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**MATANO—A Computer Code for the Analysis
of Interdiffusion and Intrinsic
Diffusion Information
in Binary Systems**

P. T. Carlson

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METALS AND CERAMICS DIVISION

MATANØ -- A COMPUTER CODE FOR THE ANALYSIS OF INTERDIFFUSION
AND INTRINSIC DIFFUSION INFORMATION IN BINARY SYSTEMS

P. T. Carlson

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MATAN~~9~~ - A COMPUTER CODE FOR THE ANALYSIS OF INTERDIFFUSION
AND INTRINSIC DIFFUSION INFORMATION IN BINARY SYSTEMS

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ABSTRACT

MATAN~~9~~ is a FORTRAN IV Computer Program written for use on the IBM 360/75 and 360/91 systems that determines interdiffusion and intrinsic diffusion coefficients from the experimental concentration-penetration profiles of infinite and semi-infinite diffusion couples. The flexibility of the code enables the user to deduce experimental values of diffusion coefficients as well as to calculate expected values for any given system. The fundamental input array consists of the experimentally determined x-ray intensity-penetration data obtained from electron microprobe analysis of the diffused couples, which the program subsequently converts to concentration-penetration profiles by comparison with standards of known composition. An analytical expression describing the concentration of each species as a function of penetration is then determined by fitting low-order polynomial splines to the experimental data by the method of least squares. Subsequent calculations are performed on the regenerated profiles. Interdiffusion coefficients are determined at incremental penetration distances by the method of Boltzmann¹ and Matano² with the use of Simpson's rule for the integration procedures. The analyses of Darken³ and Heumann⁴ are employed to calculate the experimental intrinsic diffusion coefficients at the composition of the Kirkendall⁵ reference plane. In addition, the program uses available thermodynamic and tracer diffusion coefficient information for the system of interest to generate theoretically predicted values of diffusion parameters excluding and including consideration of the vacancy wind effect through the analyses of Darken³ and Manning,⁶ respectively. Experimental vacancy wind parameters as well as atomic mobilities of the two species are determined by the method of Dayananda⁷ and are compared with the theoretical values. The extensive output of the program provides the user with a rapid summary of the experimental and calculated information in tabular as well as graphical formats. Although MATAN~~9~~ has been written with the assumption of constant molar volume across the diffusion zone, a correction can be made for molar volume changes due to composition differences by substitution of lattice spacings for diffusion distances, if this information is available.

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INTRODUCTION

In any investigation of diffusion processes occurring in the presence of chemical concentration gradients two aspects of the analysis of the experimental concentration-penetration profiles are particularly critical to an accurate calculation of the interdiffusion and intrinsic diffusion coefficients. First, a smooth curve must be drawn through the individual data points. This step is usually accomplished graphically with the use of an irregular curve and can be fairly representative of the data if the experimenter is sufficiently judicious in passing the curve through the experimental points. Second, the resultant curve must be integrated and differentiated at various positions to determine the diffusion coefficients and other kinetic parameters as functions of concentration. Generally, this part of the analysis is accomplished graphically with the use of a planimeter and straight edge and represents the major source of error in the calculation of diffusion coefficients. In many cases, two separate curves drawn through a given set of data points will differ very little to the eye, yet will yield slopes which differ by as much as a factor of two. These differences in slope can then lead to inaccuracies of as much as an order of magnitude in the calculated coefficients. In addition, the graphical methods described above become quite tedious and time-consuming when many diffusion profiles are to be treated.

MATAN~~9~~ was developed to eliminate the human inaccuracies incurred with the above methods, as well as to reduce significantly the time required to analyze experimental diffusion data. In order to provide the user with a flexible tool for the study of diffusion phenomena in a given system, the computational scheme of the program is divided into an experimental and a theoretical part. Thus, diffusion coefficients can be deduced from experimental concentration profiles or predicted from a prior knowledge of tracer diffusion and thermodynamic information. Furthermore, the user can also compute both the experimental and theoretical values and compare the results. Although the program has been

designed to accept raw intensity data from an electron microprobe, which it subsequently converts to concentration through an established correction procedure, other forms of raw data are permissible provided that relatively minor changes in the input statements are made.

To calculate experimental interdiffusion and intrinsic diffusion coefficients, the program first fits low-order polynomial splines to the concentration-penetration data of each species by the method of least squares and generates a mathematical expression which defines each profile. The regenerated profile is integrated with the use of Simpson's rule to locate the Boltzmann-Matano plane and then differentiated and integrated at incremental penetration distances to determine interdiffusion coefficients as functions of composition by the method of Boltzmann¹ and Matano.² The location of the Kirkendall⁵ reference plane, determined experimentally, is read in as input data, and the intrinsic diffusion coefficients are determined at the composition of this plane by three independent analyses. Experimental values of the various vacancy wind parameters are also calculated at the composition of the Kirkendall plane. Plotting subroutines supplement the standard printed output with plots of the concentration profiles of each species and the calculated interdiffusion coefficients as functions of composition. In addition, the user has the option of by-passing the curve fit and diffusion coefficient calculation steps and outputting only the experimental data, so in effect MATANØ can also be used as a microprobe correction program. The program has also been equipped with a group of statements to generate printout and plots of x-ray intensity versus concentration for the microprobe calibration standards used, so that the user can readily determine which mathematical expression best describes the calibration parameters of his system.

The use of the theoretical portion of MATANØ requires a knowledge of tracer diffusion and thermodynamic information at the particular temperature of interest. The computational scheme is designed to calculate, to print out and to plot interdiffusion coefficients, intrinsic diffusion coefficients and various vacancy wind parameters as predicted from the theories of Darken³ and Manning.⁶ When the user chooses

appropriate values for the internal flags, the routines will plot the various diffusion parameters as functions of concentration together with the experimental values for comparison purposes. If the theoretical portion is used separately, these plots will be generated automatically in addition to the printed output.

It should be noted that since MATANØ was originally written to aid in an investigation of diffusion in the vanadium-titanium binary system,³ the names of the arrays and program variables reflect this particular system; however, this will not affect the application of the code to other systems. Various constants, however, which apply strictly to the vanadium-titanium system (e.g. atomic weights, etc.) will need to be suitably altered for application to other binary systems. These changes have been noted wherever necessary in the text.

THEORETICAL CONSIDERATIONS

Interdiffusion Coefficients

The approach used to compute the interdiffusion coefficients as functions of concentration is that of Boltzmann¹ and Matano² in which the single parameter $\lambda = x/\sqrt{t}$ is employed in the solution of the differential equation for diffusion in an infinite system. The differential equation is

$$-\frac{\lambda}{2} \frac{dc}{d\lambda} = \frac{d}{d\lambda} \left(D \frac{dc}{d\lambda} \right) \quad (1)$$

with boundary conditions

$$\begin{aligned} c &= c_{\max} \text{ at } \lambda = -\infty \\ c &= c_{\min} \text{ at } \lambda = +\infty \end{aligned} \quad (2)$$

Suitable integration and application of the boundary conditions yields the following solution to Eq. (1), expressed in terms of the coordinate x :

$$\tilde{D}(c') = -\frac{1}{2t} \left[\left(\frac{dx}{dc} \right) \right]_{c'} \int_{c_{\min}}^{c'} x dc \quad (3)$$

where c' is the composition at which the interdiffusion coefficient, $\tilde{D}$, is to be determined. The origin of the coordinate system is termed the Boltzmann-Matano interface, and its location is based on the conservation of mass within the diffusion couple and the assumption of no volume change on mixing. It can be shown that the location of the $x = 0$ plane is defined by the following expression:

$$\int_{c_{\min}}^{c_{\max}} x dc = 0 \quad (4)$$

Strictly speaking Eq. (3) is applicable only when c' is less than the concentration of the Boltzmann-Matano interface. An equivalent expression for use when c' is greater than the concentration of the Boltzmann-Matano plane is

$$\tilde{D}(c') = \frac{1}{2t} \left[\left(\frac{dx}{dc} \right) \right]_{c'} \int_{c'}^{c_{\max}} x dc \quad (5)$$

Intrinsic Diffusion Coefficients

The classic experiments of Smigelskas and Kirkendall⁵ on movement of inert markers inspired Darken³ to point out that a meaningful study of diffusion phenomena must differentiate between intrinsic diffusion (diffusion relative to lattice planes) and mass flows demonstrated by the Kirkendall effect. The reference frame required for the investigation

of intrinsic diffusion can be identified by a moving plane of inert markers as opposed to a fixed frame of reference. The equations that result from Darken's analysis which relate intrinsic diffusion coefficients to interdiffusion coefficients and marker motion are

$$\tilde{D} = N_1 D_2 + N_2 D_1 \quad (6)$$

and

$$v = (D_1 - D_2) \frac{\partial N_1}{\partial x} \quad (7)$$

where D_1 and D_2 are intrinsic diffusivities, v is the velocity of the inert markers, and N_i are the mole fractions of components 1 and 2. From an experimental determination of marker movement and previously calculated interdiffusion coefficients (via the Boltzmann-Matano analysis), the intrinsic diffusion coefficients can be computed at the composition of the marker plane with the aid of Eqs. (6) and (7). Intrinsic diffusion coefficients can be calculated without a previous determination of interdiffusion coefficients if the method of Heumann⁴ is employed. The Heumann analysis is based on the cumulative amounts of components 1 and 2 that have diffused past the plane of inert markers during the diffusion anneal. The analysis yields the following relations

$$A_1 = -2tD_1 \left. \frac{\partial N_1}{\partial x} \right]_{\text{marker plane}} \quad (8)$$

$$A_2 = 2tD_2 \left. \frac{\partial N_1}{\partial x} \right]_{\text{marker plane}} \quad (9)$$

where A_1 and A_2 represent the cumulative intrinsic fluxes of components 1 and 2, respectively, past the plane of markers in time t . The values of A_1 and A_2 are determined from the appropriate areas under the diffusion profiles.

Interdiffusion and Intrinsic Diffusion Including Vacancy Wind Effects

In addition to providing a method for the experimental determination of intrinsic diffusion coefficients from interdiffusion coefficients and marker plane information, Darken³ also related the intrinsic diffusivities, interdiffusion and tracer diffusion coefficients through the following equations:

$$D_i = D_i^* \phi \quad (10)$$

$$\tilde{D} = (D_1^* N_2 + D_2^* N_1) \phi \quad (11)$$

where D_i , D_i^* , and $\tilde{D}$ are the intrinsic diffusion, tracer diffusion and interdiffusion coefficients, respectively. The thermodynamic factor, ϕ , is expressed by the following relation

$$\phi = \left(1 + \frac{\partial \ln \gamma_1}{\partial \ln N_1} \right) \quad (12)$$

where γ_i and N_i are the thermodynamic activity coefficient and atom fraction of component i , respectively. Manning⁶ modified Eq. (10) to include contributions to intrinsic diffusion flow arising from the vacancy wind effect and demonstrated on the basis of a random alloy model that the intrinsic diffusion coefficients D_1 and D_2 can be expressed by

$$D_1 = D_1^* \phi (1 + V_1) \quad (13)$$

$$D_2 = D_2^* \phi (1 - V_2) \quad (14)$$

where

$$V_i = \frac{2N_1(D_1^* - D_2^*)}{N_1 D_1^* + N_2 D_2^*} \quad (15)$$

and is the term which arises from the vacancy wind effect. M_0 is a constant which depends on the crystal structure of the system and for bcc systems has the value of 5.33. From Eqs. (13) through (15) it can be seen that V_i increases the intrinsic diffusion coefficient for the faster diffusing component and decreases the intrinsic diffusion coefficient for the slower diffusing component with respect to the values predicted from Darken's analysis. Insertion of Eq. (10) into Darken's expression [Eq. (6)], which relates interdiffusion and intrinsic diffusion coefficients, yields Manning's expression, which relates interdiffusion coefficients to tracer diffusion coefficients and includes the correction for vacancy wind effects:

$$\tilde{D} = (N_1 D_2^* + N_2 D_1^*) \div S \quad (16)$$

where

$$S = 1 + \frac{2N_1 N_2 (D_1^* - D_2^*)^2}{M_0 (N_1 D_2^* + N_2 D_1^*) (N_1 D_1^* + N_2 D_2^*)} \quad (17)$$

The vacancy wind parameter, S , is always greater than unity; consequently, interdiffusion coefficients predicted by Manning's theory are greater than those predicted by Darken's analysis in which the value of S was taken to be unity.

The experimental determination of the vacancy wind contributions to intrinsic fluxes is due to Dayananda⁷ who used as a starting point the equation for the intrinsic flux

$$J_i = -C_i g_i \frac{\partial \mu_i}{\partial x} + J_{iv} \quad (18)$$

where C_i is the concentration in number per unit volume, g_i is the atomic mobility and $\partial \mu_i / \partial x$ is the chemical potential gradient of component

i. The flux contribution due to the vacancy wind effect, J_{iv} , is related to the vacancy flux, J_v , by the following expression:

$$J_{iv} = - \alpha N_i \theta_i J_v \quad (19)$$

The parameter α is a function of composition and crystal structure. It can be shown on the basis of local thermodynamic equilibrium that for an n-component system

$$\alpha = \frac{\sum_{i=1}^n J_i / \theta_i}{\sum_{i=1}^n J_i} = \frac{\sum_{i=1}^n A_i / \theta_i}{\sum_{i=1}^n A_i} \quad (20)$$

where the A_i refer to the cumulative intrinsic flux of component i past the plane of markers in time t and has the same significance as the A_i in Eqs. (8) and (9). The intrinsic fluxes, J_i , are given by

$$J_i = - \sum_{j=1}^n C_j \theta_j [\delta_{ij} + \tau N_i \theta_i] \partial \mu_j / \partial x \quad (i = 1, 2, \dots, n) \quad (21)$$

where δ_{ij} is the Krönecker δ function and the parameter τ is defined as

$$\tau = \frac{\alpha}{1 - \alpha \sum_{i=1}^n N_i \theta_i} \quad (22)$$

Consideration of the Gibbs-Duhem relationship yields the following expressions for a binary system:

$$J_1 = -C_1 \bar{v}_1 [1 + \bar{v}_1 N_1 (\bar{v}_1 - \bar{v}_2)] \partial \mu_1 / \partial x \quad (23)$$

and

$$J_2 = C_1 \bar{v}_2 [1 - \bar{v}_2 N_2 (\bar{v}_1 - \bar{v}_2)] \partial \mu_1 / \partial x \quad (24)$$

The intrinsic fluxes can also be expressed in terms of Fick's⁹ law as

$$J_i = -D_i \partial C_i / \partial x \quad (25)$$

Comparison of Eqs. (23), (24), and (25) with the assumption of constant molar volume yields

$$D_1 = N_1 \bar{v}_1 \bar{v}_1 \frac{\partial \mu_1}{\partial N_1} \quad (26)$$

$$D_2 = N_1 \bar{v}_2 \bar{v}_2 \frac{\partial \mu_1}{\partial N_1} \quad (27)$$

where

$$\bar{v}_1 = 1 + \bar{v}_1 N_1 (\bar{v}_1 - \bar{v}_2) \quad (28)$$

and

$$\bar{v}_2 = 1 - \bar{v}_2 N_2 (\bar{v}_1 - \bar{v}_2) \quad (29)$$

Consequently with the use of the above expressions and experimental values for intrinsic diffusion coefficients, one can determine experimentally the vacancy wind contributions, $\bar{v}_i$, to the intrinsic fluxes of each component.

Mathematical Treatment of the Experimental Data

If the solution to Eq. (1) for the boundary conditions given in Eq. (2) is examined for the special case of constant interdiffusion coefficient, the following relationship results:

$$\frac{C - C_{\max}}{C_{\min} - C_{\max}} = \frac{1}{2} [1 - \operatorname{erf}(u)] \quad (30)$$

where

$$u = \frac{x}{2\sqrt{Dt}} \quad (31)$$

and

$$\operatorname{erf}(u) = \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2} dt \quad (32)$$

The left-hand side of Eq. (30) is termed the normalized concentration function, which can be further described by the following relation

$$\frac{C - C_{\max}}{C_{\min} - C_{\max}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^z e^{-t^2/2} dt \quad (33)$$

where $z = -u/\sqrt{2}$. In this form, Eq. (33) is termed the cumulative normal distribution with argument z . For the case of constant diffusion coefficient a plot of u or z as a function of x will be linear with the slope related to the diffusion coefficient. Hill¹⁰ has pointed out that in certain systems concentration penetration profiles across the diffusion zone can be described quite well by a series of linear segments on a probability plot in which the ordinate is linear in either z or u and the abscissa is linear in x . The implication here is that under specific conditions a diffusion couple may be treated as a combination of two or more systems in each of which the diffusivity is constant yet different

than that in the other. Baroody¹¹ extended the treatment of Hall and suggested that the segments of the u versus x plot could be fitted with a series of polynomials of second or third degree for cases in which a set of linear segments would clearly not be the best choice.

Concentration-penetration profiles could then be regenerated on cartesian coordinates by solving for the coefficients of the polynomials and inserting the results in Eq. (50). It should be noted that the use of this mathematical manipulation for a given system in which the diffusion coefficient varies with composition in no way implies that the diffusion coefficient is constant. By solving for the coefficients of the several polynomials u and thus describing the argument of the error function in terms of polynomials, the argument is permitted to vary with both distance and composition instead of merely distance as in the special case where the diffusion coefficient is a constant.

The principal advantage of this technique in arriving at a mathematical relationship which describes the concentration-penetration profiles is that plots of u or z versus x are generally much simpler than those of concentration versus x . Fewer polynomials of lower degree are required to fit the entire curve than would be necessary for a similar fit of a concentration-penetration curve, which then leads to smoother curves with fewer maxima and minima. The subsequent integration and differentiation procedures are simplified and the calculated interdiffusion and intrinsic diffusion coefficients are more accurate.

GENERAL DESCRIPTION OF THE PROGRAM

General Comments

MATAN~~9~~ is a computer program, written in FORTRAN IV for use on the IBM 360/91 or 360/75 systems, that determines interdiffusion and intrinsic diffusion coefficients for infinite and semi-infinite diffusion couples. The program is divided conceptually into six areas to provide greater flexibility in its usage: (1) data input; (2) conversion of raw intensity data into units of concentration; (3) fitting low-order polynomial splines to the corrected data by the method of least squares;

(4) determination of experimental interdiffusion and intrinsic diffusion coefficients from the regenerated curves; (5) computation of theoretically predicted values for the diffusion parameters; and (6) tabular and graphical output of results. The program has been designed in such a way that the user has the option of selecting various portions and by-passing others to suit his particular need. For example, if it is desired to compute only the theoretical values of the diffusion coefficients before the accumulation of any experimental data, steps 1 to 4 are by-passed and only steps 5 and 6 are used.

The three subroutines called by the main program are described in detail in the appendices. Briefly, the subroutine FITLOS which fits low-order polynomial splines to the experimental data by the method of least squares was rewritten by Hendricks¹² from the main program of the same name originally written by Smith.¹³ FITLOS has been designed to allow the user to divide the u versus x curve into as many as ten segments and fit each segment with a polynomial of second or third degree with the first and second derivatives continuous at each of the nine possible spline joints. It should be noted, however, that for the sake of simplicity MATAN~~OS~~ has been written to handle a maximum of six segments and five spline joints, since it has been found that this number usually suffices to provide a smooth curve fit over the diffusion zone. The user has the option of choosing either (1) the number of segments into which the u versus x curve is to be divided and FITLOS then chooses the location of the spline joints or (2) the number and location of the spline joints and FITLOS then divides the curve according to their locations. No attempt has been made to reduce the capabilities originally designed in FITLOS since the addition of a few statements in the main program will enable the user to increase the number of segments into which the u versus x curve is to be divided if he so chooses. A description of FITLOS can be found in Appendix B.

The subroutine SIMRUL provides the integration tool for the determination of diffusion coefficients through the use of Simpson's rule. A detailed description of the mechanics of this subroutine can be found in Appendix C.

The subroutine SELPD provides the main program with tracer diffusion coefficients for the two species at any temperature and composition within the range of interest. The description of this subroutine should be examined carefully by the user since the coefficients as they stand apply strictly to the vanadium-titanium system. The structure of the subroutine, however, is general and when data are furnished that correspond to the particular system of interest, the subroutine will provide MATANP with the necessary tracer diffusion coefficient information. A complete discussion and listing of this subroutine can be found in Appendix D.

Finally, to demonstrate the applicability of MATANP to diffusion studies in binary systems, three sample problems are discussed in Appendices F, G and H. Sample Problem 1 describes the case in which only theoretically predicted values of diffusion coefficients are determined. Sample Problem 2 treats the case of experimental interdiffusion and intrinsic diffusion coefficient determination in the vanadium-titanium system. Sample Problem 3 shows the results of using MATANP to print and plot the results of microprobe calibration standards in which the entire computational scheme is bypassed.

The plotting subroutines used in the program are described in extensive detail in the report on the ORNL Graphics Package¹² and are designed to be used with CALCOMP Models 765 and 763 electromechanical pen-and-ink incremental drum plotters. Minor revision in these subroutines may be necessary to facilitate plotting on other computer systems.

Input Variables and Constants

In the following tabulations, symbols are listed in the order of appearance in the program. Symbols used in the subroutines are tabulated in the appropriate appendices.

Symbol	Definition
N^o	Integer constant which determines whether the experimental or theoretical computations of MATAN o are to be used. $N^o = 0$ means the program proceeds through an analysis of the experimental data. $N^o = 1$ means the program computes, prints and plots only the theoretical diffusion values.
$N5$	Number of diffusion couples analyzed.
$N6$	Number of x-ray intensity measurements taken at each composition point.
$N8$	Number of x-ray intensity measurements taken for each of the pure elements.
$N4$	Number of x-ray intensity measurements taken for each of the background elements.
$N7$	Integer constant which determines whether experimental data or microprobe calibration standards are to be treated. $N7 = 0$ means that the calibration standards will be evaluated, printed, and plotted. $N7 > 0$ means the experimental data will be analyzed with $N7$ being the number designation of the particular diffusion couple.
T^o	Diffusion anneal temperature in $^{\circ}\text{C}$.
S	Diffusion anneal time in seconds.
N^o	Nominal weight percent of component 1 in A of couple A/B.
$N10$	Nominal weight percent of component 2 in A of couple A/B.
$N11$	Nominal weight percent of component 1 in B of couple A/B.
$N12$	Nominal weight percent of component 2 in B of couple A/B.
$N13$	Number designation of the particular profile of a given couple when more than one microprobe traverse is made.
VA, VB, VC	X-ray intensity to concentration conversion parameters for component 1 radiation from the binary alloy.
TIA, TIB, TIC	X-ray intensity to concentration conversion parameters for component 2 radiation from the binary alloy.

