.328E-07	XF=-4.155E 00	DERP=-3.490E-02	DERF=-3.644E-02	SEG	1
FOR CA=.940	D= 2.226E-07	DP= 2.236E-07	XF=-3.900E 00	DERP=-4.190E-02	DERF=-4.210E-02	SEG	1
FOR CA=.930	D= 2.222E-07	DP= 2.279E-07	XF=-3.677E 00	DERP=-4.626E-02	DERF=-4.745E-02	SEG	1
FOR CA=.920	D= 2.218E-07	DP= 2.247E-07	XF=-3.477E 00	DERP=-5.187E-02	DERF=-5.254E-02	SEG	1
FOR CA=.910	D= 2.213E-07	DP= 2.217E-07	XF=-3.295E 00	DERP=-5.729E-02	DERF=-5.740E-02	SEG	1
FOR CA=.900	D= 2.208E-07	DP= 2.245E-07	XF=-3.127E 00	DERP=-6.100E-02	DERF=-6.204E-02	SEG	1
FOR CA=.890	D= 2.203E-07	DP= 2.230E-07	XF=-2.971E 00	DERP=-6.566E-02	DERF=-6.647E-02	SEG	1
FOR CA=.880	D= 2.197E-07	DP= 2.213E-07	XF=-2.825E 00	DERP=-7.021E-02	DERF=-7.072E-02	SEG	1
FOR CA=.870	D= 2.192E-07	DP= 2.207E-07	XF=-2.688E 00	DERP=-7.429E-02	DERF=-7.479E-02	SEG	1
FOR CA=.860	D= 2.186E-07	DP= 2.190E-07	XF=-2.557E 00	DERP=-7.857E-02	DERF=-7.869E-02	SEG	1
FOR CA=.850	D= 2.181E-07	DP= 2.186E-07	XF=-2.433E 00	DERP=-8.225E-02	DERF=-8.244E-02	SEG	1
FOR CA=.840	D= 2.175E-07	DP= 2.175E-07	XF=-2.314E 00	DERP=-8.606E-02	DERF=-8.603E-02	SEG	1
FOR CA=.830	D= 2.170E-07	DP= 2.183E-07	XF=-2.200E 00	DERP=-8.894E-02	DERF=-8.948E-02	SEG	1
FOR CA=.820	D= 2.164E-07	DP= 2.176E-07	XF=-2.091E 00	DERP=-9.227E-02	DERF=-9.278E-02	SEG	1
FOR CA=.810	D= 2.158E-07	DP= 2.164E-07	XF=-1.984E 00	DERP=-9.570E-02	DERF=-9.596E-02	SEG	1
FOR CA=.800	D= 2.153E-07	DP= 2.156E-07	XF=-1.882E 00	DERP=-9.885E-02	DERF=-9.900E-02	SEG	1
FOR CA=.790	D= 2.147E-07	DP= 2.149E-07	XF=-1.782E 00	DERP=-1.018E-01	DERF=-1.019E-01	SEG	1
FOR CA=.780	D= 2.141E-07	DP= 2.148E-07	XF=-1.685E 00	DERP=-1.044E-01	DERF=-1.047E-01	SEG	1

UNSATISFACTORY XF FOR CA= .770
0.4959198E 01 0. 0. 0. 0. 0.

FOR CA=.760	D=-4.708E-07	DP= 7.616E-12	XF=-1.654E 00	DERP= 5.982E 03	DERF=-9.676E-02	SEG	2
FOR CA=.750	D= 2.418E-07	DP= 2.419E-07	XF=-1.552E 00	DERP=-9.888E-02	DERF=-9.891E-02	SEG	2
FOR CA=.740	D= 2.415E-07	DP= 2.420E-07	XF=-1.452E 00	DERP=-1.008E-01	DERF=-1.010E-01	SEG	2
FOR CA=.730	D= 2.412E-07	DP= 2.414E-07	XF=-1.353E 00	DERP=-1.028E-01	DERF=-1.029E-01	SEG	2
FOR CA=.720	D= 2.408E-07	DP= 2.409E-07	XF=-1.257E 00	DERP=-1.047E-01	DERF=-1.048E-01	SEG	2