Symbol	Definition
NC	Total number of concentration profiles for each diffusion couple for the case where more than one microprobe traverse is made.
URV1(I)	Unaveraged raw intensity measurements for component 1 radiation from pure component 1.
URV2(I)	Unaveraged raw intensity measurements for component 2 radiation from pure component 1.
UBV1(I)	Unaveraged raw intensity measurements for component 1 background radiation from pure component 1.
UBV2(I)	Unaveraged raw intensity measurements for component 2 background radiation from pure component 1.
N1	Total number of composition data points in the concentration profile.
N14	Integer constant which determines which portions of MATANP are to be bypassed. N14 = 1 means only the corrected experimental data is outputted with no attempt to solve for diffusion coefficients. N14 = 2 means the experimental data is curve fitted and the diffusion coefficients are determined, the theoretical predictions are computed and tabulated, but all plotting associated with the theoretical predictions is by-passed. N14 = 3 means both the experimental and theoretical results are printed and plotted.
XK	Location of the Kirkendall reference plane in microns.
TRANV	Logical variable which determines whether a log transformation should be made on the distance data elements for purposes of curve fitting. TRANV = .TRUE. means the transformation should be made. TRANV = .FALSE. means the transformation should not be made.
TRANU	Logical variable which indicates whether a log transformation should be made on the u variables for purposes of curve fitting. TRANU = .TRUE. means the transformation should be made. TRANU = .FALSE. means the transformation should not be made.
LREFIT	Logical variable which determines whether the FITLPS subroutine should check whether the curve of u versus x was fit in more segments than was necessary. LREFIT = .TRUE. means the check should be made. LREFIT = .FALSE. means the check should not be made.

Symbol	Definition
NS	Number of segments into which the u versus x curve is to be divided for purposes of spline fitting.
M	Degree of polynomial for spline fitting. M must be 1 or 2.
NF	Number of spline joints. NF $\neq$ 0 indicates that the user has selected the number and locations of the spline joints and these data will be read in as input data. FITPLS then divides the u versus x curve according to the chosen spline joints. NF = 0 means that FITPLS will divide the data as equally as possible among the NS segments and determines the location of the spline joints.
NP	Numerical variable which determines whether force-fitting is used to divide the u versus x data into subsets. NP < 0 means that force-fitting starts at the low end to divide the data into subsets. NP > 0 means that force-fitting starts at the high end to divide the data into subsets. NP = 0 means that the data are divided as equally as possible among the maximum number of subsets. The NP variable is ignored when either NS > 0 or NF > 0.
NP1	Numerical constant which allows for the adjustment of the x = 0 position on the distance coordinate. NP1 > 1 means that DIST(NP1) becomes the x = 0 position instead of DIST(1) with the remaining DIST(2) shifted accordingly.
NP1	Numerical constant which allows for the elimination of long tails on the concentration profiles. NP1 > 0 means that the last NP1 data points are eliminated prior to curve fitting.
DIST(I)	Distance coordinate of composition point (I) in microns. When NP = 0, DIST(I) then represents the number designation of the particular standard.
VM(I)	Location of the spline joints of the spline-fitted, polynomial u versus x curve in units of microns.
URVII(I,J)	Unaveraged raw intensity measurements for component J at DIST(I).
URVI(I,K)	Unaveraged raw intensity measurements for component 1 at DIST(I).

Symbol	Definition
C ₀ NCV(I)	Weight fraction of component 1 in microprobe calibration standard (I).
C ₀ NCTI(I)	Weight fraction of component 2 in microprobe calibration standard (I).

Variables and Constants Used for Computation and Output

Symbol	Definition
RVI ₀	Averaged raw intensity measurements for pure component 1.
RTII ₀	Averaged raw intensity measurements for pure component 2.
BGTIV	Averaged raw intensity measurements for component 1 background radiation from pure component 2.
BGVTI	Averaged raw intensity measurements for component 2 background radiation from pure component 1.
CVI ₀	Background-corrected intensity measurement for pure component 1.
CTII ₀	Background-corrected intensity measurement for pure component 2.
W(I)	Array of weights for experimental data points to be curve fitted. Since FITL ₀ S makes a weighted least squares fit, each point must have a weight. However, if all the weights are zero, FITL ₀ S will make all the weights = 1.
C ₀ NCVR(I)	Concentration ratio function for component 1 used for plotting the results of measurements on microprobe calibration standards. Mathematically, the function is given by $(1 - C_1)/C_1$ with C_1 expressed in weight fraction.
C ₀ NCTR(I)	Concentration ratio function for component 2 used for plotting the results of measurements on microprobe calibration standards. Mathematically, the function is given by $(1 - C_2)/C_2$ with C_2 expressed in weight fraction.
RVI(I)	Averaged raw intensity measurements for component 1 at DIST(I).

Symbols	Definition
RTII(I)	Averaged raw intensity measurements for component 2 at DIST(I).
CVI(I)	Background-corrected intensity measurement for component 1 at DIST(I).
CTII(I)	Background-corrected intensity measurement for component 2 at DIST(I).
C ϕ NCV(I)	Concentration of component 1 expressed in weight fraction at DIST(I).
C ϕ NCTI(I)	Concentration of component 2 expressed in weight fraction at DIST(I).
ATFRV(I)	Concentration of component 1 expressed in atom fraction at DIST(I).
ATFRTI(I)	Concentration of component 2 expressed in atom fraction at DIST(I).
CLAMB(I)	The parameter λ , defined by the expression $\lambda = x/\sqrt{t}$, at DIST(I).
CVR(I)	The normalized concentration function given by the left-hand side of Eq. (30).
UNEW(I)	The value of the variable u at DIST(I) determined by Newton-Raphson iteration techniques from the experimental concentration at each point in the concentration profile of component 1.
RCVR(I)	The regenerated normalized concentration functions using UNEW as the argument of the error function.
X(I)	The regenerated x coordinate of the concentration profiles of components 1 and 2.
A1(I), A2(I) A3(I), A4(I) A5(I), A6(I)	The coefficients of the second and third degree polynomials used to fit the six segments of the u versus x curve of component 1.
RATFRV(I)	Regenerated concentration of component 1 in units of atom fraction from the use of the calculated values UE(I) as arguments of the error function at DIST(I).
UE(I)	The calculated values of the variable u at the experimental DIST(I) using the coefficients of the polynomial spline fitting procedure.

Symbol	Definition
UX(I)	Regenerated values of the variable u at incremental distances $X(I)$ on the concentration profile of component 1. For the present program structure the incremental unit is one micron.
CPRIV(I)	The regenerated concentration of component 1 expressed in atom fraction at incremental penetration distances $X(I)$.
CPRITI(I)	The regenerated concentration of component 2 expressed in atom fraction at incremental penetration distances $X(I)$.
VERM	The location of the Boltzmann-Matano plane in microns as determined from Eq. (4).
VAREA(I)	The area under the concentration profile of component 1 necessary for the determination of the interdiffusion coefficient at point $X(I)$ and defined by the right-hand sides of Eqs. (3) and (5).
VSLØPE(I)	The slope of the concentration profile of component 1 at penetration distance $X(I)$.
D(I)	Interdiffusion coefficient at composition CPRIV(I)
EMK	Motion of the Kirkendall reference plane during the diffusion anneal in microns.
VK	Velocity of Kirkendall reference plane in cm/sec.
CPRIVK CPRITK	Concentrations of components 1 and 2, respectively, at the location of the Kirkendall reference plane.
VSLØPK	Slope of the concentration profile of component 1 at the composition of the Kirkendall reference plane.
DK DVK DTK	Experimental values of interdiffusion coefficient, intrinsic diffusion coefficient for component 1 and intrinsic diffusion coefficient for component 2, respectively, at the composition of the Kirkendall reference plane. Intrinsic coefficients computed from Eqs. (6) and (7).
PHIK	Value of the thermodynamic factor, Φ , at the composition of the Kirkendall reference plane.
DVSK DTSK	Tracer diffusion coefficients of components 1 and 2, respectively, at the composition of the Kirkendall reference plane.

Symbol	Definition
DCDK DCDVK DCDTK DCVK DCMKM	The theoretically predicted values of interdiffusion coefficient, intrinsic diffusion coefficients of components 1 and 2, respectively, the velocity of the Kirkendall reference plane and the motion of the Kirkendall reference plane, respectively, at the composition of the Kirkendall reference plane according to the theory of Darken.
VVMK VTMK	Values of the vacancy wind parameters $1 + V_1$ and $1 - V_2$, respectively, as theoretically predicted from the theory of Manning at the Kirkendall reference plane composition.
SMK	Value of the vacancy wind parameter, S , at the composition of the Kirkendall reference plane.
DCMK DVCMK DTCMK VCMK MKMKM	The theoretically predicted values of the interdiffusion coefficient, the intrinsic diffusion coefficient of components 1 and 2, respectively, the velocity of the Kirkendall reference plane and the motion of the Kirkendall reference plane, respectively, at the composition of the Kirkendall reference plane according to the theory of Manning.
DKKH DTKH	Experimental intrinsic diffusion coefficients of components 1 and 2 at the composition of the Kirkendall reference plane calculated with the analysis of Heumann [Eqs. (8) and (9)] from the standpoint of cumulative flux gain.
DVKHP DTKHP	Experimental intrinsic diffusion coefficients of components 1 and 2 at the composition of the Kirkendall reference plane calculated with the analysis of Heumann [Eqs. (8) and (9)] from the standpoint of cumulative flux loss.
BVK BTIK	Atomic mobilities of components 1 and 2 calculated from tracer diffusion coefficient information.
ALPHA ETA	Experimental vacancy wind parameters σ and τ , respectively, calculated at the composition of the Kirkendall reference plane from the analysis of Dayananada.
PSI1 PSI2	Experimental values of the parameters ψ_1 and ψ_2 , at the composition of the Kirkendall reference plane.

Symbol	Definition
DVDAY DTDAY	Experimental values of the intrinsic diffusion coefficients of components 1 and 2 at the composition of the Kirkendall reference plane by the method of Dayananda.
CVE(I) CTIE(I)	Generated incremental concentrations of components 1 and 2 in atom fraction for the purpose of calculating theoretically predicted diffusion parameters.
PHI(I)	Value of thermodynamic factor, Φ , at composition point CVE(I).
DCD(I) DCDV(I) DCDT(I)	Theoretical values of interdiffusion coefficient and intrinsic diffusion coefficients of components 1 and 2, respectively, at composition point CVE(I) according to Darken's theory.
VVM(I) VTM(I) SM(I)	Theoretical values of the vacancy wind parameters $1 + V_1$, $1 - V_2$, and S at composition point CVE(I) according to Manning's theory.
TCM(I) DVCM(I) DTCM(I)	Theoretical values of interdiffusion coefficient and intrinsic diffusion coefficients of components 1 and 2, respectively, at composition point CVE(I) according to Manning's theory.
DSRAT(I)	Ratio of the tracer diffusion coefficients of components 1 and 2 at composition point CVE(I).
DRATD(I) DRATM(I)	Ratio of the theoretical intrinsic diffusion coefficients at composition point CVE(I) according to the theories of Darken and Manning, respectively.
GAMV(I) GAMT(I)	Activity coefficients for components 1 and 2, respectively.

Sequence of Program Operations

The following list of program operations is tabulated with the assumption that no branching paths are chosen. This section should be read with reference to the program listing and flow diagram given in Appendix A which show the various computational paths available in MATAN~~0~~. In addition, the program listing includes numerous COMMENT statements to aid in the user's interpretation of the sequence of program operations. In the following order, the program will:

1. Average the N_3 raw x-ray intensity measurements for the pure components and the N_4 raw background intensity measurements for the elements used to determine background intensity and correct the x-ray intensity counts for the pure elements for background.
2. Average the N_2 raw intensity measurements for both elements at each of the N_1 points in the diffusion profile and correct the intensity counts for background radiation.
3. Convert the corrected intensity measurements to weight fraction and atom fraction for each element at each of the N_1 points in the diffusion profile, thereby generating the $ATFRV(I)$ versus $DIST(I)$ and $ATFRTI(I)$ versus $DIST(I)$ profiles.
4. Employ the Newton-Raphson iteration technique to determine the variable array $UNEW(I)$ from the array of $ATFRV(I)$ at each point in the concentration profile of component 1, thereby generating the curve of $UNEW(I)$ versus $DIST(I)$.
5. Call $FITLOS$ subroutine to divide the $UNEW(I)$ versus $DIST(I)$ curve into segments and fit the segments with polynomial splines by the method of least squares.
6. Compute the regenerated $UX(I)$ versus $X(I)$ curve in terms of polynomials of second or third degree.
7. Compute the regenerated $CPRIV(I)$ versus $X(I)$ and $CPRITI(I)$ versus $X(I)$ profiles.
8. Call $SIMRUL$ subroutine to perform the integration and locate the position of the Boltzmann-Matano plane.
9. Compute the interdiffusion coefficients $D(I)$ at incremental distances $X(I)$ in the profile of component 1, thereby generating $D(I)$ as a function of $CPRIV(I)$.
10. Calculate the experimental values of marker plane motion and velocity and the following experimental quantities at the

composition of the marker plane: concentrations of components 1 and 2, interdiffusion coefficient, intrinsic diffusion coefficients of components 1 and 2 according to the Darken analysis, thermodynamic factor Δ , and tracer diffusion coefficients of components 1 and 2.

11. Compute the following theoretical quantities at the marker plane composition according to the Darken theory: interdiffusion coefficient, intrinsic diffusion coefficients of components 1 and 2 and marker plane motion and velocity.
12. Compute the following theoretical quantities at the marker plane composition according to the theory of Manning: vacancy wind parameters $1 + V_1$, $1 - V_2$ and S , interdiffusion coefficient, intrinsic diffusion coefficients of components 1 and 2, and marker motion and velocity.
13. Compute the experimental values of the intrinsic diffusion coefficients of components 1 and 2 according to the Heumann analysis from the standpoint of both cumulative flux gain and cumulative flux loss.
14. Compute the following experimental quantities at the marker plane composition by the analysis of Dayananda: atomic mobilities of components 1 and 2, vacancy wind parameters α , τ , $\frac{1}{2}$ and $\frac{1}{2}$, and intrinsic diffusion coefficients of components 1 and 2.
15. Calculate the thermodynamics, theoretical interdiffusion coefficients, theoretical intrinsic diffusion coefficients, theoretical vacancy wind parameters and theoretical intrinsic diffusion coefficient ratios by the theories of Darken and Manning as functions of composition of component 1.

The printing and plotting statements have been omitted from the above sequence of operations in the interest of simplicity; however, the locations of these commands can be seen in the flow diagram and program listing in Appendix A.

Discussion of Program Operation

The following discussion expands the above section, which outlines the program operational sequence, and follows the same general order. As stated earlier, MATAN~~0~~ was originally written for specific application to a study of interdiffusion and intrinsic diffusion in vanadium-titanium solid solutions;⁸ therefore, the names of certain variables, arrays and constants reflect this particular system. Nevertheless, this should cause no difficulty since the mathematical operations as described by the FORTRAN IV language remain valid for other binary systems. The user is cautioned, however, to be aware of various statements within the program in which specific changes are required to apply to his chosen system, such as changes in atomic weights, thermodynamic constants, tracer diffusion parameters, and so forth. Constants of this type are shown in the program for the vanadium-titanium system and their locations have been noted in the following text to facilitate any changes that might be necessary. Furthermore, to simplify the discussion, the internal statement numbers (ISN) have been retained on the left-hand side of the program listing, given in Appendix A. These sequential numbers should not be confused with the FORTRAN IV statement numbers which appear as part of the object code.

Conversion of Electron Microprobe Intensity Data

In recent years the electron microprobe has been universally accepted as a powerful tool for the determination of concentration profiles from solid state diffusion experiments. For this reason MATAN~~0~~ has been designed to accept uncorrected x-ray intensity measurements from the microprobe as the fundamental input data and to convert these intensities to units of concentration for each component. When one makes quantitative measurements with the electron microprobe the intensity of a particular characteristic x-ray line emitted from the unknown sample is compared with the intensity of the same characteristic line emitted from a reference standard of known composition. The reference standards should be pure elements. Furthermore, since background intensity arises from the continuous x-ray spectrum generated

within a given sample, the measured intensities must be corrected for this effect before conversion to concentration units can be made. The background contribution can be determined most conveniently by setting the spectrometer for a given elemental line and measuring the intensity emitted from an element one or two atomic numbers higher or lower. For example, background for the CuK_α line ($\lambda = 1.54\text{\AA}$) may be determined by setting the spectrometer for $1.54\text{\AA}$ and measuring the intensity of x-rays emitted from pure Ni. In analyzing samples of mixed elements (as in binary alloys), it is sufficiently accurate to assume that the composite background is a weight fraction average of the backgrounds measured from each individual element. If, for example, the copper content of a copper-gold alloy is measured, the background for the CuK_α line is given as

$$B(\text{CuK}_\alpha) = C_{\text{Cu}} B_{\text{Ni}}(\text{CuK}_\alpha) + C_{\text{Au}} B_{\text{Au}}(\text{CuK}_\alpha) \quad (34)$$

where $B_{\text{Ni}}(\text{CuK}_\alpha)$ and $B_{\text{Au}}(\text{CuK}_\alpha)$ are the intensities measured from pure nickel and pure gold, respectively, at a spectrometer setting of $1.54\text{\AA}$ and C_{Cu} and C_{Au} are the weight fractions of copper and gold, respectively, in the alloy. The corrected relative intensity is given the symbol K and is computed by

$$K = I/I_0 = (N - B)/(N_0 - B_0) \quad (35)$$

where N and B are the true line and background counts from the unknown sample, and N_0 and B_0 are the true line and background counts from the pure element reference.

In order to determine composition from measured relative intensities, a calibration curve must be determined which expresses the quantity K as a function of composition weight fraction. There are essentially two methods by which this procedure can be accomplished. The first involves the calculation of the calibration parameters with theoretical or semi-empirical formulas^{15, 16} by determining backscatter-ionization, absorption and fluorescence corrections. The second method is by experimental

measurement of the x-ray intensities of a series of calibration standards of known chemical composition to arrive at the correction parameters. It has been shown by Ziebold and Ogilvie^{17,18} from a compilation of experimental calibrations of a wide variety of binary alloys that the calibration curves generally may be expressed in the following form

$$\frac{(1 - K_1)}{K_1} = a_{12} \frac{(1 - C_1)}{C_1} \quad (36)$$

where K_1 and C_1 are, respectively, the corrected relative intensity and weight fraction of component 1, and the conversion parameter, a_{12} , indicates that the correction is for measurement of element 1 in binary alloys of components 1 and 2. A similar expression can be written for the measured intensity and weight fraction of component 2. It is clear, then, from an examination of Eq. (36), that a plot of relative intensity ratios versus known chemical composition ratios from the calibration standards will yield the conversion parameters, a_{12} and a_{21} , for components 1 and 2, respectively. These parameters can then be used to determine concentrations from the measured x-ray intensities of the unknown sample and, thereby, to generate concentration profiles.

As demonstrated in the above paragraph, the quantities K_1 and a_{ij} are necessary in order to determine concentrations corresponding to the measured x-ray intensities from the microprobe. Consequently, the first series of calculations performed by MATANØ involves the determination of the quantities I_0 and B_0 in the denominator of Eq. (35) for each of the pure elements. Beginning with ISN 0028, the N3 raw intensity measurements from the pure elements are averaged, and the N4 raw intensity measurements from the elements chosen by the user to determine background intensity are averaged. For each particular system these background quantities correspond to the B_1 values given on the right-hand side of Eq. (34). It should be noted here that since

vanadium and titanium are neighbors on the periodic table, Eq. (34) reduces to the following simplified expressions for measurements in the vanadium-titanium system:

$$B(VK_g) = C_V B_{Ti}(VK_g) + C_{Ti} B_{Ti}(VK_g) = E_{Ti}(VK_g) \quad (37)$$

and

$$B(TiK_g) = C_V B_V(TiK_g) + C_{Ti} B_V(TiK_g) = E_V(TiK_g). \quad (38)$$

The corrected intensity for each of the pure element reference standards, given by the denominator of Eq. (35), is given in ISN 0046 and ISN 0047.

In similar fashion, the corrected intensity for each of the components at each point in the diffusion profile, given by the numerator of Eq. (35), is determined by averaging the N_2 raw intensity measurements for each of the elements at each of the N_1 composition points in the diffusion profile and correcting the intensities for background radiation. The quantities K_i and $(1 - K_i)/K_i$ are then determined in preparation for the computation of the weight fraction of each element according to Eq. (36). This series of calculations is given in statements ISN 0077 to ISN 0110.

As stated earlier, the microprobe correction parameters, a_{12} and a_{21} , are determined with the use of a series of calibration standards which generally span the composition range of the diffusion experiment. By plotting the relative intensity ratio, $(1 - K_i)/K_i$, against the composition ratio, $(1 - C_i)/C_i$, which is determined by independent wet chemical analysis for each element in each binary alloy standard, the correction parameters may be determined with the use of Eq. (36).

There may be some binary alloy systems for which the linear relationship suggested by Eq. (36) may not apply; consequently, a branching path has been inserted (ISN 0052) to permit the user to compute and portray graphically the relationships K_i versus C_i and $(1 - K_i)/K_i$ versus $(1 - C_i)/C_i$ for each element of the calibration standards to

determine the nature of the calibration curve. Accordingly, when $N7 = 0$, the x-ray intensities and known chemical compositions of the standards are read in as input data (ISN 0071), where DIST(I) now represents an arbitrary standard number designation chosen by the user. The K_i and $(1 - K_i)/K_i$ quantities are subsequently calculated and the appropriate plots are generated beginning with ISN 0547. In the case of the vanadium-titanium system, for example, it was found that the curves of K_V versus C_V and K_{Ti} versus C_{Ti} could be best represented by power functions (See Appendix H); therefore, the calibration equations for this system are

$$C_V = a_V [K_V]^{b_V} \quad (39)$$

and

$$C_{Ti} = a_{Ti} [K_{Ti}]^{b_{Ti}} \quad (40)$$

The constants a_V , b_V , a_{Ti} , and b_{Ti} were determined by least square fitting the experimental points of the calibration standards curves on a desk computer. The user should note here that depending on the type of calibration curve demonstrated by his particular system, the appropriate mathematical expressions will need to replace the statements presently in the listing at ISN 0111 and ISN 0112. Furthermore, the appropriate atomic weights of the components will need to be inserted in ISN 0113 to ISN 0115 which convert the concentrations from units of weight fraction to atomic fraction.

It is suggested that the user initially use MATAN~~0~~ to determine the microprobe calibration parameters as discussed above. Then the parameters may be read in as input data (ISN 0019) in subsequent computer runs without the need to regenerate the calibration curves each time. Naturally, if the calibration parameters are known a priori or if they are determined by some other method, this portion of the

program need not be used. When the calibration parameters have been determined, the program then proceeds to convert the x-ray intensities (corrected for background) to units of concentration for the points in the experimental diffusion profile beginning with ISN 0111, thereby generating the elements of the ATFRV(I) versus DIST(I) and ATFRTI(I) versus DIST(I) profiles.

Generation of the $u(x)$ Versus x Profile

As pointed out in the Theoretical Considerations, it is generally difficult to fit a set of low-order polynomials smoothly to the points of an experimental concentration-penetration curve such that the resultant mathematical expression describing the curve can be differentiated and integrated to determine diffusion parameters. Consequently, the variable $u(x)$ was introduced and is given implicitly in Eq. (30) as the argument of an error function. Since it is difficult to solve Eq. (30) explicitly in terms of $u(x)$ as a function of the normalized concentration function, the Newton-Raphson iteration technique¹⁹ is used to solve for the quantity $u(x)$ at each penetration distance, x , and the corresponding value of the concentration function. In other words, once the elements of the ATFRV(I) and ATFRTI(I) arrays have been determined as described in the above section, MATAN~~6~~ iteratively determines the variable UNEW(I) from the experimental concentrations at each point, DIST(I), in the profile of component 1. The normalized concentration function is identified by the array CVR(I). With the determination of the UNEW(I) versus DIST(I) profile, the program then fits low-order polynomial splines by the least square method to arrive at a mathematical expression that will define the argument of the error function given in Eq. (30) and yield an expression for the concentration-penetration profile.

At this point the comment should be made again that suitable choice of the value of N14 allows the user to compute and display in tabular and graphical formats either: (1) the experimental points only; (2) the

experimental data fit with a least squares curve and all resultant diffusion coefficient and vacancy wind information; or (3) the experimental data fit with a least squares curve, all experimentally computed diffusion parameters, and the theoretically predicted diffusion coefficients. Furthermore, if $N99 = 1$, only the theoretically predicted values at a given temperature are computed. Since the number and location of the segments into which the $UNEW(I)$ versus $DIST(I)$ curve is to be divided are generally not known prior to plotting the experimental points of the diffusion profile, it is suggested that $N14$ initially be set equal to one so that only the experimental data will be displayed. Then one can determine the appropriate number of segments and locations of spline joints which best describe the experimental data. Once this information has been determined, $MATANP$ proceeds to the curve-fitting routine as described in the following section.

Mathematical Expression of Concentration as a Function of Distance

As described above, the first step in arriving at a mathematical expression for the concentration-penetration profiles of the diffusing species is to determine an expression for the argument of the error function given in Eq. (30). Since in general the curve of $u(x)$ versus x cannot be represented by a single polynomial over the entire range of x values, it is usually necessary to divide the experimental data into two or more segments and fit each segment with a low-order polynomial. To this end, the subroutine $FITLOS^{12,13}$ (see Appendix B) is used to fit low-order polynomial splines to the segments of the $UNEW(I)$ versus $DIST(I)$ data by the method of least squares. The use of this subroutine ensures the existence of continuous first and second derivatives at all spline joints of the resultant curve.

$MATANP$ has been designed to allow the user to divide the $UNEW(I)$ versus $DIST(I)$ curve for component 1 into from two to six segments for purposes of spline fitting with polynomials of degree two or three. Furthermore, the user has the option of either (1) selecting the maximum number of segments into which the $u(x)$ curve is to be divided and

allowing FITLPS to determine the locations of the spline joints or (2) selecting the locations of the spline joints and allowing FITLPS to divide the experimental data into segments according to the chosen XM(I) values. If the user chooses the former option, the values of NS $\neq$ 0 and NB = 0 are read in as input data. If the latter option is chosen, the values of NS $\neq$ 0 and NB $\neq$ 0 are used and, in addition, the values of XM(I) must be read in as input data. When FITLPS has completed its task, the elements of the polynomial coefficient array are used to compute the quantity UX(I) at distance increments of 1 micron, where the distance array is denoted as X (I). The $u_i(x)$ polynomials have the following form for each segment i of the UX(I) versus X(I) curve:

$$u_i(x) = \sum_{n=0}^m A_{in} x^n \quad (41)$$

where $m = 2$ or $m = 3$. Following the generation of the UX(I) array for the data of component 1, these elements are inserted in Eq. (30) to arrive at the array of calculated concentrations, CPRIV(I). The result is a mathematical expression for the concentration of component 1 as a function of diffusion penetration which is necessary for the subsequent differentiation and integration procedures leading to the determination of diffusion coefficients. The calculated concentration profile of component 2, CPRITI(I) versus X(I), is obtained by difference and results in a good fit to the experimental data (see Appendix G).

Location of the Boltzmann-Matano Plane

The origin of the coordinate system for the determination of interdiffusion coefficients is termed the Boltzmann-Matano plane and its location is based on the conservation of mass within the diffusion couple with the assumption of negligible volume changes on mixing. The

computer program computes the location of this interface by setting the areas A_1 and A_2 equal in the schematic given in Fig. 1 according to the definition given in Eq. (4) in the following fashion:

$$A_1 = (c_{\max}) (x_{\text{BM}}) - \int_0^{x_{\text{BM}}} c(x) dx \quad (42)$$

and

$$A_2 = \int_{x_{\text{BM}}}^{x_{\max}} c(x) dx - (c_{\min}) (x_{\max} - x_{\text{BM}}) \quad (43)$$

Fig. 1. Diffusion profile schematic demonstrating location of Boltzmann-Matano plane.

Setting Eqs. (42) and (43) equal gives

$$\int_0^{x_{\max}} c(x) dx = x_{\text{BM}} (c_{\max} - c_{\min}) + (c_{\min}) (x_{\max}) \quad (44)$$

which after suitable rearrangement yields

$$x_{\text{BM}} = \left[\int_0^{x_{\max}} c(x) dx - (c_{\min}) (x_{\max}) \right] \frac{1}{c_{\max} - c_{\min}} \quad (45)$$

The subroutine SIMRUL is used to perform this and subsequent integrations in accordance with Simpson's rule.²⁰ The operational characteristics of this subroutine are described in Appendix C. The user should note that MATANO has been designed such that the component chosen to be designated as number 1 and, hence, used for the determination of the diffusion coefficients must have the concentration points of the profile in order of decreasing magnitude with increasing values of x .

Calculation of Experimental Interdiffusion Coefficients

The determination of the experimental interdiffusion coefficients at each composition, c' , of the diffusion profile of component 1 is accomplished with the use of either Eq. (5) or Eq. (3) depending on whether c' is greater than or less than the composition at the Boltzmann-Matano plane, respectively. The computation of the integrals in Eqs. (5) and (3) are thus divided into two cases: Case 1 applies when $c' \geq c_{\text{BM}}$ and $x' \leq x_{\text{BM}}$ and Case 2 is used when $c' < c_{\text{BM}}$ and $x' > x_{\text{BM}}$. For Case 1 the integral is shown schematically as the shaded area in Fig. 2 and is computed as

$$A_1 = (c_{\max}) (x') - \int_0^{x'} c(x) dx + (x_{\text{BM}} - x') [c_{\max} - c'] \quad (46)$$

Fig. 2. Diffusion profile schematic demonstrating calculation of interdiffusion coefficients for Case 1.

The integral which comprises the second term is determined with the subroutine SIMRUL. The integral for Case 2 is shown in Fig. 3 and is computed from the following expression:

$$A_2 = [c' - c_{\min}](x' - x_{\text{BM}}) + \int_{x'}^{x_{\max}} c(x) dx - (x_{\max} - x')(c_{\min}) \quad (47)$$

where the integral in the third term is determined with SIMRUL.

Fig. 3. Diffusion profile schematic demonstrating calculation of interdiffusion coefficients for Case 2.

Furthermore, since the $u(x)$ polynomial, which describes the argument of the error function and, ultimately, the concentration profile in Eq. (30), is different for each segment of the $u(x)$ versus x curve, the derivative appearing in Eqs. (3) and (5) must be computed separately for each of the segments. Although the polynomial coefficients vary, the general expression for dc/dx remains unchanged and the manner of computing the slope is given as follows:

For the general polynomial

$$u(x) = A + Bx + Cx^2 + Dx^3 \quad (4c)$$

used as the argument of the error function in Eq. (3), the derivative of c with respect to x is given as

$$\left. \frac{dc}{dx} \right|_{c'} = \frac{d}{dx} \left[\frac{c - c_{\max}}{c_{\min} - c_{\max}} \right]_{c'} = \frac{1}{\sqrt{\pi}} \frac{d}{du} \frac{du}{dx} \left[1 - \operatorname{erf} u(x) \right] \quad (49)$$

and

$$\left. \frac{dc}{dx} \right|_{c'} = \frac{-(c_{\min} - c_{\max})}{\sqrt{\pi}} \exp(-u^2) \frac{du}{dx} \quad (50)$$

The derivative of the $u(x)$ polynomial is

$$\frac{du(x)}{dx} = B + 2Cx + 3Dx^2 \quad (51)$$

which when inserted into Eq. (50) gives the slope of the concentration profile at composition point c' :

$$\left. \frac{dc}{dx} \right|_{c'} = - \frac{(c_{\min} - c_{\max})}{\sqrt{\pi}} \exp(-u^2) (B + 2Cx + 3Dx^2) \quad (52)$$

MATANØ selects the values of the polynomial coefficients appropriate to the particular segment in which c' happens to lie and computes the concentration gradient with Eq. (52).

Following the computation of the appropriate area and slope corresponding to the particular composition, c' , MATANØ combines these two pieces of information with the diffusion anneal time to determine the interdiffusion coefficient according to Eq. (3) or (5). This process is repeated at increments of the penetration distance to yield tabular and graphical representations of the interdiffusion coefficient as a function of composition.

Calculation of Experimental Intrinsic Diffusion Coefficients and Vacancy Wind Parameters

The experimental intrinsic diffusion coefficients of the two components are computed with the use of three separate methods of analysis to provide a cross check. In the following discussion of the Darken analysis, Heumann analysis and Dayananda analysis, the user is advised to consult the lists of variables, arrays, and constants tabulated earlier.

Darken analysis. Of the three analyses, the Darken method is probably the most straightforward from the standpoint of necessary mathematical manipulations. The location of the Kirkendall reference plane and its movement during the diffusion process have been read in as input data earlier. Having already computed the array of inter-diffusion coefficients, the slopes of the concentration profile and the concentrations at incremental penetration distances, MATANØ simply selects the value corresponding to the marker plane location and inserts these values in Eqs. (6) and (7). These equations are then simultaneously solved for D_1 and D_2 at the marker plane composition.

Heumann analysis. As stated in the Theoretical Considerations, the Heumann analysis is based on the cumulative amounts of components 1 and 2 that have diffused past the plane of inert markers during the diffusion anneal and are represented by A_1 and A_2 in Eqs. (8) and (9), respectively. The areas A_1 and A_2 are shown in Fig. 4 as the shaded and cross hatched regions, respectively, of a typical concentration profile and are computed as follows by MATANØ:

$$A_1 = \text{CUMF1} = \int_{x_M}^{x_{\max}} N_1 dx - (x_{\max} - x_{BM}) N_{1\min} \quad (53)$$

and

$$A_2 = \text{CUMF2} = x_M N_{1 \max} - \int_0^{x_M} N_2 dx + (x_M - x_{BM}) (1 - N_{1 \max}) \quad (54)$$

Fig. 4. Diffusion profile schematic showing calculation of intrinsic diffusion coefficients according to the Heumann Analysis.

The integrals in Eqs. (53) and (54) are determined with the use of the subroutine SIMFOL. Once again, the cumulative amounts of the two components, denoted as CUMF1 and CUMF2, refer to the net amount of component 1 gained by the right-hand side and the net amount of component 2 gained by the left-hand side of the diffusion couple. Since there is a mass balance within the system, the net amount of component 1 gained by the right-hand side of the couple must equal the net amount

of component 1 lost by the left-hand side of the couple. Similar reasoning exists for the net amount of component 2 transferred. In this sense, the cumulative amounts of components 1 and 2 lost from the appropriate sides of the couple during diffusion are CUMF1P and CUMF2P and are given as

$$\text{CUMF1P} = (x_M)(N_{1_{\max}}) - \int_0^{x_M} N_1 dx + (x_{BM} - x_M)N_{1_{\max}} \quad (55)$$

and

$$\text{CUMF2P} = \int_{x_M}^{x_{\max}} N_1 dx - (x_{\max} - x_M)N_{1_{\min}} + (x_M - x_{BM})(1 - N_{1_{\min}}) \quad (56)$$

The values thus computed are inserted into Eqs. (8) and (9) to determine the intrinsic diffusivities, D_1 and D_2 .

Dayananda analysis. For the Dayananda analysis and the theoretical calculations to be discussed in the next section it is necessary that the tracer diffusion coefficients of the two components be known as functions of composition and temperature in the alloys of interest. To this end, the subroutine SELFD has been designed to supply the main program with tracer coefficients; however, SELFD as it is written applies strictly to the vanadium-titanium system based on the work of Murdock and McHargue.²¹ The user will need to alter the subroutine for application to his particular system. The subroutine SELFD is discussed in detail in Appendix D. For the calculation of intrinsic diffusion coefficients and vacancy wind parameters with the Dayananda analysis, MATAN~~0~~ first determines the atomic mobilities, μ_i , of the two components according to the following expression:

$$\mu_i = \frac{D_i^*}{kT} \quad (57)$$

where D_i^* and k are the tracer diffusivity of component i and Boltzmann's constant, respectively. The vacancy wind parameter, γ , is then determined with the aid of Eq. (20) which then allows the calculation of the parameter $\bar{\gamma}$ with the use of Eq. (22). The quantities $\bar{t}_1$ and $\bar{t}_2$ are determined from Eqs. (23) and (24), respectively. The intrinsic diffusivities, D_1 and D_2 , are obtained by inserting the above quantities in Eqs. (26) and (27) together with the proper value of the thermodynamic quantity $\partial\mu_1/\partial N_1$. It should be noted that the statements for DVDAY and DTDAY are presently written in light of the thermodynamics of the vanadium-titanium system, and the user will have to insert the appropriate values or expressions corresponding to his system.

Calculation of Theoretically Predicted Values of Diffusion Coefficients

The inclusion in MATANØ of a series of statements which determines the theoretically predicted diffusion parameters serves two useful purposes. First, the calculations permit comparisons to be made between the experimentally determined diffusion information and the values predicted on the basis of different theories. Second, MATANØ is designed so that the user can employ this portion of the program separately from the experimental portion (by setting $N_{20} = 1$), generate expected values of the diffusion coefficients and, thereby, be able to plan his experimental program more judiciously. The theoretical calculations begin with FORTRAN statement 17. As discussed in the previous section, the user must alter the definitions of the thermodynamic quantities $\text{PHI}(I)$, $\text{GAMV}(I)$ and $\text{GAMT}(I)$ as well as the expressions for $\text{DVS}(I)$ and $\text{DTS}(I)$ in the SELFD subroutine to correspond to his particular system. The various FORTRAN statements corresponding to Eqs. (1) through (17) can be readily interpreted by reference to the list of variables and arrays presented earlier. In addition, the theoretical predictions at the composition of the plane of inert markers are automatically computed together with the experimental quantities.

Input Data Format

The following section is presented to aid the user in the preparation of the FORTRAN card deck when using MATAN~~50~~. On each card where more than one variable, array or constant appears, the order of tabulation below is the same as the order of appearance on the card when read from left to right.

<u>Card</u>	<u>Variable, Array or Constant Name</u>	<u>Columns</u>	<u>Field Specification</u>
1	N99	5	I5
2	N5	1-5	I5
3	N2	1-5	3I5
	N3	6-10	
	N4	11-15	
4	N7	5	I5, F9.3, E11.5, 5I5
	T8	6-14	
	S	15-25	
	N9	26-30	
	N10	31-35	
	N11	36-40	
	N12	41-45	
	N13	46-50	
5	VA	1-10	6F10.7
	VB	11-20	
	VC	21-30	
	T1A	31-40	
	T1B	41-50	
	T1C	51-60	
6	N6	1-5	I5
7	URVI 0	1-60	6F10.0
8	URTI 0	1-60	6F10.0
9	UBTIV	1-60	6F10.0
10	UBVTI	1-60	6F10.0
11	N1	1-5	I5
12	N14	1-5	I5

<u>Card</u>	<u>Variable, Array Constant Name</u>	<u>Columns</u>	<u>Field Specification</u>
13	XK	1-10	F10.4
14	TRANX	1-10	3L10
	TRANY	11-20	
	LREFIT	21-30	
15	NS	1-5	6I5
	M	6-10	
	NB	11-15	
	NF	16-20	
	N20	21-25	
	N21	26-30	

Beginning with card 16, the next N1 cards read in the raw intensity-penetration data:

16	DIST	1-10	5F10.0
	URTII	11-30	
	URVI	31-50	

It is emphasized that the 5F10.0 field specification for the quantities URVI ϕ , URTII ϕ , UBTIV and UBTVI in no way limits the number of independent measurements to six for each of the arrays. Insertion of the appropriate number of continuation cards after each of the cards 7 through 10 enables the user to select any value for either N ϕ or N4. In similar fashion, the value for N2 may be increased with suitable continuation cards following each of the N1 cards beginning with card 16. Also, in accordance with the earlier discussion of the program operation and, specifically, the purpose of the N14 parameter, when N14 = 1, cards 13 through 15 should not be included since these pertain to the curve fitting and subsequent diffusion coefficient determination steps.

Discussion of Output

An adequate understanding of the tabular and graphical output of MATAN ϕ can be obtained from an examination of the three sample problems given in Appendices F, G, and H. Because the program was originally written for the study of diffusion in the vanadium-titanium

binary system, the table headings and coordinate labels for the plots reflect this system. This should not cause the user serious difficulty, however, since these various labels can be altered to suit his particular system merely by inserting the proper Hollerith field specifications in the appropriate printing and plotting statements.

APPLICATIONS AND LIMITATIONS OF MATANØ

As its name implies, the primary function of MATANØ is to determine interdiffusion and intrinsic diffusion coefficients from the experimental concentration profiles of solid state diffusion experiments. Many times, however, the experimentalist may desire to estimate the various diffusion parameters prior to the execution of any experiments in order to better plan his research program. In addition, he might wish to compare his experimental results with theoretical predictions to determine the validity of the measured values or the theoretical approach. To accommodate these possibilities, MATANØ has been designed to handle experimental data, theoretical information or a combination of the two aspects. Furthermore, the entire diffusion coefficient determination process can be bypassed, and MATANØ can be used to determine the various correction parameters necessary for conversion of microprobe x-ray intensity data to concentrations. It should be remarked here that the inclusion of the intensity-to-penetration scheme at the beginning of the program in no way limits the user to data gathering via the electron microprobe. The user may input concentration versus distance data directly by eliminating the microprobe correction portion and suitably altering the READ statements which are currently written in terms of x-ray intensities.

In the construction of any computer program certain limitations are necessary to prevent excessive length, memory requirements and running times. One such limitation is that the maximum number of experimental data points is 200. This upper limit can be increased by alteration of the DIMENSION statements at the beginning of the program; however, in normal diffusion couple analyses the total number of data points is usually well below this value.

To facilitate the use of the integration subroutine `SIMUL` and the Boltzmann-Matano analysis, the concentration profile of the component chosen for the interdiffusion coefficient determination must have its data points decreasing in value with increasing values of x . Furthermore, the subroutine `FITLPS` is capable of dividing the u versus x curve into as many as ten segments; however, `MATANØ` limits the maximum number of segments to six in the interest of efficiency. This limitation should cause little difficulty, since most u versus x curves can be adequately described by two or three segments. If the user chooses to increase the maximum number of segments above six, `FITLPS` will fit the u versus x curve accordingly, but `MATANØ` will not accept the results of these types of fit for subsequent treatment. In short, the program will abort.

As explained in Appendix C, the computational limitations of `SIMUL` make it necessary to limit the determination of interdiffusion coefficients to distance increments of $2 \mu\text{m}$. That is, interdiffusion values will be computed only at even numerical values of $X(I)$. Furthermore, calls to the plotting subroutines of `ØRGRAPH` will result in only every fourth value of $D(I)$ being plotted. This has been implemented in the interest of memory space and clarity of the plots. Even with these two restrictions; however, the tabular and graphical results of `MATANØ` give good representations of interdiffusion coefficients as functions of composition, as demonstrated by Sample Problem 2 (Appendix G).