FOR CA=.710	D= 2.403E-07	DP= 2.404E-07	XF=-1.162E 00	DERP=-1.065E-01	DERF=-1.065E-01	SEG 2
FOR CA=.700	D= 2.398E-07	DP= 2.397E-07	XF=-1.069E 00	DERP=-1.082E-01	DERF=-1.082E-01	SEG 2
FOR CA=.690	D= 2.392E-07	DP= 2.394E-07	XF=-9.773E-01	DERP=-1.097E-01	DERF=-1.098E-01	SEG 2
FOR CA=.680	D= 2.386E-07	DP= 2.387E-07	XF=-8.868E-01	DERP=-1.113E-01	DERF=-1.113E-01	SEG 2
FOR CA=.670	D= 2.379E-07	DP= 2.379E-07	XF=-7.975E-01	DERP=-1.127E-01	DERF=-1.127E-01	SEG 2
FOR CA=.660	D= 2.372E-07	DP= 2.373E-07	XF=-7.092E-01	DERP=-1.140E-01	DERF=-1.140E-01	SEG 2
FOR CA=.650	D= 2.364E-07	DP= 2.365E-07	XF=-6.220E-01	DERP=-1.153E-01	DERF=-1.153E-01	SEG 2
FOR CA=.640	D= 2.356E-07	DP= 2.357E-07	XF=-5.357E-01	DERP=-1.164E-01	DERF=-1.164E-01	SEG 2
FOR CA=.630	D= 2.348E-07	DP= 2.348E-07	XF=-4.502E-01	DERP=-1.175E-01	DERF=-1.175E-01	SEG 2
FOR CA=.620	D= 2.339E-07	DP= 2.340E-07	XF=-3.655E-01	DERP=-1.185E-01	DERF=-1.185E-01	SEG 2
FOR CA=.610	D= 2.330E-07	DP= 2.330E-07	XF=-2.814E-01	DERP=-1.194E-01	DERF=-1.194E-01	SEG 2
FOR CA=.600	D= 2.320E-07	DP= 2.320E-07	XF=-1.980E-01	DERP=-1.202E-01	DERF=-1.202E-01	SEG 2
FOR CA=.590	D= 2.310E-07	DP= 2.310E-07	XF=-1.152E-01	DERP=-1.210E-01	DERF=-1.210E-01	SEG 2
FOR CA=.580	D= 2.299E-07	DP= 2.299E-07	XF=-3.282E-02	DERP=-1.216E-01	DERF=-1.217E-01	SEG 2
FOR CA=.570	D= 2.288E-07	DP= 2.288E-07	XF= 4.910E-02	DERP=-1.222E-01	DERF=-1.222E-01	SEG 2
FOR CA=.560	D= 2.276E-07	DP= 2.276E-07	XF= 1.306E-01	DERP=-1.227E-01	DERF=-1.228E-01	SEG 2
FOR CA=.550	D= 2.264E-07	DP= 2.264E-07	XF= 2.118E-01	DERP=-1.232E-01	DERF=-1.232E-01	SEG 2
FOR CA=.540	D= 2.251E-07	DP= 2.251E-07	XF= 2.928E-01	DERP=-1.235E-01	DERF=-1.235E-01	SEG 2
FOR CA=.530	D= 2.238E-07	DP= 2.237E-07	XF= 3.735E-01	DERP=-1.238E-01	DERF=-1.238E-01	SEG 2
FOR CA=.520	D= 2.224E-07	DP= 2.223E-07	XF= 4.540E-01	DERP=-1.240E-01	DERF=-1.240E-01	SEG 2
FOR CA=.510	D= 2.209E-07	DP= 2.209E-07	XF= 5.344E-01	DERP=-1.242E-01	DERF=-1.241E-01	SEG 2
FOR CA=.500	D= 2.194E-07	DP= 2.193E-07	XF= 6.147E-01	DERP=-1.242E-01	DERF=-1.242E-01	SEG 2
FOR CA=.490	D= 2.179E-07	DP= 2.178E-07	XF= 6.950E-01	DERP=-1.242E-01	DERF=-1.241E-01	SEG 2
FOR CA=.480	D= 2.162E-07	DP= 2.162E-07	XF= 7.755E-01	DERP=-1.240E-01	DERF=-1.240E-01	SEG 2
FOR CA=.470	D= 2.145E-07	DP= 2.145E-07	XF= 8.560E-01	DERP=-1.238E-01	DERF=-1.238E-01	SEG 2
FOR CA=.460	D= 2.127E-07	DP= 2.128E-07	XF= 9.367E-01	DERP=-1.235E-01	DERF=-1.235E-01	SEG 2
FOR CA=.450	D= 2.109E-07	DP= 2.110E-07	XF= 1.018E 00	DERP=-1.231E-01	DERF=-1.232E-01	SEG 2
FOR CA=.440	D= 2.090E-07	DP= 2.090E-07	XF= 1.099E 00	DERP=-1.227E-01	DERF=-1.228E-01	SEG 2
FOR CA=.430	D= 2.069E-07	DP= 2.071E-07	XF= 1.180E 00	DERP=-1.222E-01	DERF=-1.222E-01	SEG 2
FOR CA=.420	D= 2.048E-07	DP= 2.048E-07	XF= 1.262E 00	DERP=-1.217E-01	DERF=-1.217E-01	SEG 2
FOR CA=.410	D= 2.026E-07	DP= 2.027E-07	XF= 1.345E 00	DERP=-1.209E-01	DERF=-1.210E-01	SEG 2