APPENDIX A

Flow Chart for MATANØ

CRN-DSG 75-2334

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ORNL-DWG 75-2337

```

15N 0034      102 CONTINUE
15N 0035      RV10 = SUMV0/Y
15N 0036      RT10 = SUMT10/Y
15N 0037      SUM1 = 0.0
15N 0038      SUM2 = 0.0
15N 0039      Z = N4
15N 0040      DO 103 I = 1,N4
15N 0041      SUM1 = SUM1 + URTV(I)
15N 0042      SUM2 = SUM2 + UHVT(I)
15N 0043      103 CONTINUE
15N 0044      BGTIV = SUM1/Z
15N 0045      HGVTI = SUM2/Z
15N 0046      CV10 = RV10 - BGTIV
15N 0047      CT10 = RT10 - HGVTI
15N 0048      2000 READ 7,N1
15N 0049      7 FORMAT (15)
15N 0050      READ 8,N14
15N 0051      8 FORMAT (15)
15N 0052      IF (N7 .EQ. 0) GO TO 1051
15N 0053      IF (N14 .EQ. 1) GO TO 1050
15N 0054      READ 14,XX
15N 0055      14 FORMAT (F10.4)
15N 0056      READ 11,TRANX,TRANV,LPFFIT
15N 0057      11 FORMAT (3L10)
15N 0058      READ 16,NS,M,NB,NF,N20,N21
15N 0059      16 FORMAT (6I5)
15N 0060      IF (NB.NE.0) READ 4,(XM(I), I=1,NB)
15N 0061      DO 15 I=1,N1
15N 0062      W(I) = 0.0
15N 0063      15 CONTINUE
15N 0064      1050 READ 9,(DIST(I), (URT(I),J), J=1,N2),
15N 0065      1 (URV(I,K), K=1,N2), I=1,N1)
15N 0066      9 FORMAT (5F10.0)
15N 0067      IF (N7 .GT. 0) GO TO 1052
15N 0068      1051 READ 9,(DIST(I), (URT(I),J), J=1,N2),
15N 0069      1 (URV(I,K), K=1,N2), CONCV(I), CONCT(I), I=1,N1)
15N 0070      9 FORMAT (5F10.0, 2F10.7)
15N 0071      DO 1053 I=1,N1
15N 0072      CONCV(I) = (1.0 - CONCV(I))/CONCV(I)
15N 0073      CONCT(I) = (1.0 - CONCT(I))/CONCT(I)
15N 0074      1053 CONTINUE
15N 0075
15N 0076
C
C
C THE FOLLOWING STATEMENTS(UP TO STATEMENT 9700) AVERAGE THE N2 RAD
C INTENSITY MEASUREMENTS FOR BOTH ELEMENTS AT EACH OF THE N1 POINTS
C IN THE DIFFUSION PROFILE AND CORRECT THE COUNTS FOR BACKGROUND
C INTENSITY.
C
C
15N 0077      1052 X20 = N2
15N 0078      DO 101 I = 1,N1
15N 0079      SUMV = 0.0
15N 0080      SUMT = 0.0
15N 0081      DO 100 J = 1,N2
15N 0082      SUMV = SUMV + URV(I,J)
15N 0083      SUMT = SUMT + URT(I,J)
15N 0084      100 CONTINUE
15N 0085      RV(I) = SUMV/X20

```

```

15N 0086      P711(1) = S0MT/AN20
15N 0087      CONTINUE
15N 0088      IF (N7.GT. 0) GO TO 97
15N 0090      DO 104 I = 1,N1
15N 0091      C711(I) = P71(I) - AGTIV
15N 0092      CT11(I) = RT11(I) - AGVTI
15N 0093      SV11(I) = C711(I)/CV10
15N 0094      ST11(I) = CT11(I)/CT10
15N 0095      TV11(I) = (1.0 - SV11(I))/SV11(I)
15N 0096      TT11(I) = (1.0 - ST11(I))/ST11(I)
15N 0097      ASV11(I) = ABS(SV11(I))
15N 0098      AST11(I) = ABS(ST11(I))
15N 0099      90 CONTINUE
15N 0100      IF (N7.EQ. 0) GO TO 2049
15N 0102      97 DO 104 I = 1,N1
15N 0103      C711(I) = P71(I) - AGTIV
15N 0104      CT11(I) = RT11(I) - AGVTI
15N 0105      SV11(I) = C711(I)/CV10
15N 0106      ST11(I) = CT11(I)/CT10
15N 0107      TV11(I) = (1.0 - SV11(I))/SV11(I)
15N 0108      TT11(I) = (1.0 - ST11(I))/ST11(I)
15N 0109      ASV11(I) = ABS(SV11(I))
15N 0110      AST11(I) = ABS(ST11(I))

C
C
C      THE FOLLOWING STATEMENTS (UP TO STATEMENT 104) EMPLOY THE CORREC-
C      TION PROCEDURES OF ZIFOLD TO CONVERT THE CORRECTED INTENSITIES
C      OF THE TWO COMPONENTS TO CONCENTRATION EXPRESSED IN WEIGHT
C      FRACTION AT EACH POINT IN THE CONCENTRATION PROFILE. THE CONCEN-
C      TRATIONS ARE THEN CONVERTED TO UNITS OF ATOM FRACTION.
C
15N 0111      CONCV(I) = VAPASV11(PVMI)
15N 0112      CONCT(I) = VAPAST11(PVMI)
15N 0113      DUM1(I) = (CONCV(I)/50.942) + (CONCT(I)/67.90)
15N 0114      ATRV1(I) = (CONCV(I)/50.942)/(DUM1(I))
15N 0115      ATRT1(I) = (CONCT(I)/67.90)/(DUM1(I))
15N 0116      DUM4 = SORT(S)
15N 0117      CLAMP(I) = (DIST(I))/DUM4
15N 0118      104 CONTINUE
15N 0119      CVMAX = 1.0
15N 0120      CVMIN = 0.0
15N 0121      XMAX = DIST(N1)
15N 0122      DO 110 I = 1,N1
15N 0123      CV11(I) = (ATRV1(I) - CVMIN)/(CVMAX - CVMIN)
15N 0124      IF (CV11(I).GT. 1.0) CV11(I) = 1.0
15N 0126      110 CONTINUE

C
C
C      THE FOLLOWING STATEMENTS (UP TO STATEMENT 250) ITERATIVELY DETER-
C      MINE THE VARIABLE D FROM THE EXPERIMENTAL CONCENTRATIONS AT EACH
C      POINT IN THE VANADIUM PROFILE BY THE NEWTON-RAPHSON METHOD.
C
15N 0127      D(1) = 1
15N 0128      DO 127 I = 1,N1
15N 0129      IF (I.EQ. 1) D(I) = D(I)-1
15N 0131      NS(I) = 1

```



```

15N 0132      106  FU = 1.0 - ERFC(U(1)) - 2.0*CVR(1)
15N 0133      3FU = (-2.0/1.772454)*EXP(-U(1)**2)
15N 0134      ZZ = FU/DFU
15N 0135      IF (ABS(ZZ) .GT. 1.0) ZZ = SIGN(1.0,ZZ)
15N 0137      UNFW(1) = U(1) - ZZ
15N 0138      IF (ABS(U(1)-UNFW(1)) .LT. 1.0E-6 .OR. NN(1) .GT. 50) GO TO 105
15N 0140      IF (ABS(UNFW(1)) .GT. 10.0) GO TO 105
15N 0142      U(1) = UNFW(1)
15N 0143      NN(1) = NN(1) + 1
15N 0144      GO TO 106
15N 0145      105  RCVR(1) = (10.5)*(1.0 - ERFC(UNFW(1)))
15N 0146      107  CONTINUE
15N 0147      470  CVMAX = ATRV(1)
15N 0148      CVMIN = ATRV(N1)
15N 0149      471  PRINT 480,N7,T8,S,N9,N10,N11,N12,N13
15N 0150      480  FORMAT (1H1,5X,13HDIFFUSION RUN,2X,15,///6X,
1          1      19HMINOMIAL TEMPERATURE,2X,F9.3,///6X,
2          2      21HDIFFUSION TIME IN SEC,2X,1E14.5,///6X,
3          3      25HMINOMIAL WT PERCENT V IN A,2X,15,///6X,
4          4      26HMINOMIAL WT PERCENT TI IN A,2X,15,///6X,
5          5      25HMINOMIAL WT PERCENT V IN B,2X,15,///6X,
6          6      24HMINOMIAL WT PERCENT TI IN B,2X,15,///6X,
7          7      14HPROFILE NUMBER,15,///)
15N 0151      PRINT 500
15N 0152      500  FORMAT (6X,8HDISTANCE,4X,11HINT RATIO V,3X,
1          1      12HINT RATIO TI,3X,9HWT FRAC V,5X,10HWT FRAC TI,
2          2      4X,9HAT FRAC V,5X,10HAT FRAC TI,///)
15N 0153      PRINT 501,(DIST(1),SV(1),ST(1),CONCV(1),CONCTI(1),
1          1      ATRV(1), ATRTI(1), I = 1,N1)
15N 0154      501  FORMAT (7F14.5)
15N 0155      PRINT 502
15N 0156      502  FORMAT (1H1,5X,8HDISTANCE,5X,4HK RATIO V,3X,10HK RATIO TI,
1          1      9X,6HCLAMROA,9X,9HAT FRAC V,5X,10HAT FRAC TI,///)
15N 0157      PRINT 503,(DIST(1),TV(1),TT(1),CLAMB(1),
1          1      ATRV(1), ATRTI(1), I = 1,N1)
15N 0158      503  FORMAT (3F14.5, F18.5, 2F14.5)
15N 0159      PRINT 508,CVMAX,CVMIN,XMAX
15N 0160      508  FORMAT (1H1,5X,30HMAXIMUM ATOM FRACTION VANADIUM,2X,F14.5,///6X,
1          1      30HMINIMUM ATOM FRACTION VANADIUM,2X,F14.5,///6X,
2          2      38HMAXIMUM VANADIUM PENETRATION (MICRONS),2X,F14.5,///9X,
3          3      8HDISTANCE,14X,4HUNFW, 9X,17HNORMALIZED CONC V, 4X,
4          4      17HNORMALIZED CONC V,743X,12HEXPERIMENTAL, 6X,
5          5      18HCOMPUTED FROM UNFW,///)
15N 0161      PRINT 509,(DIST(1),UNFW(1),CVR(1),RCVR(1), I=1,N1)
15N 0162      509  FORMAT (F14.6,3F20.6)
15N 0163      IF (N14 .EQ. 1) GO TO 520

```

C
C
C
C
C
C
C
C
C

THE FOLLOWING STATEMENTS (UP TO STATEMENT 211) DETERMINE THE
VARIABLE U AS A FUNCTION OF THE PENETRATION DISTANCE FOR THE
SEGMENTS OF THE U VS X CURVE BY FITTING LOW ORDER POLYNOMIAL
SPLINES BY THE METHOD OF LEAST SQUARES. THE CONCENTRATIONS
OF VANADIUM AND TITANIUM ARE THEN COMPUTED AT INCREMENTAL
PENETRATION DISTANCES.

15N 0165
15N 0166

CVMAX=1.0
CVMIN=0.0

```

154 0167      N=1
154 0168      DISTZ = DIST(N20)
154 0169      N1M = N1-N21
154 0170      DO 30 I=N20,N1M
154 0171      DISTIN) = DIST(I)-DISTZ
154 0172      UNEMIN) = UNEM(I)
154 0173      ATRPV(N) = ATRPV(I)
154 0174      ATRPT(N) = ATRPT(I)
154 0175      N=N+1
154 0176      30 CONTINUE
154 0177      N1 = N1-(N20-N21)+1
154 0178      XMAX = DIST(N1)
154 0179      X(1) = 0.0
154 0180      DUM10 = 0.0
154 0181      NXLM = XMAX+1
154 0182      DO 250 I=2,NXLM
154 0183      X(I) = DUM10 + 1.0
154 0184      DUM10 = X(I)
154 0185      250 CONTINUE
154 0186      IENTRY=0
154 0187      CALL FITLOS(DIST,UNFW,W,N1,NS,M,NR,NF,TRANX,TRANX,LRFFIT,0.01,
1      IENTRY,UF,XM,A,200)
1      IF (M.EQ.3) GO TO 33
1      DO 32 I=1,NS
1      A(I,4) = 0.0
1      32 CONTINUE
1      33 DO 31 I=1,4
1      A(1,I) = A(1,I)
1      A(2,I) = A(2,I)
1      A(3,I) = A(3,I)
1      A(4,I) = A(4,I)
1      A(5,I) = A(5,I)
1      A(6,I) = A(6,I)
1      31 CONTINUE
1      X1 = XM(1)
1      X2 = XM(2)
1      X3 = XM(3)
1      X4 = XM(4)
1      X5 = XM(5)
1      DO 210 I=1,N1
1      RATPRV(I) = CVMIN + ((CVMAX-CVMIN)/2.0)*1.0 -DPRF(UE(I))
1      CDFV(I) = (RATPRV(I) - ATRPV(I))
1      PCDFV(I) = ((RATPRV(I) - ATRPV(I))/ATRPV(I))*100
1      210 CONTINUE
1      DO 211 I=1,NXLM
1      IF (NS .EQ. 2 .AND. X(I) .GT. X1) GO TO 212
1      IF (NS .GT. 3) GO TO 214
1      IF (X(I) .GT. X2) GO TO 213
1      214 IF (X(I) .GT. X1 .AND. X(I) .LT. X2) GO TO 212
1      IF (X(I) .GT. X2 .AND. X(I) .LE. X3) GO TO 213
1      IF (X(I) .GT. X3 .AND. NS .EQ. 4) GO TO 215
1      IF (X(I) .GT. X3 .AND. X(I) .LT. X4) GO TO 215
1      IF (X(I) .GT. X4 .AND. NS .EQ. 5) GO TO 217
1      IF (X(I) .GT. X4 .AND. X(I) .LT. X5) GO TO 217
1      IF (X(I) .GT. X5) GO TO 218
1      UX(I) = A(1) + A(2)*X(I) + A(3)*(X(I)**2) + A(4)*(X(I)**3)
1      GO TO 214
1      217 UX(I) = A(1) + A(2)*X(I) + A(3)*(X(I)**2) + A(4)*(X(I)**3)

```


ISN 0387

DCXKM = (DCVK*2*5)*1E4

C
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C
C
C
C
C
C

THE FOLLOWING STATEMENTS COMPUTE THE FOLLOWING THEORETICAL QUANTITIES AT THE MARKER PLANE COMPOSITION ACCORDING TO THE HANNING THEORY- VACANCY WIND PARAMETERS, $1-V1$ AND $1-V2$ FOR V AND T, RESPECTIVELY, VACANCY WIND PARAMETER, S, INTERDIFFUSION COEFFICIENT, INTRINSIC DIFFUSION COEFFICIENTS FOR V AND T, AND MARKER PLANE MOTION AND VELOCITY.

ISN 0388

VVMK = (2.0*CPRIVK*(DVSK-DTSK))/(5.33*(CPRIVK*DVSK + CPRTK*DTSK)) + 1.0

ISN 0389

VTKM = (2.0*CPRTK*(DVSK-DTSK))/(5.33*(CPRIVK*DVSK + CPRTK*DTSK))*(-1.0) + 1.0

ISN 0390

SMK = 1.0 + (2.0*CPRIVK*CPRTK*((DVSK-DTSK)**2))/
1 (5.33*(CPRIVK*DVSK + CPRTK*DTSK) + CPRTK*DVSK +
2 CPRTK*DTSK)

ISN 0391

DCMK = (CPRIVK*DTSK + CPRTK*DVSK)*PHIK*SMK

ISN 0392

DVCHK = DVSK*PHIK*VVMK

ISN 0393

DTCMK = DTSK*PHIK*VTKM

ISN 0394

VCHK = (DVSK - DTSK)*PHIK*1.3/5*VSLIPK

ISN 0395

XXMCM = (VCHK*2*5)*1E4

C
C
C
C
C
C
C

THE FOLLOWING STATEMENTS COMPUTE THE EXPERIMENTAL INTRINSIC DIFFUSION COEFFICIENTS OF V AND T BASED ON THE HUMANN ANALYSIS.

ISN 0396

MIN = XK*1.0

ISN 0397

MAX = XMAX*1.0

ISN 0398

NT = MAX-MIN

ISN 0399

CALL SIMRUL(X,CPRIV,MIN,MAX,NT,1,AREA)

ISN 0400

CUMF1 = AREA - (XMAX-VXBH)*CVMIN

ISN 0401

CUMF2P = AREA - (XMAX-XK)*CVMIN + (XK-VXBH)*(1.0-CVMIN)

ISN 0402

DVKH = (-0.5/(5*VSLDPK))*CUMF1*1E-4

ISN 0403

DTKHP = (-0.5/(5*VSLDPK))*CUMF2P*1E-4

ISN 0404

MIN = 1.0

ISN 0405

MAX = XK*1.0

ISN 0406

NT = MAX-MIN

ISN 0407

CALL SIMRUL(X,CPRTV,MIN,MAX,NT,1,AREA)

ISN 0408

CUMF1P = (XK*CVMAX) - AREA + (VXBH-XK)*CVMAX

ISN 0409

CUMF2 = (XK*CVMAX) - AREA + (XK-VXBH)*(1.0-CVMAX)

ISN 0410

DVKHP = (-0.5/(5*VSLDPK))*CUMF1P*1E-4

ISN 0411

DTKH = (-0.5/(5*VSLDPK))*CUMF2*1E-4

C
C
C
C
C
C
C

THE FOLLOWING STATEMENTS COMPUTE THE EXPERIMENTAL VACANCY WIND PARAMETERS AND INTRINSIC DIFFUSION COEFFICIENTS ACCORDING TO THE THEORY OF DAYANANDA AT THE MARKER PLANE COMPOSITION.

ISN 0412

BVK = DVSK/((TB*273)*(1.38E-16))

ISN 0413

BTIK = DTSK/((TB*273)*(1.38E-16))

ISN 0414

ALPHA = (CUMF1/BVK - CUMF2/BTIK)/(CUMF1-CUMF2)

ISN 0415

ETA = ALPHA/(1.0 - ALPHA*(CPRIVK*BVK + CPRTK*BTIK))

ISN 0416

PS11 = 1.0 - ETA*CPRIVK*(BVK-BTIK)

ISN 0417

PS12 = 1.0 - ETA*CPRTK*(BVK-BTIK)

CCCCCCCC


```

15N 0483  DVCMI(1) = DVS(1)*CM(1)*VVM(1)
15N 0484  DTCMI(1) = DTS(1)*DM(1)*VCM(1)
15N 0485  IF(DVCM(1) .LE. 0.0) DVCMI(1) = 1.0
15N 0486  IF(DTCMI(1) .LE. 0.0) DTCMI(1) = 1.0
15N 0487  DSRAT(1) = DVS(1)/DTS(1)
15N 0488  GAMV(1) = EXP((CTIF(1)*D2)/(1.021)/(1.98697-30180+27311)
15N 0489  GAMT(1) = EXP((CTIF(1)*D2)/(1.021)/(1.98697-30180+27311)
15N 0490  DRATD(1) = EXP((CVE(1)*D2)/(1.021)/(1.98697-30180+27311)
15N 0491  DRATM(1) = DCDV(1)/DCDT(1)
15N 0492  DRAT(1) = DVCMI(1)*DTCMI(1)
15N 0493  IF(DRATD(1) .GT. 10.0) DRATD(1) = 0.0
15N 0494  IF(DRATM(1) .GT. 10.0) DRATM(1) = 0.0
15N 0495  616 CONTINUE
15N 0496  619 PRINT 620
15N 0497  620 FORMAT(1H,17X,10HTRACER COEFFICIENTS,5X,
15N 0500
15N 0501
15N 0502
15N 0503
15N 0504
15N 0505
15N 0506
15N 0507
15N 0508
15N 0509
15N 0510
15N 0511
15N 0512
15N 0513
15N 0514
15N 0515
15N 0516
15N 0517
15N 0518
15N 0519
15N 0520
15N 0521
15N 0522
15N 0523
15N 0524
15N 0525
15N 0526
15N 0527
15N 0528
15N 0529
15N 0530
15N 0531
15N 0532
15N 0533
15N 0534
15N 0535
15N 0536

15N 0501  611 FORMAT(14,5,2E13,5,5F10,5,2F13,5)
15N 0502  612 PRINT 612
15N 0503  612 FORMAT(1H,13X,22HINTRINSIC COEFFICIENTS,77X,PHAT FR V,XX,7HVV,
15N 0504  1 12X,2HVV,13X,3HDT,12X,3HOT(,7X,6HVV/DT,4X,6HVV/DT,5X,
15N 0505  2 2HT(,7X,7HVV/DT,5X,7HMGAMMA V,2X,6HMGAMMA V,5X,7HMMT,6X,
15N 0506  3 1MS,10X,1MD,12X,1MD,796X,6HDARKEN,7X,7HMMANNING,77X)
15N 0507  1 PRINT 613,(CVE(1),DVS(1),DSRAT(1),GAMV(1),GAMT(1),PHI(1),
15N 0508  2 5X(1),DCD(1),DCM(1), 1-1,101)
15N 0509  613 FORMAT(14,5,2E13,5,5F10,5,2F13,5)
15N 0510  614 PRINT 614
15N 0511  614 FORMAT(14,5,4F15,5,4F10,5)
15N 0512  615 CALL QDCPA(9,0.05)
15N 0513  616 CALL QDCPA(5,10.0)
15N 0514  617 IF(N99 .EQ. 1) GO TO 618
15N 0515  618 N40 = XMAX/500
15N 0516  619 N40 = (2*N40) + 2
15N 0517  620 N=0
15N 0518  621 DO 800 I=3,NX1M,N40
15N 0519  622 XIN(1) = X(I)
15N 0520  623 CPRIV(1) = CPRIV(1)
15N 0521  624 IF (DI(1) .LE. 0.0) DI(1) = 1.0
15N 0522  625 DI(1) = DI(1)
15N 0523  800 CONTINUE
15N 0524  1 MAX = XMAX/N40
15N 0525  1 CALL FIXPLT(0.0,1.0,1.0E-11,1.0E-5,1VLOT,1MFCH,20.0,6.0,HUFFP,10,
15N 0526  2 'CARLSBURG')
15N 0527  1 CALL TITLE(0.2,1,INTERDIFFUSION COEFFICIENTS,1,'ATOM FRACTION VS',
15N 0528  2 'ID, CMO2/SFC')
15N 0529  1 CALL LIMPLT(CPRIV,0,(MAX,-1,0)
15N 0530  1 CALL LIMPLT(CVE,DCD,1,1,0,-1)
15N 0531  1 CALL LIMPLT(CVE,DCM,101,2,-1)
15N 0532  1 CALL QDCSYM(7,0,9,5,0,10,'RUMS',0,0,3)
15N 0533  1 CALL QDCSYM(99,999,0,1,0,0,7,(15))
15N 0534  1 CALL QDCSYM(7,0,9,3,0,10,'PERFILF',0,0,7)
15N 0535  1 CALL QDCSYM(99,999,0,1,0,0,13,0,0,(15))
15N 0536  1 CALL QDCSYM(7,0,9,1,0,10,'TEMPERATURE',0,0,11)
15N 0537  1 CALL QDCSYM(99,999,0,1,0,18,0,0,(19,3))
15N 0538  1 CALL QDCSYM(7,0,9,0,10,'TIME,SFC',0,0,8)
15N 0539  1 CALL QDCSYM(99,999,0,10,5,0,0,(15,5))

```



```

ISN 0589      CALL TITLE(0.2,'MICROPROBE CALIBRATIONS','CVS','KVS')
ISN 0590      CALL LINPLT(CONCV,SV,N1,0,-1)
ISN 0591      CALL SETPLT(CONCTI,STI,N1,'LINEAR','MECH',20.,20.,BUFFER,10,
              'CARLSONS')
ISN 0592      CALL TITLE(0.2,'MICROPROBE CALIBRATIONS','CTIS','KTI')
ISN 0593      CALL LINPLT(CONCTI,STI,N1,0,-1)
ISN 0594      CALL SETPLT(CONCVR,TV,N1,'LINEAR','MECH',20.,20.,BUFFER,10,
              'CARLSONS')
ISN 0595      CALL TITLE(0.2,'MICROPROBE CALIBRATIONS','(1-CV)/CVI',
              '(1-KV)/KVS')
ISN 0596      CALL LINPLT(CONCVR,TV,N1,0,-1)
ISN 0597      CALL SETPLT(CONCTH,TTI,N1,'LINEAR','MECH',20.,20.,BUFFER,10,
              'CARLSONS')
ISN 0598      CALL TITLE(0.2,'MICROPROBE CALIBRATIONS','(1-CTI)/CTIS',
              '(1-KTI)/KTI')
ISN 0599      CALL LINPLT(CONCTR,TTI,N1,0,-1)
ISN 0600      2050 IF (L .GE. N6) GO TO 1001
ISN 0602      L = L + 1
ISN 0603      N13 = N13 + 1
ISN 0604      GO TO 2000
ISN 0605      1001 IF (KCYCLE .GE. N5) GO TO 3000
ISN 0607      KCYCLE = KCYCLE + 1
ISN 0608      GO TO 1000
ISN 0609      3000 CALL ADVANS
ISN 0610      CALL EXIT
ISN 0611      RETURN
ISN 0612      FNO

```

APPENDIX B

Description of FITLOS Subroutine

The following appendix is, for the most part, excerpted from the original publication of Smith¹³ and is presented here for the convenience of the reader. Naturally a more detailed account, particularly from the standpoint of the mathematical foundations of the routine, may be found in the original document.

The subroutine FITLOS is designed to fit polynomial splines of second or third degree to experimental data points. The method of least squares is combined with the segmented curve of the theory of splines to obtain a smooth curve across the region of interest with no points of discontinuity. The data points are divided into subsets and a polynomial of degree two or three is fitted on each subset by the method of least squares. A smooth curve is obtained by forcing the polynomials and their first derivatives to be equal at the break points between the segments of the curve. In the case of polynomials of degree three, the second derivatives are also made equal at the spline joints. The above constraints are imposed with the use of Lagrangian multipliers.

Definition of Variables Used by FITLOS

The following section tabulates the variables used by the subroutine FITLOS in order of their appearance in the argument list.

<u>Symbol</u>	<u>Definition</u>
DIST(I)	Distance coordinate of composition point I in microns.
UNEW(I)	The value of the variable u at DIST(I) determined by the Newton-Raphson iteration technique from the experimental concentration at each point in the concentration profile of component 1.
W(I)	Array of weights. Since FITLOS makes a weighted least

<u>Symbol</u>	<u>Definition</u>
	squares fit, each point must have a weight. If all the weights are zero, FITLPS will make all the weights equal to 1.
NI	Total number of composition data points in the concentration profile.
NS	Number of segments if the user selects the number of segments. NS $\neq$ 0 means the curve will be fit in NS segments. If NS = 0, the program will select the largest possible number of segments.
M	Degree of polynomial. M must be 2 or 3.
NB	Number of spline joints. NB $\neq$ 0 indicates the user has selected the spline joints and these data will be read in as part of the input data. NB = 0 means that the program will set NB = NS - 1.
NF	Numerical variable which decides whether force-fitting is used to divide the u versus x curve into subsets. NF < 0 means that force-fitting starts at the low end to divide the data into subsets. NF > 0 means that force-fitting starts at the high end to divide the data into subsets. NF = 0 means that the data are divided as equally as possible among the maximum number of subsets. The NF variable is ignored by FITLPS when either NS > 0 or NB > 0.
TRANX	Logical variable which indicates whether a log transformation should be made on the distance data elements for purposes of curve fitting. TRANX = .TRUE. means the transformation should be made. TRANX = .FALSE. means the transformation should not be made.
TRANY	Logical variable which indicates whether a log transformation should be made on the u element for purposes of curve fitting. TRANY = .TRUE. means the transformation should be made. TRANY = .FALSE. means the transformation should not be made.
LREFIT	Logical variable which determines whether FITLPS subroutine should check whether the u versus x curve was fit in more segments than was necessary. LREFIT = .TRUE. means the check should be made. LREFIT = .FALSE. means the check should not be made.

Symbol	Definition
IENTRY	Variable which is used within FITLPS such that the arrays called by the various subroutines within FITLPS are dimensioned only once in cases where successive calls to FITLPS are made. IENTRY should be set equal to zero initially in the argument list.
UE(I)	The values calculated by FITLPS of the variable u at the experimental DIST(I) using the coefficients of the polynomial spline fitting procedure.
XM(I)	Location of the spline joints of the spline-fitted, polynomial u versus x curve in units of microns. If NB = 0, FITLPS determines the values of XM(I). If NB > 0, the user reads the XM(I) as input data.
A	The array of polynomial coefficients obtained from spline fitting the various segments of the u versus x curve of component 1.

Discussion of Program Operation of FITLPS

The subroutine FITLPS itself is written as a series of subprograms each of which performs a separate function in the spline fitting procedure. In order to make the various subroutines as flexible as possible, the arrays used by them are variably dimensioned. Every such subprogram with a dimensioned array is called only once by its subroutine name to conserve execution time; thereafter, the subroutines are called by their entry names which does not affect the size of the variably dimensioned arrays set up by the first call.

FITLPS is designed to read the input data given in the argument list, call the subroutines to make the spline fit and generate the output data. Following the reading of the data presented in the argument list, FITLPS first checks the logical variables TRANX and TRANY to determine whether a log transformation should be made on the variables DIST(I) or UNEW(I), respectively. If either variable is .TRUE., the subroutine TRANSF is called to perform this transformation; however, this particular aspect of FITLPS is not needed for most chemical diffusion applications.

The next subroutine called is SEGMENT which divides the data into subsets in accordance with the particular method specified by the user by his choice of the values of NS, NB and NF in the argument list of FITLPS. SEGMENT provides four possible ways to divide the data into subsets: (1) selection of the number and locations of the spline joints of the segmented curve; (2) selection of the number of segments into which the curve is to be divided; (3) force-fitting the data points beginning at either the high or low end of the data set; and (4) a special division for cases where the total number of data elements is less than $2M + 1$.

If the user elects to divide his experimental data by specifying the number and locations of the spline joints (case 1), $NB \neq 0$ in the argument list, and the subroutine DIVM is called by SEGMENT to perform this division. Naturally, when this course is chosen, the values of the spline joint locations, $XM(I)$, must be read in as part of the input data. DIVM sets $NS = NB + 1$ and proceeds to divide the data elements into subsets in accordance with the values of NB and the prechosen spline joints. If the user instead wishes to specify the number of segments into which the data set is to be divided (case 2), $NB = 0$ and $NS \neq 0$ in the argument list, and the subroutine DIVNS is called by SEGMENT to divide the data as evenly as possible among the NS subsets. DIVNS sets $NB = NS - 1$ and proceeds to divide the data according to the prechosen number of segments, NS. It should be noted here that SEGMENT first interrogates NB; consequently, when $NB \neq 0$ the subroutine DIVM is called to perform the data division into subsets and the subroutine DIVNS is bypassed. The consequence of this program structure is that when $NB \neq 0$, the value of NS in the argument list is ignored. Similarly, when SEGMENT interrogates NB and discovers that $NB = 0$, it then interrogates NS to test whether DIVNS is to be used.

The remaining two methods of dividing the data into subsets (cases 3 and 4) cannot be used by MATANØ for reasons to be discussed below; nevertheless, they are included here in the event the user wishes to modify MATANØ accordingly. If neither the number of spline joints

(and their locations) nor the number of segments is specified ($NB = NS = 0$), SEGMENT automatically chooses the largest possible number of segments based on the number of data points and the degree of the polynomial. SEGMENT first checks the number of data elements (N). If $N < 3M + 1$, where M is the degree of the polynomial, the subroutine SPESHL is called to make a special division of the data into subsets (case 4). If $N > M$, then SEGMENT interrogates NF to see if force-fitting of the data is to be begun at the high or low end of the data set (case 3). If force-fitting is to be begun at the high end of the data set, $NF > 0$ and the subroutine FFHIGH is called to make this division; likewise, if force-fitting is to be begun at the low end of the data, $NF < 0$ and FFL~~OW~~ is called for this division. If $NF = 0$, DIVNS is used to divide the elements along the maximum possible number of subsets.

Finally, it is important to note that since MATAN~~0~~ is currently designed to treat a maximum of six segments, NS and NB cannot both equal zero. The consequence of selecting neither the number of spline joints nor the number of segments (i.e., $NB = NS = 0$) would be to force SEGMENT to choose the maximum number of segments (10) with the result that MATAN~~0~~ would abort. Since NF is not interrogated unless $NB = NS = 0$, the subroutines SPESHL, FFHIGH and FFL~~OW~~ are not used by MATAN~~0~~; nevertheless, they have been included in the event that the user may wish to expand MATAN~~0~~ to treat data division into more than six segments. Also, in light of the above comments, the value of NF in the argument list is ignored by SEGMENT.

Once proper division of the data into subsets has been accomplished, the subroutines DEFMAT and AS~~OL~~VE are called to define the appropriate matrices and perform the necessary matrix manipulations, respectively, to produce the fitted curve. The reader is referred to the complete documentation of FITL~~OS~~¹³ for a more detailed description of the operation of the above subroutines.


```

15N 0002      SUBROUTINE FITLOS(XX,VV,WW,NX,NS,M,NB,NF,TRANX,TRANV,LREFIT,TOL,
15N 0003      1 (ENTRY,YC,XM,A,INX)
15N 0004      DIMENSION XX(INX),VV(INX),WW(INX),YC(INX)
15N 0005      DIMENSION XM(11),LLOW(10),LHIGH(10)
15N 0006      DIMENSION A(10,4),XWX(10,4,4),VWX(10,4),C(9,1,4),R(9,1,1,1),
15N 0007      1 BB(4,4,3,3)
15N 0008      DOUBLE PRECISION H,RR,A,YC,XWX,VWX,C
15N 0009      DOUBLE PRECISION DEV,FRR,VAR,STDEV,CORP,CORPAX,SJAX,SUMV,SUMWV,
15N 0010      1 SUMX2,SUMY2,SUMW,SUMW2,FN,FX
15N 0011      LOGICAL LREFIT,TRANX,TRANV
15N 0012      INX = 10
15N 0013
15N 0014      C
15N 0015      C
15N 0016      C
15N 0017      SET DIMENSIONS OF ARRAYS IN SUBROUTINES
15N 0018
15N 0019      IF (ENTRY .NE. 0) GO TO 315
15N 0020      ENTRY=1
15N 0021      CALL SEG(XX,VV,XM,LLOW,LHIGH,INX,11,10)
15N 0022      CALL DEF(XX,VV,WW,XM,LLOW,LHIGH,XWX,VWX,C,INX,11,10,4,1,9)
15N 0023      CALL SLVIC,XWX,VWX,A,B,RR,9,3,4,10)
15N 0024      CALL RPT(XX,A,XM,LLOW,LHIGH,INX,10,11,4)
15N 0025      CALL DXM(XX,XM,LLOW,LHIGH,INX,11,10)
15N 0026      CALL DSPL(XX,XM,LLOW,LHIGH,INX,11,10)
15N 0027      CALL DNS(XX,XM,LLOW,LHIGH,INX,11,10)
15N 0028      CALL DM(XX,VV,XM,LLOW,LHIGH,INX,11,10)
15N 0029      CALL DL(XX,VV,XM,LLOW,LHIGH,INX,11,10)
15N 0030
15N 0031      C
15N 0032      C
15N 0033      C
15N 0034      IF ALL WEIGHTS ARE READ AS 0, SET ALL WEIGHTS TO 1
15N 0035
15N 0036      315 NW = 0
15N 0037      DO 82 I=1,NX
15N 0038      1 IF(WW(I) .LT. 0) NW=NW+1
15N 0039      82 CONTINUE
15N 0040      IF (NW.NE.NX) GO TO 84
15N 0041      DO 83 I=1,NX
15N 0042      83 WW(I)=1.
15N 0043
15N 0044      C
15N 0045      C
15N 0046      C
15N 0047      TEST INPUT TRIGGERS TO SEE IF ADDITIONAL DATA IS NEEDED TO DIVIDE
15N 0048      THE CURVE INTO SEGMENTS
15N 0049
15N 0050      C
15N 0051      C
15N 0052      C
15N 0053      84 IF(NS.GT.1XMI) NB=1XMI
15N 0054      IF(TRANX .OR. TRANV) CALL TRANS(XX,VV,NX,XM,NB,TRANX,TRANV)
15N 0055
15N 0056      C
15N 0057      C
15N 0058      C
15N 0059      CHECK FOR SUFFICIENT NUMBER OF DATA POINTS AND CORRECT ORDER OF
15N 0060      POLYNOMIALS
15N 0061
15N 0062      C
15N 0063      C
15N 0064      C
15N 0065      WRITE(6,24)
15N 0066      IF (INX.GT.M.AND.(M.EQ.2.OR.M.EQ.3)) GO TO 85
15N 0067      WRITE (6,23) M,NX
15N 0068      GO TO 80
15N 0069
15N 0070      C
15N 0071      C
15N 0072      C
15N 0073      85 CALL SEGMENT(XX,VV,XM,LLOW,LHIGH,NX,NS,NB,NF,M,TOL,FXM)
15N 0074      CALL DEFMAT(XX,VV,WW,XM,LLOW,LHIGH,NX,NS,M,XWX,VWX,C)
15N 0075      XM(IAM-1) = XX(I)
15N 0076      CALL ASOLVE(C,XWX,VWX,A,NS,M)
15N 0077      IF (NS.EQ.1) LREFIT=.FALSE.
15N 0078      IF (LREFIT) CALL RPT(XX,A,XM,LLOW,LHIGH,NX,NS,NS,M,TOL)
15N 0079

```


	1 =,15)		310
ISN 0149	12 FORMAT (1H0,4HSEGMENT COEFFICIENTS IN ASCENDING ORDER =)		311
ISN 0150	13 FORMAT (1H ,1P3D25,15)		312
ISN 0151	14 FORMAT (1H ,1P4D25,15)		313
ISN 0152	15 FORMAT (1H0,1HMSPLINE JOINTS ARE -)		314
ISN 0153	16 FORMAT (1H ,2IX,2G15,7)		315
ISN 0154	17 FORMAT (1H ,1P2(17,7,1P2D25,15,3PD25,15)		316
ISN 0155	21 FORMAT (1H0,4X,1HX,14X,1HY,21X,2HY,21X,1HDEV,21X,5HR-FRR)		317
ISN 0156	22 FORMAT (1H0,7,1H0,5HOCORRELATION OF FITTED DATA TO ORIGINAL DATA 1 7,1H0,16X,10HVARVANCE =,1P025,15,12X,19HOCORRELATION IND 2FX =,OPD25,15,7,1H ,6X,20HSTANDARD DEVIATION =,1P025,15,10X, 32HMAXIMUM CORRELATION =,OPD25,15)		318 319 320 321
ISN 0157	23 FORMAT (1H0,10HCANNOT MAKE VALID FIT WITH M =,13,9H AND N =,13)		322
ISN 0158	24 FORMAT (1H1)		323
ISN 0159	36 FORMAT (1H ,82H DUPLICATION OCCURRED IN FIRST SET OF COEFFICIENTS - 1CURVE WAS REFIT IN NEW SEGMENTS)		324 325
ISN 0160	37 FORMAT (1H ,4HNO DUPLICATION IN FIRST SET OF COEFFICIENTS)		326
ISN 0161	38 FORMAT (1H0,20HREIT CHECK WAS MADE)		327
ISN 0162	39 FORMAT (1H0,6HEQUATION FITTED IS 1) + A2 (LOG X1002)	LOG Y = A0 + A1 (LOG X	328 329
ISN 0163	40 FORMAT (1H0,6HEQUATION FITTED IS 1A2 (LOG X1002)	Y = A0 + A1 (LOG X) +	330 331
ISN 0164	41 FORMAT (1H0,5HEQUATION FITTED IS 1 X002)	LOG Y = A0 + A1 X + A2	332 333
ISN 0165	42 FORMAT (1H0,5HEQUATION FITTED IS 1)	Y = A0 + A1 X + A2 X00	334 335
ISN 0166	43 FORMAT (1H0,1HNO REFIT CHECK MADE)		336
ISN 0167	44 FORMAT (1H0,10X,2HMO,21X,2HA1,21X,2HA2)		337
ISN 0168	45 FORMAT (1H0,10X,2HMO,21X,2HA1,21X,2HA2,21X,2HA3)		338
ISN 0169	46 FORMAT (1H0,8HEQUATION FITTED IS 1) + A2 (LOG X1002 + A3 (LOG X1003)	LOG Y = A0 + A1 (LOG X	339 340
ISN 0170	47 FORMAT (1H0,8HEQUATION FITTED IS 1A2 (LOG X1002 + A3 (LOG X1003)	Y = A0 + A1 (LOG X) +	341 342
ISN 0171	48 FORMAT (1H0,6HEQUATION FITTED IS 1 X002 + A3 X003)	LOG Y = A0 + A1 X + A2	343 344
ISN 0172	49 FORMAT (1H0,6HEQUATION FITTED IS 12 + A3 X003)	Y = A0 + A1 X + A2 X00	345 346
ISN 0173	C END		347 348 349 350 351 352

15N 0030	1M NUMBER OF SUBSETS)	57
15N 0039	26 FORMAT (1M0,75M DATA DIVIDED INTO SUBSETS BY FORCE FITTING STARTING	58
15N 0040	1 AT THE HIGH END OF DATA)	59
	27 FORMAT (1M0,15,24,32M POINTS REQUIRES SPECIAL DIVISION)	60
	C	61
	END	62

ISS 0002	SUBROUTINE DSPL(X,M,LLW,HIGH,X,LM,TL)	1
ISS 0003	DIMENSION A(1),X(M),LLW(1),HIGH(1)	2
ISS 0004	RETURN	3
	C	4
	C SPECIAL DIVISION INTO SEGMENTS WHEN NUMBER OF POINTS IS BETWEEN	5
	C M+1 AND M	6
	C	7
ISS 0005	ENTRY SPDSPL(X,A,LLW,HIGH,NX,NS,NH,M)	8
	C	9
	C NUMBER OF POINTS LESS THAN 2M+1 REQUIRES ONE SEGMENT	10
	C	11
ISS 0006	100 IF (NX.GT.2*M) GO TO 200	12
ISS 0008	NS = 1	13
ISS 0009	NH = 0	14
ISS 0010	XM(1) = X(NX)	15
ISS 0011	LLW(1) = 1	16
ISS 0012	HIGH(1) = NX	17
ISS 0013	RETURN	18
	C	19
ISS 0014	200 NS = 2	20
ISS 0015	NH = 1	21
ISS 0016	GO TO (1,2,3),M	22
	C	23
ISS 0017	1 WRITE (6,10)	24
ISS 0018	10 FORMAT (1H0,13M: CANNOT BE 1)	25
ISS 0019	CALL EXIT	26
	C	27
	C M = 2	28
	C	29
ISS 0020	2 LLW(1) = 1	30
ISS 0021	LLW(2) = 3	31
ISS 0022	HIGH(2) = NX	32
ISS 0023	XM(2) = X(NX)	33
ISS 0024	IF (NX.GT.5) GO TO 210	34
ISS 0025	XM(1) = X(3)	35
ISS 0026	HIGH(1) = 3	36
ISS 0028	RETURN	37
	C	38
ISS 0029	210 XM(1) = .5*(X(3)+X(4))	39
ISS 0030	HIGH(1) = 4	40
ISS 0031	RETURN	41
	C	42
	C M = 3	43
	C	44
ISS 0032	3 LLW(1) = 1	45
ISS 0033	XM(2) = X(NX)	46
ISS 0034	HIGH(2) = NX	47
ISS 0035	IF (NX.GT.8) GO TO 310	48
ISS 0037	IF (NX.GT.7) GO TO 300	49
ISS 0039	XM(1) = X(4)	50
ISS 0040	LLW(2) = 4	51
ISS 0041	HIGH(1) = 4	52
ISS 0042	RETURN	53
	C	54
ISS 0043	300 XM(1) = .5*(X(4)+X(5))	55
ISS 0044	LLW(2) = 5	56

47
 48
 49
 50
 51
 52
 53
 54

LHIGH(1) = 4
 RETURN
 C 310 LLOW(2) = 5
 LHIGH(1) = 5
 KM(1) = X(5)
 RETURN
 END

ISN 0045
 ISN 0046
 ISN 0047
 ISN 0048
 ISN 0049
 ISN 0050
 ISN 0051


```

154 0002 SURROUTINE OM(X,Y,XA,LCOM,LCHIGH,X,Y,IXM,IL)
155 0003 DIMENS:OM X(1),Y(1),X(1),Y(1),LCOM(1),LCHIGH(1),
156 0004 RETURN
157
158 0005 C DETERMINE SUMSETS BY FORCE FITTING STARTING AT HIGH END OF DATA
159 0006 C
160 0007 C
161 0008 C
162 0009 C
163 0010 C
164 0011 C
165 0012 C
166 0013 C
167 0014 C
168 0015 C
169 0016 C
170 0017 C
171 0018 C
172 0019 C
173 0020 C
174 0021 C
175 0022 C
176 0023 C
177 0024 C
178 0025 C
179 0026 C
180 0027 C
181 0028 C
182 0029 C
183 0030 C
184 0031 C
185 0032 C
186 0033 C
187 0034 C
188 0035 C
189 0036 C
190 0037 C
191 0038 C
192 0039 C
193 0040 C
194 0041 C
195 0042 C
196 0043 C
197 0044 C
198 0045 C
199 0046 C
200 0047 C
201 0048 C
202 0049 C
203 0050 C
204 0051 C
205 0052 C
206 0053 C
207 0054 C
208 0055 C
209 0056 C
210 0057 C
211 0058 C
212 0059 C
213 0060 C
214 0061 C
215 0062 C
216 0063 C
217 0064 C
218 0065 C
219 0066 C
220 0067 C
221 0068 C
222 0069 C
223 0070 C
224 0071 C
225 0072 C
226 0073 C
227 0074 C
228 0075 C
229 0076 C
230 0077 C
231 0078 C
232 0079 C
233 0080 C
234 0081 C
235 0082 C
236 0083 C
237 0084 C
238 0085 C
239 0086 C
240 0087 C
241 0088 C
242 0089 C
243 0090 C
244 0091 C
245 0092 C
246 0093 C
247 0094 C
248 0095 C
249 0096 C
250 0097 C
251 0098 C
252 0099 C
253 0100 C
254 0101 C
 
```



```

15N 0039      TT = WIK)
15N 0040      DO 220 J=1,M1
15N 0041      T(I,J) = T(I,J)+TT
15N 0042      WIK(M,J) = WIK(M,J)+TT+VY(K)
15N 0043      220 TT = VTX(K)
15N 0044      DO 230 I=2,M1
15N 0045      T(I,M1) = T(I,M1)+TT
15N 0046      TT = VTX(K)
15N 0047      230 CONTINUE
15N 0048      240 CONTINUE
15N 0049      C
15N 0050      DO 270 I=2,M1
15N 0051      DO 260 J=1,M1
15N 0052      260 T(I,J) = T(I-1,J+1)
15N 0053      270 CONTINUE
15N 0054      CALL MINVRT(M1,DET,ERR)
15N 0055      DO 290 I=1,M1
15N 0056      WIK(M,I) = T(I,J)
15N 0057      290 CONTINUE
15N 0058      300 CONTINUE
15N 0059      C
15N 0060      400 RETURN
15N 0061      END

```

```

15N 0039
15N 0040
15N 0041
15N 0042
15N 0043
15N 0044
15N 0045
15N 0046
15N 0047
15N 0048
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15N 0050
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15N 0052
15N 0053
15N 0054
15N 0055
15N 0056
15N 0057
15N 0058
15N 0059
15N 0060

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```

15N 0002 SUBROUTINE SLVIC,XXX,VMX,A,B,MINV,IC,IM,IMI,1,
15N 0003 DIMENSION C(1C,1M,1M),XMX(1C,1M),YMX(1C,1M),XIL(1C,1M),XIL(1M),
15N 0004 1 B(1C,1M,1M),B(1C,1M),B(1C,1M),B(1C,1M),B(1C,1M),B(1C,1M),
15N 0005 DIMENSION T(4,4),T(4,4),E(4,4),DELTA(3,3),V(4),V(4),
15N 0006 DOUBLE PRECISION C,XXX,VMX,A,B,MINV,T,TT,F,DELTA,V,VM,TS,CT,DEV, DBM
15N 0007 1 SIGN
15N 0008 GO TO 540
15N 0009
15N 0010 C SOLVE MATRIX EQUATION FOR A-TRANSPOSE
15N 0011 C
15N 0012 FENTRY ASOLVEIC,XXX,VMX,A,AS,M)
15N 0013 C
15N 0014 FOR ONE SEGMENT, DO A SIMPLE LEAST SQUARES FIT
15N 0015 C
15N 0016 IF (MS.GT.1) GO TO 100
15N 0017 M1 = M+1
15N 0018 DO 95 I=1,M1
15N 0019 A(I,1) = 0.00
15N 0020 DO 90 K=1,M1
15N 0021 A(I,1) = A(I,1)+XXX(I,1,K)*VMX(I,K)
15N 0022 90 CONTINUE
15N 0023 95 CONTINUE
15N 0024 RETURN
15N 0025 C
15N 0026 C DEFINE B MATRIX
15N 0027 C
15N 0028 100 NN = NS-1
15N 0029 MM = M
15N 0030 M1 = M+1
15N 0031 DO 200 N=1,NN
15N 0032 DO 190 L=1,3
15N 0033 MIND = (L-1)/2+N
15N 0034 GO TO (1,2,3),L
15N 0035 1 IF (N.EQ.1) GO TO 190
15N 0036 JIND = N-1
15N 0037 GO TO 120
15N 0038 C
15N 0039 2 SIGN = 1.00
15N 0040 JIND = N
15N 0041 DO 110 I=1,M1
15N 0042 DO 110 J=1,M1
15N 0043 Y(I,J) = XXX(N,1,J)+XXX(N+1,1,J)
15N 0044 110 CONTINUE
15N 0045 GO TO 140
15N 0046 C
15N 0047 3 IF (N.EQ.NN) GO TO 200
15N 0048 JIND = N+1
15N 0049 120 SIGN = -1.00
15N 0050 DO 130 I=1,M1
15N 0051 DO 130 J=1,M1
15N 0052 Y(I,J) = XXX(NIND,1,J)
15N 0053 130 CONTINUE
15N 0054 C
15N 0055 140 DO 160 I=1,M1
15N 0056 DO 150 J=1,MM
15N 0057 Y(I,J) = 0.00