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        FOR CA=.400      D= 1.472E-07     DP=-0.            XF= 1.427E 00     DERP= 0.            DERF=-1.202E-01     SEG   2
UNSATISFACTORY XF FOR CA= .390
     0.6301813E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .380
     0.6424545E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .370
     0.6548283E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .360
     0.6673130E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .350
     0.6799195E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .340
     0.6926591E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .330
     0.7055443E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .320
     0.7185883E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .310
     0.7318050E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .300
     0.7452099E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .290
     0.7588195E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .280
     0.7726518E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .270
     0.7867265E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .260
     0.8010653E 01       0.               0.                0.                0.                  0.

        FOR CA=.250      D= 3.872E-06     DP=-1.813E-11     XF= 1.439E 00     DERP= 1.446E 04     DERF=-6.773E-02     SEG   3

        FOR CA=.240      D= 2.558E-07     DP= 2.560E-07     XF= 1.589E 00     DERP=-6.622E-02     DERF=-6.626E-02     SEG   3

        FOR CA=.230      D= 2.540E-07     DP= 2.540E-07     XF= 1.741E 00     DERP=-6.471E-02     DERF=-6.471E-02     SEG   3

        FOR CA=.220      D= 2.515E-07     DP= 2.516E-07     XF= 1.898E 00     DERP=-6.308E-02     DERF=-6.310E-02     SEG   3

        FOR CA=.210      D= 2.484E-07     DP= 2.485E-07     XF= 2.059E 00     DERP=-6.140E-02     DERF=-6.142E-02     SEG   3
UNSATISFACTORY XF FOR CA= .200
     0.8393864E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .190
     0.8427216E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .180
     0.8461664E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .170
     0.8497336E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .160
     0.8534381E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .150
     0.8572971E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .140
     0.8613318E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .130
     0.8655672E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .120
     0.8700346E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .110
     0.8747726E 01       0.               0.                0.                0.                  0.
UNSATISFACTORY XF FOR CA= .100
     0.8798305E 01       0.               0.                0.                0.                  0.
```

FOR CA=.090	D= 4.739E-06	DP=-1.968E-11	XF= 2.135E 00	DERP= 4.256E 04	DERF=-1.767E-01	SEG	4
FOR CA=.080	D= 1.046E-06	DP=-2.184E-11	XF= 2.194E 00	DERP= 7.747E 03	DERF=-1.618E-01	SEG	4
FOR CA=.070	D= 3.959E-08	DP= 3.959E-08	XF= 2.259E 00	DERP=-1.461E-01	DERF=-1.461E-01	SEG	4
FOR CA=.060	D= 3.914E-08	DP= 3.914E-08	XF= 2.332E 00	DERP=-1.296E-01	DERF=-1.296E-01	SEG	4
FOR CA=.050	D= 3.865E-08	DP= 3.866E-08	XF= 2.414E 00	DERP=-1.122E-01	DERF=-1.122E-01	SEG	4
FOR CA=.040	D= 3.813E-08	DP= 3.815E-08	XF= 2.512E 00	DERP=-9.368E-02	DERF=-9.374E-02	SEG	4
FOR CA=.030	D= 3.753E-08	DP= 3.752E-08	XF= 2.631E 00	DERP=-7.403E-02	DERF=-7.401E-02	SEG	4
FOR CA=.020	D= 3.681E-08	DP= 3.679E-08	XF= 2.790E 00	DERP=-5.269E-02	DERF=-5.266E-02	SEG	4
FOR CA=.010	D= 3.583E-08	DP= 3.577E-08	XF= 3.041E 00	DERP=-2.903E-02	DERF=-2.898E-02	SEG	4