```

[illegible]

```

155 290 RINV(N,N,I,J)= RINV(N,N,I,J) + F(I,K)*DELTA(K,J)
156 300 CONTINUE
157 C
158 IF (I=EQ-1) GO TO 500
159 L=NM-1
160 310 LAST=L
161 DO 306 LL=1, LAST
162 320 IF (L=1) GO TO 340
163 DO 330 J=1, MM
164 DO 340 J=1, MM
165 F(I,J)=G(I,J,I,J)
166 DELTA(I,J)=0.00
167 IF (L=EQ,N,AND,I,FQ,J) DELTA(I,J)=1.00
168 330 CONTINUE
169 GO TO 390
170 C
171 340 DO 360 I=1, MM
172 DO 350 J=1, MM
173 T(I,J)=0.00
174 T(I,J)=0.00
175 DO 350 K=1, MM
176 T(I,J)=T(I,J)+F(I,K)*DELTA(K,J)
177 350 T(I,J)=T(I,J)+DELTA(I,K)*DELTA(K,J)
178 360 CONTINUE
179 DO 380 I=1, MM
180 DO 380 J=1, MM
181 DELTA(I,J)=0.00
182 T(I,J)=0.00
183 DO 370 K=1, MM
184 DELTA(I,J)=DELTA(I,J)+R(I,I,K)*T(K,J)
185 370 F(I,J)=F(I,J)+R(I,I,K)*T(K,J)
186 F(I,J)=F(I,J)+T(I,J)
187 TS=0.00
188 IF (L=EQ,N,AND,I,FQ,J) TS=L.00
189 DELTA(I,J)=TS-DELTA(I,J)
190 380 CONTINUE
191 390 CALL MINV(TL,MM,DT,DFV)
192 396 CONTINUE
193 C
194 400 DO 420 I=1, MM
195 DO 410 J=1, MM
196 DO 410 K=1, MM
197 DELTA(I,J)=DELTA(I,J)+R(I,I,K)*RINV(L+1,N,K,J)
198 410 CONTINUE
199 420 CONTINUE
200 C
201 DO 440 I=1, MM
202 DO 430 J=1, MM
203 RINV(L,N,I,J)=0.00
204 DO 430 K=1, MM
205 RINV(L,N,I,J)=RINV(L,N,I,J)+F(I,K)*DELTA(K,J)
206 430 CONTINUE
207 440 CONTINUE
208 C
209 IF (L=FQ-1) GO TO 450
210 L=L-1
211 GO TO 110
212 450 CONTINUE
213

```


930.00000	0.17019	0.42941	-0.27770F-03	0.12951F 03	0.26782F-07
934.00000	0.16908	0.43092	-0.27791F-03	0.12902F 03	0.26653F-07
938.00000	0.16797	0.43203	-0.27810F-03	0.12752F 03	0.26533F-07
942.00000	0.16685	0.43315	-0.27827F-03	0.12702F 03	0.26414F-07
946.00000	0.16574	0.43426	-0.27844F-03	0.12652F 03	0.26294F-07
950.00000	0.16463	0.43537	-0.27856F-03	0.12500F 03	0.26174F-07
954.00000	0.16351	0.43649	-0.27867F-03	0.12449F 03	0.26060F-07
958.00000	0.16240	0.43760	-0.27875F-03	0.12497F 03	0.25944F-07
962.00000	0.16128	0.43872	-0.27882F-03	0.12444F 03	0.25828F-07
966.00000	0.16017	0.43983	-0.27890F-03	0.12391F 03	0.25714F-07
970.00000	0.15905	0.44095	-0.27890F-03	0.12338F 03	0.25601F-07
974.00000	0.15793	0.44207	-0.27890F-03	0.12284F 03	0.25488F-07
978.00000	0.15682	0.44318	-0.27890F-03	0.12230F 03	0.25377F-07
982.00000	0.15570	0.44430	-0.27885F-03	0.12175F 03	0.25266F-07
986.00000	0.15459	0.44541	-0.27880F-03	0.12120F 03	0.25154F-07
990.00000	0.15347	0.44653	-0.27872F-03	0.12064F 03	0.25041F-07
994.00000	0.15236	0.44764	-0.27863F-03	0.12009F 03	0.24928F-07
998.00000	0.15124	0.44876	-0.27851F-03	0.11952F 03	0.24814F-07
1002.00000	0.15013	0.44987	-0.27837F-03	0.11895F 03	0.24699F-07
1006.00000	0.14902	0.45098	-0.27821F-03	0.11837F 03	0.24584F-07
1010.00000	0.14790	0.45210	-0.27803F-03	0.11780F 03	0.24468F-07
1014.00000	0.14679	0.45321	-0.27783F-03	0.11721F 03	0.24351F-07
1018.00000	0.14568	0.45432	-0.27761F-03	0.11663F 03	0.24234F-07
1022.00000	0.14457	0.45543	-0.27737F-03	0.11604F 03	0.24117F-07
1026.00000	0.14346	0.45654	-0.27711F-03	0.11545F 03	0.24000F-07
1030.00000	0.14236	0.45764	-0.27684F-03	0.11485F 03	0.23882F-07
1034.00000	0.14125	0.45875	-0.27654F-03	0.11425F 03	0.23764F-07
1038.00000	0.14014	0.45985	-0.27622F-03	0.11364F 03	0.23645F-07
1042.00000	0.13904	0.46096	-0.27588F-03	0.11304F 03	0.23526F-07
1046.00000	0.13794	0.46206	-0.27552F-03	0.11242F 03	0.23407F-07
1050.00000	0.13683	0.46317	-0.27514F-03	0.11179F 03	0.23287F-07
1054.00000	0.13573	0.46427	-0.27474F-03	0.11119F 03	0.23167F-07
1058.00000	0.13464	0.46536	-0.27432F-03	0.11057F 03	0.23046F-07
1062.00000	0.13354	0.46646	-0.27388F-03	0.10994F 03	0.22925F-07
1066.00000	0.13245	0.46755	-0.27342F-03	0.10931F 03	0.22804F-07
1070.00000	0.13135	0.46865	-0.27294F-03	0.10868F 03	0.22682F-07
1074.00000	0.13026	0.46974	-0.27245F-03	0.10804F 03	0.22560F-07
1078.00000	0.12917	0.47083	-0.27194F-03	0.10740F 03	0.22438F-07
1082.00000	0.12809	0.47191	-0.27140F-03	0.10676F 03	0.22315F-07
1086.00000	0.12700	0.47300	-0.27083F-03	0.10612F 03	0.22192F-07
1090.00000	0.12592	0.47408	-0.27028F-03	0.10547F 03	0.22069F-07
1094.00000	0.12484	0.47516	-0.26969F-03	0.10482F 03	0.21946F-07
1098.00000	0.12376	0.47624	-0.26908F-03	0.10416F 03	0.21823F-07
1102.00000	0.12268	0.47731	-0.26845F-03	0.10351F 03	0.21700F-07
1106.00000	0.12161	0.47839	-0.26781F-03	0.10285F 03	0.21577F-07
1110.00000	0.12054	0.47946	-0.26714F-03	0.10219F 03	0.21454F-07
1114.00000	0.11948	0.48052	-0.26644F-03	0.10152F 03	0.21331F-07
1118.00000	0.11841	0.48159	-0.26570F-03	0.10085F 03	0.21208F-07
1122.00000	0.11735	0.48265	-0.26500F-03	0.10019F 03	0.21085F-07
1126.00000	0.11629	0.48371	-0.26431F-03	0.99511F 02	0.20962F-07
1130.00000	0.11524	0.48476	-0.26361F-03	0.98936F 02	0.20839F-07
1134.00000	0.11418	0.48582	-0.26292F-03	0.98361F 02	0.20716F-07
1138.00000	0.11313	0.48687	-0.26221F-03	0.97786F 02	0.20593F-07
1142.00000	0.11209	0.48791	-0.26149F-03	0.97211F 02	0.20470F-07
1146.00000	0.11105	0.48894	-0.26073F-03	0.96636F 02	0.20347F-07
1150.00000	0.11001	0.48999	-0.25993F-03	0.96061F 02	0.20224F-07
1154.00000	0.10897	0.49103	-0.25916F-03	0.95486F 02	0.20101F-07
1158.00000	0.10794	0.49206	-0.25836F-03	0.94911F 02	0.19978F-07
1162.00000	0.10691	0.49307	-0.25759F-03	0.94336F 02	0.19855F-07
1166.00000	0.10588	0.49412	-0.25680F-03	0.93761F 02	0.19732F-07

1170.00000	0.10486	0.89314	-0.25490E-03	0.91974E 02	0.20862E-07
1174.00000	0.10394	0.89616	-0.25415E-03	0.91243E 02	0.20794E-07
1178.00000	0.10283	0.89717	-0.25320E-03	0.90586E 02	0.20704E-07
1182.00000	0.10162	0.89818	-0.25223E-03	0.89887E 02	0.20627E-07
1186.00000	0.10081	0.89919	-0.25125E-03	0.89187E 02	0.20542E-07
1190.00000	0.09960	0.90020	-0.25025E-03	0.88486E 02	0.20466E-07
1194.00000	0.09881	0.90119	-0.24924E-03	0.87784E 02	0.20382E-07
1198.00000	0.09781	0.90219	-0.24821E-03	0.87080E 02	0.20307E-07
1202.00000	0.09682	0.90318	-0.24717E-03	0.86376E 02	0.20223E-07
1206.00000	0.09582	0.90417	-0.24612E-03	0.85671E 02	0.20144E-07
1210.00000	0.09485	0.90515	-0.24505E-03	0.84964E 02	0.20068E-07
1214.00000	0.09387	0.90613	-0.24396E-03	0.84257E 02	0.19994E-07
1218.00000	0.09290	0.90710	-0.24286E-03	0.83549E 02	0.19909E-07
1222.00000	0.09193	0.90807	-0.24175E-03	0.82841E 02	0.19830E-07
1226.00000	0.09097	0.90903	-0.24063E-03	0.82132E 02	0.19753E-07
1230.00000	0.09001	0.90999	-0.23949E-03	0.81422E 02	0.19675E-07
1234.00000	0.08905	0.91095	-0.23833E-03	0.80712E 02	0.19598E-07
1238.00000	0.08810	0.91190	-0.23717E-03	0.80002E 02	0.19521E-07
1242.00000	0.08715	0.91285	-0.23600E-03	0.79291E 02	0.19444E-07
1246.00000	0.08621	0.91379	-0.23480E-03	0.78580E 02	0.19367E-07
1250.00000	0.08527	0.91473	-0.23360E-03	0.77869E 02	0.19290E-07
1254.00000	0.08434	0.91566	-0.23239E-03	0.77158E 02	0.19214E-07
1258.00000	0.08341	0.91659	-0.23117E-03	0.76447E 02	0.19138E-07
1262.00000	0.08249	0.91751	-0.22993E-03	0.75736E 02	0.19062E-07
1266.00000	0.08158	0.91842	-0.22868E-03	0.75025E 02	0.18986E-07
1270.00000	0.08066	0.91934	-0.22742E-03	0.74314E 02	0.18910E-07
1274.00000	0.07974	0.92024	-0.22615E-03	0.73604E 02	0.18835E-07
1278.00000	0.07883	0.92115	-0.22487E-03	0.72894E 02	0.18759E-07
1282.00000	0.07794	0.92204	-0.22358E-03	0.72185E 02	0.18684E-07
1286.00000	0.07707	0.92291	-0.22228E-03	0.71476E 02	0.18609E-07
1290.00000	0.07618	0.92382	-0.22097E-03	0.70768E 02	0.18533E-07
1294.00000	0.07530	0.92470	-0.21965E-03	0.70060E 02	0.18458E-07
1298.00000	0.07442	0.92558	-0.21832E-03	0.69353E 02	0.18382E-07
1302.00000	0.07355	0.92645	-0.21698E-03	0.68647E 02	0.18306E-07
1306.00000	0.07269	0.92731	-0.21561E-03	0.67942E 02	0.18230E-07
1310.00000	0.07183	0.92817	-0.21428E-03	0.67238E 02	0.18154E-07
1314.00000	0.07097	0.92903	-0.21291E-03	0.66535E 02	0.18078E-07
1318.00000	0.07012	0.92988	-0.21154E-03	0.65832E 02	0.18002E-07
1322.00000	0.06928	0.93072	-0.21016E-03	0.65132E 02	0.17926E-07
1326.00000	0.06844	0.93156	-0.20877E-03	0.64432E 02	0.17850E-07
1330.00000	0.06761	0.93239	-0.20737E-03	0.63734E 02	0.17774E-07
1334.00000	0.06678	0.93322	-0.20597E-03	0.63037E 02	0.17698E-07
1338.00000	0.06596	0.93404	-0.20456E-03	0.62341E 02	0.17622E-07
1342.00000	0.06513	0.93485	-0.20314E-03	0.61644E 02	0.17546E-07
1346.00000	0.06434	0.93566	-0.20172E-03	0.60955E 02	0.17470E-07
1350.00000	0.06353	0.93647	-0.20028E-03	0.60265E 02	0.17394E-07
1354.00000	0.06273	0.93727	-0.19885E-03	0.59574E 02	0.17318E-07
1358.00000	0.06194	0.93806	-0.19741E-03	0.58884E 02	0.17242E-07
1362.00000	0.06115	0.93885	-0.19596E-03	0.58203E 02	0.17166E-07
1366.00000	0.06037	0.93963	-0.19450E-03	0.57520E 02	0.17090E-07
1370.00000	0.05960	0.94040	-0.19304E-03	0.56839E 02	0.17014E-07
1374.00000	0.05883	0.94117	-0.19158E-03	0.56159E 02	0.16938E-07
1378.00000	0.05807	0.94193	-0.19011E-03	0.55482E 02	0.16862E-07
1382.00000	0.05731	0.94269	-0.18864E-03	0.54807E 02	0.16786E-07
1386.00000	0.05656	0.94344	-0.18716E-03	0.54135E 02	0.16710E-07
1390.00000	0.05581	0.94419	-0.18568E-03	0.53464E 02	0.16634E-07
1394.00000	0.05507	0.94493	-0.18420E-03	0.52796E 02	0.16558E-07
1398.00000	0.05434	0.94564	-0.18271E-03	0.52131E 02	0.16482E-07
1402.00000	0.05361	0.94639	-0.18122E-03	0.51468E 02	0.16406E-07
1406.00000	0.05289	0.94711	-0.17973E-03	0.50807E 02	0.16330E-07

1410.00000	0.05217	0.94783	-0.17423E-03	0.50149E 02	0.1628W -07
1414.00000	0.05146	0.94854	-0.17673E-03	0.49494E 02	0.1620W -07
1418.00000	0.05076	0.94924	-0.17923E-03	0.48847E 02	0.1613W -07
1422.00000	0.05006	0.94994	-0.17173E-03	0.48192E 02	0.1605W -07
1426.00000	0.04937	0.95063	-0.17223E-03	0.47535E 02	0.1597W -07
1430.00000	0.04868	0.95137	-0.17072E-03	0.46880E 02	0.1589W -07
1434.00000	0.04800	0.95207	-0.16921E-03	0.46226E 02	0.1581E -07
1438.00000	0.04733	0.95267	-0.16771E-03	0.45562E 02	0.1574W -07
1442.00000	0.04666	0.95331	-0.16620E-03	0.44896E 02	0.1566W -07
1446.00000	0.04600	0.95400	-0.16469E-03	0.44234E 02	0.1558W -07
1450.00000	0.04534	0.95466	-0.16318E-03	0.43572E 02	0.1550W -07
1454.00000	0.04469	0.95531	-0.16167E-03	0.42910E 02	0.1542W -07
1458.00000	0.04405	0.95594	-0.16016E-03	0.42247E 02	0.1534W -07
1462.00000	0.04341	0.95659	-0.15865E-03	0.41584E 02	0.1526W -07
1466.00000	0.04278	0.95722	-0.15714E-03	0.40921E 02	0.1518W -07
1470.00000	0.04216	0.95784	-0.15563E-03	0.40259E 02	0.1510W -07
1474.00000	0.04154	0.95846	-0.15412E-03	0.39596E 02	0.1502W -07
1478.00000	0.04092	0.95908	-0.15261E-03	0.38934E 02	0.1494W -07
1482.00000	0.04031	0.95969	-0.15110E-03	0.38271E 02	0.1486W -07
1486.00000	0.03971	0.96029	-0.14959E-03	0.37609E 02	0.1478W -07
1490.00000	0.03912	0.96088	-0.14808E-03	0.36947E 02	0.1469W -07
1494.00000	0.03853	0.96147	-0.14657E-03	0.36285E 02	0.1461W -07
1498.00000	0.03795	0.96205	-0.14506E-03	0.35623E 02	0.1453W -07
1502.00000	0.03737	0.96263	-0.14355E-03	0.34961E 02	0.1445W -07
1506.00000	0.03680	0.96320	-0.14204E-03	0.34299E 02	0.1437W -07
1510.00000	0.03623	0.96377	-0.14053E-03	0.33637E 02	0.1429W -07
1514.00000	0.03567	0.96433	-0.13902E-03	0.32975E 02	0.1421W -07
1518.00000	0.03512	0.96488	-0.13751E-03	0.32313E 02	0.1413W -07
1522.00000	0.03457	0.96543	-0.13600E-03	0.31651E 02	0.1405W -07
1526.00000	0.03403	0.96597	-0.13449E-03	0.30989E 02	0.1397W -07
1530.00000	0.03349	0.96651	-0.13297E-03	0.30327E 02	0.1389W -07
1534.00000	0.03296	0.96704	-0.13146E-03	0.29665E 02	0.1381W -07
1538.00000	0.03244	0.96756	-0.12995E-03	0.29003E 02	0.1373W -07
1542.00000	0.03192	0.96808	-0.12844E-03	0.28341E 02	0.1365W -07
1546.00000	0.03141	0.96859	-0.12693E-03	0.27679E 02	0.1357W -07
1550.00000	0.03090	0.96910	-0.12542E-03	0.27017E 02	0.1349W -07
1554.00000	0.03040	0.96960	-0.12391E-03	0.26355E 02	0.1341W -07
1558.00000	0.02990	0.97010	-0.12240E-03	0.25693E 02	0.1333W -07
1562.00000	0.02941	0.97059	-0.12089E-03	0.25031E 02	0.1325W -07
1566.00000	0.02893	0.97107	-0.11938E-03	0.24369E 02	0.1317W -07
1570.00000	0.02845	0.97155	-0.11787E-03	0.23707E 02	0.1309W -07
1574.00000	0.02798	0.97202	-0.11636E-03	0.23045E 02	0.1301W -07
1578.00000	0.02751	0.97249	-0.11485E-03	0.22383E 02	0.1293W -07
1582.00000	0.02705	0.97294	-0.11334E-03	0.21721E 02	0.1285W -07
1586.00000	0.02659	0.97341	-0.11183E-03	0.21059E 02	0.1277W -07
1590.00000	0.02614	0.97386	-0.11032E-03	0.20397E 02	0.1269W -07
1594.00000	0.02570	0.97430	-0.10881E-03	0.19735E 02	0.1261W -07
1598.00000	0.02526	0.97474	-0.10730E-03	0.19073E 02	0.1253W -07
1602.00000	0.02483	0.97517	-0.10579E-03	0.18411E 02	0.1245W -07
1606.00000	0.02440	0.97560	-0.10428E-03	0.17749E 02	0.1237W -07
1610.00000	0.02398	0.97602	-0.10277E-03	0.17087E 02	0.1229W -07
1614.00000	0.02356	0.97644	-0.10126E-03	0.16425E 02	0.1221W -07
1618.00000	0.02315	0.97685	-0.09975E-03	0.15763E 02	0.1213W -07
1622.00000	0.02274	0.97726	-0.09824E-03	0.15101E 02	0.1205W -07
1626.00000	0.02234	0.97766	-0.09673E-03	0.14439E 02	0.1197W -07
1630.00000	0.02194	0.97806	-0.09522E-03	0.13777E 02	0.1189W -07
1634.00000	0.02155	0.97845	-0.09371E-03	0.13115E 02	0.1181W -07
1638.00000	0.02117	0.97883	-0.09220E-03	0.12453E 02	0.1173W -07
1642.00000	0.02078	0.97922	-0.09069E-03	0.11791E 02	0.1165W -07
1646.00000	0.02041	0.97959	-0.08918E-03	0.11129E 02	0.1157W -07

1650.00000	0.02004	0.37996	-0.019431-04	0.17116F 02	0.10773-07
1654.00000	0.01987	0.08033	-0.008811-04	0.16591F 02	0.10652F-07
1658.00000	0.01931	0.08069	-0.04928E-04	0.16771F 02	0.10428F-07
1662.00000	0.01896	0.08104	-0.08185F-04	0.19955F 02	0.10409F-07
1666.00000	0.01861	0.08134	-0.06950F-04	0.19544F 02	0.10279F-07
1670.00000	0.01826	0.08174	-0.05724F-04	0.19336F 02	0.10151F-07
1674.00000	0.01792	0.08208	-0.04507F-04	0.19036F 02	0.10021F-07
1678.00000	0.01759	0.08241	-0.03100F-04	0.18735F 02	0.09899F-08
1682.00000	0.01726	0.08274	-0.02102E-04	0.18434F 02	0.09756F-08
1686.00000	0.01693	0.08307	-0.00914F-04	0.18134F 02	0.09620F-08
1690.00000	0.01661	0.08339	-0.07973E-04	0.17834F 02	0.09483F-08
1694.00000	0.01629	0.08371	-0.07866E-04	0.17534F 02	0.09346F-08
1698.00000	0.01594	0.08402	-0.07740E-04	0.17234F 02	0.09209F-08
1702.00000	0.01567	0.08433	-0.07625E-04	0.16934F 02	0.09072F-08
1706.00000	0.01537	0.08463	-0.07511E-04	0.16634F 02	0.08935F-08
1710.00000	0.01507	0.08493	-0.07396F-04	0.16334F 02	0.08798F-08
1714.00000	0.01474	0.08522	-0.07281E-04	0.16034F 02	0.08661F-08
1718.00000	0.01440	0.08551	-0.07165E-04	0.15734F 02	0.08524F-08
1722.00000	0.01403	0.08580	-0.07049E-04	0.15434F 02	0.08387F-08
1726.00000	0.01362	0.08608	-0.06934F-04	0.15134F 02	0.08250F-08
1730.00000	0.01365	0.08635	-0.06818E-04	0.14834F 02	0.08113F-08
1734.00000	0.01318	0.08662	-0.06701E-04	0.14534F 02	0.07976F-08
1738.00000	0.01311	0.08689	-0.06584E-04	0.14234F 02	0.07839F-08
1742.00000	0.01284	0.08716	-0.06467E-04	0.13934F 02	0.07702F-08
1746.00000	0.01253	0.08743	-0.06350E-04	0.13634F 02	0.07565F-08
1750.00000	0.01233	0.08767	-0.06231E-04	0.13334F 02	0.07428F-08
1754.00000	0.01204	0.08794	-0.06110E-04	0.13034F 02	0.07291F-08
1758.00000	0.01183	0.08817	-0.06021E-04	0.12734F 02	0.07154F-08
1762.00000	0.01154	0.08841	-0.05923E-04	0.12434F 02	0.07017F-08
1766.00000	0.01135	0.08864	-0.05824E-04	0.12134F 02	0.06880F-08
1770.00000	0.01112	0.08888	-0.05725E-04	0.11834F 02	0.06743F-08
1774.00000	0.01089	0.08911	-0.05626E-04	0.11534F 02	0.06606F-08
1778.00000	0.01066	0.08934	-0.05527E-04	0.11234F 02	0.06469F-08
1782.00000	0.01043	0.08957	-0.05428E-04	0.10934F 02	0.06332F-08
1786.00000	0.01022	0.08979	-0.05319E-04	0.10634F 02	0.06195F-08
1790.00000	0.01000	0.09000	-0.05202E-04	0.10334F 02	0.06058F-08
1794.00000	0.00974	0.09021	-0.05094E-04	0.10034F 02	0.05921F-08
1798.00000	0.00958	0.09043	-0.04985E-04	0.09734F 02	0.05784F-08
1802.00000	0.00937	0.09063	-0.04876E-04	0.09434F 02	0.05647F-08
1806.00000	0.00917	0.09083	-0.04767E-04	0.09134F 02	0.05510F-08
1810.00000	0.00897	0.09103	-0.04658E-04	0.08834F 02	0.05373F-08
1814.00000	0.00874	0.09122	-0.04549E-04	0.08534F 02	0.05236F-08
1818.00000	0.00854	0.09141	-0.04440E-04	0.08234F 02	0.05099F-08
1822.00000	0.00840	0.09160	-0.04331E-04	0.07934F 02	0.04962F-08
1826.00000	0.00827	0.09178	-0.04222E-04	0.07634F 02	0.04825F-08
1830.00000	0.00804	0.09198	-0.04113E-04	0.07334F 02	0.04688F-08
1834.00000	0.00786	0.09214	-0.04004E-04	0.07034F 02	0.04551F-08
1838.00000	0.00769	0.09232	-0.03895E-04	0.06734F 02	0.04414F-08
1842.00000	0.00751	0.09249	-0.03786E-04	0.06434F 02	0.04277F-08
1846.00000	0.00731	0.09264	-0.03677E-04	0.06134F 02	0.04140F-08
1850.00000	0.00714	0.09282	-0.03568E-04	0.05834F 02	0.04003F-08
1854.00000	0.00702	0.09298	-0.03459E-04	0.05534F 02	0.03866F-08
1858.00000	0.00686	0.09316	-0.03350E-04	0.05234F 02	0.03729F-08
1862.00000	0.00670	0.09330	-0.03241E-04	0.04934F 02	0.03592F-08
1866.00000	0.00655	0.09345	-0.03132E-04	0.04634F 02	0.03455F-08
1870.00000	0.00640	0.09360	-0.03023E-04	0.04334F 02	0.03318F-08

DATA DIVIDED AS EVENLY AS POSSIBLE AMONG THE NUMBER OF SUBSETS CHOSEN BY PROGRAMMER

DEGREE OF POLYNOMIAL = 2 NUMBER OF SEGMENTS = 2

EQUATION FITTED IS $Y = A0 + A1 X + A2 X^2$

SEGMENT COEFFICIENTS IN ASCENDING ORDER -

$A0$
 $-1.7057615939919550 \quad 01 \quad -9.1144418368298930 \quad 01 \quad -5.23358203111430 \quad 00$
 $-1.7433493054966105 \quad 01 \quad 5.4366571181089970 \quad 01 \quad -6.9281695340201210 \quad 00$

$A1$
 $A2$
 SPLINE JOINTS ARE - $0.0 \quad 0.4999995 \quad 0.9999990$

X	Y	DEF	P-FIT
0.0	-1.6928452E 01	-1.2896450181241150-01	0.761804272402 480-02
1.0	-1.6928452E 01	-1.0492931111203580-01	0.41846117606506500-02
2.0	-1.6928452E 01	-8.0435562399805400-02	0.47550178297094020-02
3.0	-1.7033035E 01	-5.6605361750809760-02	0.1123249213145440-02
4.0	-1.7033035E 01	-3.2178174008194540-02	0.1849030655548460-02
5.0	-1.7101315E 01	-7.416673071323290-03	0.4314919249321710-03
6.0	-1.7101315E 01	1.7755444006293480-02	0.1015340007270720-02
7.0	-1.7191240E 01	4.367554466265750-02	0.2028931999154360-02
8.0	-1.7280533E 01	6.9896183827712100-02	0.4055491407607150-02
9.0	-1.7309537E 01	9.7154641043005100-02	0.5622220160712970-02
1.0	-1.7318726E 01	1.0515513091123210-01	0.6074534316481160-02
2.0	-1.7329590E 01	9.5521532144646800-02	0.4500867231851630-02
3.0	-1.7340576E 01	8.4698736934808100-02	0.4447452114726920-02
4.0	-1.7351654E 01	7.1011252273837500-02	0.4710628494552400-02
5.0	-1.7362854E 01	6.0310599771620500-02	0.3476936007946490-02
6.0	-1.7374161E 01	4.8647250010271570-02	0.2688915082725420-02
7.0	-1.7385574E 01	3.2045912073171740-02	0.1945611516571260-02
8.0	-1.7397110E 01	1.6466725136305550-02	0.9671487110261660-03
9.0	-1.7408748E 01	-7.518177387038560-03	0.4471125602518700-03
1.0	-1.7420428E 01	-1.7011776149835050-02	0.1012120297846460-02
2.0	-1.7432094E 01	-1.7169238816147650-02	0.9959834008126750-03
3.0	-1.7443806E 01	-1.660128720222210-02	0.9501376063016400-03
4.0	-1.7455595E 01	-1.5911035082551960-02	0.789649017459460-03
5.0	-1.7467426E 01	-1.5206819721610520-02	0.6670420281693460-03
6.0	-1.7479364E 01	-1.4477459613654500-02	0.4209640054152710-03
7.0	-1.7491409E 01	-1.3687701073983900-02	0.7654549590114310-03
8.0	-1.7503553E 01	-1.2261361352949460-02	0.6945564296465040-03
9.0	-1.7515804E 01	-1.0649493384742360-02	0.6066174541018460-03
1.0	-1.7528202E 01	-8.6942625381874200-03	0.4473106745707000-03
2.0	-1.7540778E 01	-7.7911235757608900-03	0.4344048696419100-03
3.0	-1.7553491E 01	-1.1308018833400260-02	0.4350080393410510-03
4.0	-1.7566348E 01	-1.4595849068914500-02	0.4128234900094820-03
5.0	-1.7579351E 01	-1.7247271180748100-02	0.4642241204970530-03
6.0	-1.7592507E 01	-1.9410274856395460-02	0.1082493083701190-02
7.0	-1.7605820E 01	-2.0812729783356190-02	0.1161311020643460-02
8.0	-1.7619291E 01	-2.1436231701821550-02	0.1149623346818490-02
9.0	-1.7632945E 01	-2.0933119381028200-02	0.1158657102724800-02
1.0	-1.7646733E 01	-1.9149593576491720-02	0.1056935716491720-02
2.0	-1.7660711E 01	-1.5826270793620700-02	0.8709570141248420-03
3.0	-1.7674801E 01	-1.5556131508209960-02	0.8516860151293430-03
4.0	-1.7689037E 01	-1.4948347476337630-02	0.1064600917207640-02
5.0	-1.7703407E 01	-2.2130459284583360-02	0.1294949457941400-02

CORRELATION OF FITTED DATA TO ORIGINAL DATA

VARIANCE = 6.174227957118400-03
 STANDARD DEVIATION = 6.6145905966938100-02

NO REFIT CHECK MADE

CORRELATION INDEX = 0.974680452289780 00
 MAXIMUM CORRELATION = 0.980198019801980 00

DATA DIVIDED AS EVENLY AS POSSIBLE AMONG THE NUMBER OF SPLINES CHOSEN BY PROGRAMMER

DEGREE OF POLYNOMIAL = 2 NUMBER OF SEGMENTS = 2

EQUATION FITTED IS $Y = A0 + A1 \cdot X + A2 \cdot X^2$

SEGMENT COEFFICIENTS IN ASCENDING ORDER -

A0		A1		A2	
-1.720179070420900 01	-2.2309322910896780 00	-1.858567150409830 00			
-1.8069520366124011 01	4.479960754958484 00	-8.5694671968411470 00			
SPLINE JOINTS ARE -					
0.0	Y	Y ²	NEV		
9.9999979E-03	-1.72249538E 01	-1.7291798704620500 01	-6.22637407537111010-02	0.26134047804597180-01	0.26134047804597180-01
9.9999996E-01	-1.72645350E 01	-1.7314290709575020 01	-4.63433317778146490-02	0.281429830344810550-02	0.281429830344810550-02
2.9999994E-02	-1.73024294E 01	-1.733716070747924180 01	-3.47371968705428370-02	0.2007372366896570-02	0.2007372366896570-02
3.9999992E-02	-1.73409174E 01	-1.73603399369606360 01	-1.94875244333989500-02	0.1133747756111260-02	0.1133747756111260-02
4.9999990E-02	-1.73808745E 01	-1.7384009684067580 01	-3.13503101852124500-01	0.1807176014194690-01	0.1807176014194690-01
5.9999987E-02	-1.74224406E 01	-1.7407991713341830 01	1.4447861853479790-02	0.420267439343580-03	0.420267439343580-03
6.9999983E-02	-1.7465759E 01	-1.7432345455271110 01	3.3413322072638780-02	0.19131046465832330-02	0.19131046465832330-02
7.9999979E-02	-1.7510986E 01	-1.74570707880672780 01	5.391556745271620-02	0.3078055468782450-01	0.3078055468782450-01
8.9999974E-02	-1.7558289E 01	-1.74821697928616100 01	7.612065602586000-02	0.4333311224131640-02	0.4333311224131640-02
9.9999969E-02	-1.7607644E 01	-1.7507636784040680 01	1.0022759048213460-01	0.5693209955234760-02	0.5693209955234760-02
1.0999960E-01	-1.7652530E 01	-1.7533477363024330 01	1.027510572364790-01	0.5826251018081120-02	0.5826251018081120-02
1.1999959E-01	-1.7694509E 01	-1.7559689696493110 01	8.5406175702146700-02	0.4844021689044260-02	0.4844021689044260-02
1.2999950E-01	-1.7736407E 01	-1.758627364801040 01	6.773329206776200-02	0.38152734259090-02	0.38152734259090-02
1.3999941E-01	-1.77783010E 01	-1.7613229368050080 01	4.780292604596100-02	0.281935246425730-02	0.281935246425730-02
1.4999932E-01	-1.7820258E 01	-1.7640556785940280 01	3.1501314528460150-02	0.1782549567254270-02	0.1782549567254270-02
1.5999923E-01	-1.7861198E 01	-1.7668235923771610 01	1.2944713455576910-02	0.7319750764430180-03	0.7319750764430180-03
1.6999914E-01	-1.7903039E 01	-1.7696326774446400 01	5.5272604527195400-03	0.3357466149824200-01	0.3357466149824200-01
1.7999905E-01	-1.7945677E 01	-1.7724769337957660 01	2.5392824285798570-02	0.1417649594630870-02	0.1417649594630870-02
1.8999896E-01	-1.7987030E 01	-1.7753581414312390 01	4.4553452945206230-02	0.2515861261988230-02	0.2515861261988230-02
1.9999887E-01	-1.8028940E 01	-1.7782769803503260 01	6.4309320490744740-02	0.3674979911947010-02	0.3674979911947010-02
2.0999878E-01	-1.8070732E 01	-1.7812327305545260 01	6.5324957728083920-02	0.3674703765286770-02	0.3674703765286770-02
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CORRELATION OF FITTED DATA TO ORIGINAL DATA

VARIANCE = 3.1380924645761170-03
STANDARD DEVIATION = 5.6018679604004570-02

CORRELATION INDEX = 0.9796420042993660 00
MAXIMUM CORRELATION = 0.9801980198019800 00

NO REFIT CHECK MADE

INTRINSIC DIFFUSION AND VACANCY KIN.

MARKER PLANE POSITION, MICRONS= 426.0000
 MARKER PLANE COMP. AT FRAC V= 0.38045
 MARKER PLANE VELOCITY, CM/SEC= -0.36457E-07
 MARKER PLANE MOTION, MICRONS= -62.9976

AT MARKER PLANE COMP
 THERMODYNAMIC FACTOR= 0.73442E 00
 V TRACER DIFFUSION COEFFICIENT= 0.12605E-07
 TI TRACER DIFFUSION COEFFICIENT= 0.10112E-07

EXPERIMENTAL DETERMINATION AT MARKER PLANE
 INTERDIFFUSION COEFFICIENT= 0.10620E-07
 DARKEN ANALYSIS
 V INTRINSIC DIFFUSION COEFFICIENT= 0.12242E-07
 TI INTRINSIC DIFFUSION COEFFICIENT= 0.79781E-08
 HEUMANN ANALYSIS
 BASED ON CUMULATIVE FLUX GAIN
 V INTRINSIC DIFFUSION COEFFICIENT= 0.12242E-07
 TI INTRINSIC DIFFUSION COEFFICIENT= 0.79781E-08
 BASED ON CUMULATIVE FLUX LOSS
 V INTRINSIC DIFFUSION COEFFICIENT= 0.12242E-07
 TI INTRINSIC DIFFUSION COEFFICIENT= 0.79782E-08

DARKEN THEORETICAL CALCULATIONS AT MARKER PLANE
 INTERDIFFUSION COEFFICIENT= 0.85607E-08
 V INTRINSIC DIFFUSION COEFFICIENT= 0.92572E-08
 TI INTRINSIC DIFFUSION COEFFICIENT= 0.74246E-08
 VELOCITY OF MARKER PLANE, CM/SEC= -0.15652E-07
 MARKER PLANE MOTION, MICRONS= -27.0473

MANNING THEORETICAL CALCULATIONS AT MARKER PLANE
 INTERDIFFUSION COEFFICIENT= 0.85772E-08
 V INTRINSIC DIFFUSION COEFFICIENT= 0.95550E-08
 TI INTRINSIC DIFFUSION COEFFICIENT= 0.70375E-08
 VELOCITY OF MARKER PLANE, CM/SEC= -0.21522E-07
 MARKER PLANE MOTION, MICRONS= -37.1900

DAYANANDA CALCULATIONS AT MARKER PLANE
 VANADIUM MOBILITY= 0.56176E 05
 TITANIUM MOBILITY= 0.45067E 05
 VACANCY WIND FACTOR, ALPHA= 0.95910E-05
 VACANCY WIND FACTOR, ETA= 0.18191E-04
 VANADIUM PSI FACTOR= 1.0769
 TITANIUM PSI FACTOR= 0.8748
 V INTRINSIC DIFFUSION COEFFICIENT= 0.99753E-08
 TI INTRINSIC DIFFUSION COEFFICIENT= 0.65009E-08

INTERDIFFUSION COEFFICIENTS

TRACE COEFFICIENTS

AT PR V	V	TI	QVS/ITS	GAMMA V	GAMMA TI	PHI	S	D _{AB/PM}	D _{MAN/PM}
0.0	0.39000E-07	0.10922E-07	1.26414	1.75654	1.00000	1.00000	1.00000	0.39000E-07	0.39000E-07
0.01000	0.38715E-07	0.10219E-07	1.28049	1.73699	1.00006	0.98867	1.00023	0.38199E-07	0.38208E-07
0.02000	0.38301E-07	0.79531E-07	1.29609	1.71742	1.00023	0.97792	1.00050	0.37244E-07	0.37303E-07
0.03000	0.37851E-07	0.28877E-07	1.31099	1.69905	1.00051	0.96721	1.00080	0.36350E-07	0.36379E-07
0.04000	0.37365E-07	0.26199E-07	1.32597	1.68068	1.00090	0.95673	1.00115	0.35398E-07	0.35428E-07
0.05000	0.36846E-07	0.27530E-07	1.33934	1.66269	1.00141	0.94645	1.00152	0.34433E-07	0.34463E-07
0.06000	0.36295E-07	0.26868E-07	1.35085	1.64508	1.00203	0.93645	1.00192	0.33459E-07	0.33489E-07
0.07000	0.35712E-07	0.26212E-07	1.36244	1.62784	1.00276	0.92665	1.00234	0.32477E-07	0.32507E-07
0.08000	0.35102E-07	0.25562E-07	1.37310	1.61096	1.00361	0.91707	1.00274	0.31491E-07	0.31521E-07
0.09000	0.34464E-07	0.24920E-07	1.38301	1.59446	1.00457	0.90772	1.00309	0.30504E-07	0.30534E-07
0.10000	0.33801E-07	0.24244E-07	1.39193	1.57827	1.00565	0.89866	1.00349	0.29518E-07	0.29548E-07
0.11000	0.33115E-07	0.23566E-07	1.39989	1.56243	1.00684	0.88966	1.00395	0.28533E-07	0.28563E-07
0.12000	0.32408E-07	0.22835E-07	1.40689	1.54693	1.00817	0.88102	1.00441	0.27548E-07	0.27578E-07
0.13000	0.31681E-07	0.22055E-07	1.41292	1.53175	1.00957	0.87257	1.00490	0.26563E-07	0.26593E-07
0.14000	0.30938E-07	0.21218E-07	1.41799	1.51690	1.01110	0.86434	1.00548	0.25578E-07	0.25608E-07
0.15000	0.30179E-07	0.20322E-07	1.42205	1.50235	1.01276	0.85634	1.00606	0.24593E-07	0.24623E-07
0.16000	0.29406E-07	0.20614E-07	1.42509	1.48812	1.01453	0.84857	1.00664	0.23608E-07	0.23638E-07
0.17000	0.28622E-07	0.20046E-07	1.42715	1.47418	1.01641	0.84102	1.00722	0.22623E-07	0.22653E-07
0.18000	0.27829E-07	0.19486E-07	1.42819	1.46054	1.01842	0.83369	1.00780	0.21638E-07	0.21668E-07
0.19000	0.27029E-07	0.18925E-07	1.42819	1.44712	1.02054	0.82660	1.00838	0.20653E-07	0.20683E-07
0.20000	0.26223E-07	0.18374E-07	1.42715	1.43412	1.02274	0.81972	1.00896	0.19668E-07	0.19698E-07
0.21000	0.25414E-07	0.17833E-07	1.42513	1.42136	1.02514	0.81308	1.00954	0.18683E-07	0.18713E-07
0.22000	0.24603E-07	0.17300E-07	1.42209	1.40882	1.02764	0.80666	1.01012	0.17698E-07	0.17728E-07
0.23000	0.23791E-07	0.16776E-07	1.41804	1.39657	1.03035	0.80046	1.01070	0.16713E-07	0.16743E-07
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0.25000	0.22176E-07	0.15762E-07	1.40896	1.37286	1.03584	0.78874	1.01186	0.14743E-07	0.14773E-07
0.26000	0.21367E-07	0.15269E-07	1.40496	1.36138	1.03884	0.78322	1.01244	0.13758E-07	0.13788E-07
0.27000	0.20552E-07	0.14786E-07	1.39910	1.35015	1.04197	0.77792	1.01302	0.12773E-07	0.12803E-07
0.28000	0.19739E-07	0.14312E-07	1.39231	1.33917	1.04516	0.77285	1.01360	0.11788E-07	0.11818E-07
0.29000	0.19019E-07	0.13869E-07	1.38324	1.32842	1.04852	0.76804	1.01418	0.10803E-07	0.10833E-07
0.30000	0.18253E-07	0.13439E-07	1.37257	1.31791	1.05201	0.76359	1.01476	0.09818E-07	0.09848E-07
0.31000	0.17498E-07	0.12953E-07	1.35996	1.30763	1.05563	0.75949	1.01534	0.08833E-07	0.08863E-07
0.32000	0.16757E-07	0.12519E-07	1.34648	1.29752	1.05939	0.75582	1.01592	0.07848E-07	0.07878E-07
0.33000	0.16030E-07	0.12096E-07	1.33223	1.28775	1.06327	0.75269	1.01650	0.06863E-07	0.06893E-07
0.34000	0.15318E-07	0.11683E-07	1.31713	1.27814	1.06729	0.74976	1.01708	0.05878E-07	0.05908E-07
0.35000	0.14621E-07	0.11280E-07	1.29925	1.26876	1.07145	0.74716	1.01766	0.04893E-07	0.04923E-07
0.36000	0.13941E-07	0.10886E-07	1.28064	1.25955	1.07574	0.74460	1.01824	0.03908E-07	0.03938E-07
0.37000	0.13278E-07	0.10502E-07	1.26131	1.25057	1.08014	0.73734	1.01882	0.02923E-07	0.02953E-07
0.38000	0.12631E-07	0.10128E-07	1.24173	1.24180	1.08475	0.73454	1.01940	0.01938E-07	0.01968E-07
0.39000	0.12007E-07	0.97635E-07	1.22065	1.23322	1.08947	0.73195	1.02000	0.00953E-07	0.00983E-07
0.40000	0.11399E-07	0.94047E-07	1.21138	1.22486	1.09433	0.72948	1.02060	0.00968E-07	0.00998E-07
0.41000	0.10812E-07	0.90546E-07	1.19252	1.21666	1.09934	0.72746	1.02120	0.00983E-07	0.01013E-07
0.42000	0.10240E-07	0.87249E-07	1.17314	1.20866	1.10444	0.72553	1.02180	0.00998E-07	0.01028E-07
0.43000	0.96907E-07	0.84026E-07	1.15324	1.20086	1.10974	0.72384	1.02240	0.01013E-07	0.01043E-07
0.44000	0.91546E-07	0.80844E-07	1.13285	1.19326	1.11524	0.72237	1.02300	0.01028E-07	0.01058E-07
0.45000	0.86381E-07	0.77733E-07	1.11204	1.18580	1.12084	0.72117	1.02360	0.01043E-07	0.01073E-07
0.46000	0.81326E-07	0.74787E-07	1.09085	1.17854	1.12660	0.72012	1.02420	0.01058E-07	0.01088E-07
0.47000	0.76381E-07	0.71874E-07	1.06924	1.17146	1.13260	0.71913	1.02480	0.01073E-07	0.01103E-07
0.48000	0.71538E-07	0.69063E-07	1.04747	1.16455	1.13860	0.71847	1.02540	0.01088E-07	0.01118E-07
0.49000	0.66804E-07	0.66312E-07	1.02526	1.15781	1.14464	0.71784	1.02600	0.01103E-07	0.01133E-07
0.50000	0.62186E-07	0.63636E-07	1.00284	1.15124	1.15124	0.71733	1.02660	0.01118E-07	0.01148E-07
0.51000	0.57695E-07	0.61084E-07	0.98073	1.14484	1.15781	0.71683	1.02720	0.01133E-07	0.01163E-07
0.52000	0.53311E-07	0.58544E-07	0.94947	1.13860	1.16455	0.71677	1.02780	0.01148E-07	0.01178E-07

0.53000	0.52484F-08	0.55901E-08	0.93888	1.13252	1.17146	0.71913	1.00037	0.39044F-09	0.19070F-08
0.53400	0.47324F-08	0.53340E-08	0.91908	1.12661	1.17854	0.72012	1.00066	0.36491F-08	0.17006F-08
0.55000	0.45728E-08	0.50808E-08	0.90000	1.12684	1.18580	0.72113	1.00103	0.36491F-08	0.15027F-08
0.56000	0.42595E-08	0.48315E-08	0.88161	1.11524	1.19324	0.72313	1.00146	0.33084F-08	0.13112F-08
0.57000	0.39622E-08	0.45866E-08	0.86387	1.10574	1.20046	0.72346	1.00196	0.31254F-08	0.11117F-08
0.58000	0.36855E-08	0.43446E-08	0.84636	1.10448	1.20866	0.72533	1.00252	0.29506F-08	0.09580F-08
0.59000	0.34141E-08	0.41120E-08	0.83028	1.09933	1.21666	0.72744	1.00312	0.27831F-08	0.07918F-08
0.60000	0.31624E-08	0.38835E-08	0.81437	1.09433	1.22484	0.72954	1.00377	0.26210F-08	0.06248F-08
0.61000	0.29254E-08	0.36614E-08	0.79905	1.08947	1.23322	0.73195	1.00446	0.24699F-08	0.04600F-08
0.62000	0.27026E-08	0.34461E-08	0.78425	1.08475	1.24179	0.73454	1.00511	0.23188F-08	0.03121F-08
0.63000	0.24931E-08	0.32379E-08	0.76949	1.08017	1.25057	0.73734	1.00581	0.21643F-08	0.02045F-08
0.64000	0.22967E-08	0.30370E-08	0.75623	1.07574	1.25959	0.74040	1.00647	0.20191F-08	0.01438F-08
0.65000	0.21129E-08	0.28438E-08	0.74288	1.07145	1.26874	0.74367	1.00714	0.18739F-08	0.01048F-08
0.66000	0.19410E-08	0.26593E-08	0.73018	1.06729	1.27814	0.74716	1.00781	0.17382F-08	0.01818F-08
0.67000	0.17807E-08	0.24804E-08	0.71784	1.06327	1.28775	0.75088	1.00849	0.16042F-08	0.01704E-08
0.68000	0.16313E-08	0.23108E-08	0.70594	1.05939	1.29754	0.75482	1.00916	0.14801F-08	0.01595F-08
0.69000	0.14924E-08	0.21490E-08	0.69446	1.05563	1.30763	0.75899	1.00981	0.13669F-08	0.014921F-08
0.70000	0.13634E-08	0.19951E-08	0.68340	1.05201	1.31791	0.76339	1.01047	0.12593F-08	0.01306F-08
0.71000	0.12439E-08	0.18490E-08	0.67273	1.04852	1.32842	0.76801	1.01121	0.11572F-08	0.01212F-08
0.72000	0.11333E-08	0.17107E-08	0.66245	1.04516	1.33917	0.77285	1.01257	0.10597F-08	0.01128F-08
0.73000	0.10311E-08	0.15801E-08	0.65253	1.04192	1.35015	0.77792	1.01370	0.09678F-08	0.010494F-08
0.74000	0.93675E-08	0.14569E-08	0.64298	1.03882	1.36134	0.78327	1.01479	0.08808F-08	0.097461F-08
0.75000	0.84889E-08	0.13410E-08	0.63378	1.03584	1.37286	0.78874	1.01532	0.07995F-08	0.09061F-08
0.76000	0.77002E-08	0.12322E-08	0.62491	1.03298	1.38454	0.79444	1.01587	0.07249F-08	0.08374F-08
0.77000	0.69670E-08	0.11303E-08	0.61637	1.03025	1.39657	0.80044	1.01609	0.06501F-08	0.07748F-08
0.78000	0.62947E-08	0.10351E-08	0.60814	1.02764	1.40882	0.80665	1.01587	0.05767F-08	0.07145F-08
0.79000	0.56794E-08	0.94623E-08	0.60023	1.02516	1.42133	0.81307	1.01609	0.05041F-08	0.06534F-08
0.80000	0.51174E-08	0.86353E-08	0.59262	1.02279	1.43412	0.81972	1.01624	0.04322F-08	0.05908F-08
0.81000	0.46045E-08	0.78672E-08	0.58527	1.02054	1.44719	0.82661	1.01630	0.03608F-08	0.05280F-08
0.82000	0.41373E-08	0.71550E-08	0.57823	1.01842	1.46044	0.83369	1.01628	0.02904F-08	0.04647F-08
0.83000	0.37122E-08	0.64962E-08	0.57145	1.01641	1.47414	0.84097	1.01617	0.02202F-08	0.04022F-08
0.84000	0.33263E-08	0.58879E-08	0.56493	1.01453	1.48814	0.84857	1.01597	0.01502F-08	0.03399F-08
0.85000	0.29764E-08	0.53275E-08	0.55868	1.01276	1.50235	0.85634	1.01567	0.00809F-08	0.02781F-08
0.86000	0.26595E-08	0.48121E-08	0.55267	1.01110	1.51689	0.86434	1.01528	0.00122F-08	0.02161F-08
0.87000	0.23731E-08	0.43392E-08	0.54691	1.00957	1.53175	0.87257	1.01479	0.00056F-08	0.01505F-08
0.88000	0.21147E-08	0.39060E-08	0.54139	1.00815	1.54693	0.88099	1.01419	0.00016F-08	0.00843F-08
0.89000	0.18817E-08	0.35101E-08	0.53609	1.00684	1.56243	0.88969	1.01344	0.00000F-08	0.00183F-08
0.90000	0.16721E-08	0.31489E-08	0.53102	1.00565	1.57826	0.89854	1.01267	0.00000F-08	0.00000F-08
0.91000	0.14830E-08	0.28200E-08	0.52618	1.00457	1.59444	0.90772	1.01174	0.00000F-08	0.00000F-08
0.92000	0.13149E-08	0.25212E-08	0.52195	1.00361	1.61096	0.91707	1.01070	0.00000F-08	0.00000F-08
0.93000	0.11636E-08	0.22501E-08	0.51712	1.00274	1.62786	0.92645	1.00954	0.00000F-08	0.00000F-08
0.94000	0.10283E-08	0.20048E-08	0.51291	1.00203	1.64508	0.93645	1.00826	0.00000F-08	0.00000F-08
0.95000	0.90745E-08	0.17831E-08	0.50891	1.00141	1.66269	0.94644	1.00686	0.00000F-08	0.00000F-08
0.96000	0.79970E-08	0.15833E-08	0.50509	1.00090	1.68068	0.95671	1.00533	0.00000F-08	0.00000F-08
0.97000	0.70376E-08	0.14034E-08	0.50147	1.00051	1.69905	0.96721	1.00364	0.00000F-08	0.00000F-08
0.98000	0.61848E-08	0.12418E-08	0.49803	1.00023	1.71782	0.97792	1.00191	0.00000F-08	0.00000F-08
0.99000	0.54277E-08	0.10970E-08	0.49478	1.00006	1.73699	0.98864	1.00000	0.00000F-08	0.00000F-08
1.00000	0.47568E-08	0.96739E-08	0.49177	1.00000	1.75657	1.00000	1.00000	0.00000F-08	0.00000F-08

INTRINSIC COEFFICIENTS

AT 14 V	IV UG-4 KEV	ON MANNING	DTI MANNING	OV/DTI DARLEN	OV/DTI MANNING	1+VI	1+V2
0.0	0.39040E-07	0.59390E-07	0.30922E-07	0.27847E-07	1.26414	1.00000	0.90089
0.31000	0.38283E-07	0.58323E-07	0.29897E-07	0.26791E-07	1.28046	1.00105	0.89610
0.62000	0.37455E-07	0.57335E-07	0.28899E-07	0.25711E-07	1.29609	1.00221	0.89176
0.93000	0.36610E-07	0.56311E-07	0.27926E-07	0.24794E-07	1.31099	1.00447	0.88789
0.00000	0.35749E-07	0.55321E-07	0.26979E-07	0.23860E-07	1.32507	1.00682	0.88441
0.00000	0.34874E-07	0.54309E-07	0.26051E-07	0.22966E-07	1.33838	1.00924	0.88138
0.00000	0.33988E-07	0.53271E-07	0.25095E-07	0.22111E-07	1.35085	1.01174	0.87880
0.00000	0.33094E-07	0.52208E-07	0.24280E-07	0.21293E-07	1.36244	1.01428	0.87665
0.00000	0.32191E-07	0.51121E-07	0.23442E-07	0.20510E-07	1.37319	1.01688	0.87490
0.00000	0.31284E-07	0.50015E-07	0.22602E-07	0.19760E-07	1.38301	1.01950	0.87357
0.10000	0.30373E-07	0.48890E-07	0.21761E-07	0.19042E-07	1.39193	1.02214	0.87263
0.10000	0.29458E-07	0.47745E-07	0.20928E-07	0.18354E-07	1.40084	1.02481	0.87208
0.10000	0.28539E-07	0.46580E-07	0.20101E-07	0.17695E-07	1.40984	1.02750	0.87190
0.10000	0.27616E-07	0.45395E-07	0.19280E-07	0.17062E-07	1.41799	1.03024	0.87207
0.10000	0.26689E-07	0.44190E-07	0.18458E-07	0.16455E-07	1.42205	1.03296	0.87340
0.10000	0.25758E-07	0.42965E-07	0.17635E-07	0.15873E-07	1.42509	1.03564	0.87455
0.10000	0.24823E-07	0.41720E-07	0.16810E-07	0.15313E-07	1.42715	1.03827	0.87597
0.10000	0.23884E-07	0.40465E-07	0.16000E-07	0.14775E-07	1.42818	1.04083	0.87768
0.10000	0.22941E-07	0.39190E-07	0.15200E-07	0.14261E-07	1.42818	1.04341	0.87965
0.10000	0.21994E-07	0.37905E-07	0.14410E-07	0.13761E-07	1.42715	1.04593	0.88187
0.20000	0.21044E-07	0.36610E-07	0.13630E-07	0.13282E-07	1.42513	1.04839	0.88431
0.20000	0.20091E-07	0.35305E-07	0.12860E-07	0.12822E-07	1.42209	1.05079	0.88686
0.20000	0.19134E-07	0.34000E-07	0.12100E-07	0.12378E-07	1.41804	1.05311	0.88981
0.20000	0.18173E-07	0.32695E-07	0.11350E-07	0.11950E-07	1.41300	1.05534	0.89284
0.20000	0.17208E-07	0.31390E-07	0.10600E-07	0.11538E-07	1.40796	1.05750	0.89605
0.20000	0.16240E-07	0.30085E-07	0.09850E-07	0.11140E-07	1.40296	1.05959	0.89940
0.20000	0.15269E-07	0.28780E-07	0.09100E-07	0.10756E-07	1.39796	1.06159	0.90290
0.20000	0.14294E-07	0.27475E-07	0.08350E-07	0.10388E-07	1.39291	1.06359	0.90653
0.20000	0.13315E-07	0.26170E-07	0.07600E-07	0.10027E-07	1.38784	1.06559	0.91027
0.20000	0.12332E-07	0.24865E-07	0.06850E-07	0.96818E-08	1.38278	1.06759	0.91411
0.20000	0.11347E-07	0.23560E-07	0.06100E-07	0.93478E-08	1.37774	1.06959	0.91805
0.20000	0.10360E-07	0.22255E-07	0.05350E-07	0.90252E-08	1.37265	1.07159	0.92207
0.20000	0.09371E-07	0.20950E-07	0.04600E-07	0.87146E-08	1.36759	1.07359	0.92616
0.20000	0.08380E-07	0.19645E-07	0.03850E-07	0.84135E-08	1.36253	1.07559	0.93032
0.20000	0.07387E-07	0.18340E-07	0.03100E-07	0.81207E-08	1.35747	1.07759	0.93453
0.20000	0.06394E-07	0.17035E-07	0.02350E-07	0.78391E-08	1.35241	1.07959	0.93879
0.20000	0.05400E-07	0.15730E-07	0.01600E-07	0.75667E-08	1.34730	1.08159	0.94308
0.20000	0.04406E-07	0.14425E-07	0.00850E-07	0.73033E-08	1.34224	1.08359	0.94741
0.20000	0.03412E-07	0.13120E-07	0.00100E-07	0.70484E-08	1.33719	1.08559	0.95176
0.20000	0.02418E-07	0.11815E-07	0.00000E-07	0.68022E-08	1.33214	1.08759	0.95612
0.20000	0.01424E-07	0.10510E-07	0.00000E-07	0.65639E-08	1.32709	1.08959	0.96050
0.20000	0.00430E-07	0.09205E-07	0.00000E-07	0.63335E-08	1.32204	1.09159	0.96487
0.20000	0.00000E-07	0.07900E-07	0.00000E-07	0.61100E-08	1.31700	1.09359	0.96925
0.20000	0.00000E-07	0.06595E-07	0.00000E-07	0.58915E-08	1.31200	1.09559	0.97362
0.20000	0.00000E-07	0.05290E-07	0.00000E-07	0.56730E-08	1.30700	1.09759	0.97798
0.20000	0.00000E-07	0.03985E-07	0.00000E-07	0.54545E-08	1.30200	1.09959	0.98233
0.20000	0.00000E-07	0.02680E-07	0.00000E-07	0.52360E-08	1.29700	1.10159	0.98668
0.20000	0.00000E-07	0.01375E-07	0.00000E-07	0.50175E-08	1.29200	1.10359	0.99095
0.20000	0.00000E-07	0.00000E-07	0.00000E-07	0.47990E-08	1.28700	1.10559	0.99522
0.20000	0.00000E-07	0.00000E-07	0.00000E-07	0.45805E-08	1.28200	1.10759	0.99947
0.20000	0.00000E-07	0.00000E-07	0.00000E-07	0.43620E-08	1.27700	1.10959	1.00358
 						

0.51000	0.37.54E-08	0.17274E-03	0.40211E-08	0.40649E-08	0.93988	0.01645	0.98744	1.01114
0.54000	0.3510E-08	0.1469E-08	0.18611E-08	0.18972E-08	0.91908	0.08012	0.79285	1.01460
0.57000	0.3291E-08	0.1229E-08	0.16640E-08	0.16640E-08	0.3279E-08	0.32070	0.86489	1.01747
0.60000	0.30770E-08	0.99450E-08	0.14902E-08	0.14902E-08	0.35633E-08	0.88161	0.84052	1.02091
0.63000	0.28680E-08	0.27773E-08	0.37190E-08	0.37190E-08	0.33990E-08	0.86387	0.81715	1.02381
0.66000	0.26703E-08	0.25720E-08	0.31536E-08	0.31536E-08	0.32772E-08	0.84676	0.79470	1.02651
0.69000	0.24834E-08	0.23790E-08	0.29912E-08	0.29912E-08	0.30700E-08	0.83024	0.77319	1.02902
0.72000	0.23074E-08	0.2198E-08	0.28133E-08	0.28133E-08	0.29222E-08	0.81631	0.75249	1.03144
0.75000	0.21414E-08	0.20291E-08	0.26799E-08	0.26799E-08	0.27694E-08	0.79904	0.73261	1.03352
0.78000	0.19832E-08	0.18701E-08	0.25313E-08	0.25313E-08	0.26212E-08	0.78625	0.71347	1.03551
0.81000	0.18383E-08	0.17214E-08	0.23875E-08	0.23875E-08	0.24766E-08	0.76989	0.69507	1.03735
0.84000	0.17005E-08	0.15823E-08	0.22466E-08	0.22466E-08	0.23365E-08	0.75623	0.67735	1.03951
0.87000	0.15717E-08	0.14530E-08	0.21146E-08	0.21146E-08	0.22003E-08	0.74298	0.66010	1.04188
0.90000	0.14502E-08	0.13321E-08	0.19862E-08	0.19862E-08	0.20693E-08	0.73014	0.64395	1.04408
0.93000	0.13371E-08	0.12201E-08	0.18626E-08	0.18626E-08	0.19429E-08	0.71784	0.62799	1.04618
0.96000	0.12314E-08	0.11159E-08	0.17443E-08	0.17443E-08	0.18213E-08	0.70594	0.61270	1.04813
0.99000	0.11327E-08	0.10192E-08	0.16311E-08	0.16311E-08	0.17045E-08	0.69446	0.59797	1.05004
1.00000	0.10400E-08	0.92963E-08	0.15230E-08	0.15230E-08	0.15928E-08	0.68340	0.58366	1.05179
0.10000	0.95333E-09	0.84982E-09	0.14201E-08	0.14201E-08	0.14860E-08	0.67271	0.56988	1.05349
0.20000	0.8754E-09	0.77034E-09	0.13221E-08	0.13221E-08	0.13841E-08	0.66245	0.55657	1.05505
0.30000	0.80208E-09	0.69979E-09	0.12292E-08	0.12292E-08	0.12871E-08	0.65253	0.54367	1.05647
0.40000	0.7356E-09	0.63483E-09	0.11311E-08	0.11311E-08	0.11951E-08	0.64278	0.53121	1.05774
0.50000	0.67034E-09	0.57409E-09	0.10377E-08	0.10377E-08	0.11070E-08	0.63314	0.51914	1.05886
0.60000	0.61177E-09	0.52023E-09	0.97898E-09	0.97898E-09	0.10252E-08	0.62491	0.50743	1.05984
0.70000	0.55767E-09	0.46994E-09	0.90477E-09	0.90477E-09	0.94728E-09	0.61637	0.49610	1.06069
0.80000	0.50774E-09	0.42389E-09	0.83494E-09	0.83494E-09	0.87386E-09	0.60814	0.48509	1.06142
0.90000	0.46174E-09	0.38181E-09	0.76836E-09	0.76836E-09	0.80478E-09	0.60021	0.47441	1.06204
0.95000	0.4194E-09	0.3433E-09	0.70745E-09	0.70745E-09	0.73998E-09	0.59262	0.46406	1.06255
0.98000	0.38060E-09	0.30836E-09	0.65030E-09	0.65030E-09	0.67928E-09	0.58527	0.45397	1.06297
0.99000	0.34492E-09	0.27649E-09	0.59650E-09	0.59650E-09	0.62489E-09	0.57821	0.44414	1.06334
0.99500	0.31220E-09	0.24743E-09	0.54634E-09	0.54634E-09	0.56952E-09	0.57164	0.43463	1.06367
0.99800	0.28276E-09	0.22126E-09	0.49963E-09	0.49963E-09	0.52029E-09	0.56403	0.42544	1.06395
0.99900	0.2548E-09	0.19746E-09	0.45622E-09	0.45622E-09	0.47435E-09	0.55664	0.41624	1.06419
0.99950	0.22987E-09	0.17493E-09	0.41593E-09	0.41593E-09	0.43143E-09	0.54967	0.40745	1.06440
0.99980	0.20707E-09	0.15451E-09	0.37862E-09	0.37862E-09	0.39243E-09	0.54291	0.39883	1.06458
0.99990	0.18631E-09	0.13908E-09	0.34413E-09	0.34413E-09	0.35604E-09	0.53609	0.39041	1.06472
0.99995	0.16742E-09	0.12324E-09	0.31229E-09	0.31229E-09	0.32248E-09	0.52969	0.38216	1.06483
0.99998	0.15024E-09	0.10908E-09	0.28296E-09	0.28296E-09	0.29157E-09	0.52310	0.37411	1.06491
0.99999	0.13469E-09	0.96379E-10	0.25498E-09	0.25498E-09	0.26318E-09	0.51618	0.36621	1.06496
0.999995	0.12059E-09	0.85008E-10	0.23121E-09	0.23121E-09	0.23716E-09	0.50915	0.35847	1.06499
0.999998	0.10742E-09	0.74844E-10	0.20831E-09	0.20831E-09	0.21331E-09	0.50217	0.35087	1.06500
0.999999	0.96293E-10	0.65770E-10	0.18473E-09	0.18473E-09	0.19154E-09	0.49591	0.34340	1.06500
0.9999995	0.8588E-10	0.57703E-10	0.16473E-09	0.16473E-09	0.17186E-09	0.48941	0.33610	1.06500
0.9999998	0.7651E-10	0.50523E-10	0.15146E-09	0.15146E-09	0.15932E-09	0.48309	0.32949	1.06500
0.9999999	0.6804E-10	0.44192E-10	0.13574E-09	0.13574E-09	0.14372E-09	0.47681	0.32317	1.06500
0.99999995	0.6048E-10	0.38508E-10	0.12144E-09	0.12144E-09	0.12734E-09	0.47061	0.31675	1.06500
0.99999998	0.5367E-10	0.33517E-10	0.10846E-09	0.10846E-09	0.10899E-09	0.46454	0.31073	1.06500
0.99999999	0.4768E-10	0.29117E-10	0.96879E-10	0.96879E-10	0.96739E-10	0.45874	0.30499	1.06500
0.999999995					1E-10	0.45312	0.29944	1.06500
0.999999998					1E-10	0.44761	0.29401	1.06500
0.999999999					1E-10	0.44219	0.28869	1.06500
0.9999999995					1E-10	0.43686	0.28347	1.06500
0.9999999998					1E-10	0.43161	0.27834	1.06500
0.9999999999					1E-10	0.42644	0.27331	1.06500
0.99999999995					1E-10	0.42134	0.26837	1.06500
0.99999999998					1E-10	0.41631	0.26352	1.06500
0.99999999999					1E-10	0.41134	0.25876	1.06500
0.999999999995					1E-10	0.40644	0.25409	1.06500
0.999999999998					1E-10	0.40164	0.24950	1.06500
0.999999999999					1E-10	0.39691	0.24500	1.06500
0.9999999999995					1E-10	0.39224	0.24059	1.06500
0.9999999999998					1E-10	0.38764	0.23626	1.06500
0.9999999999999					1E-10	0.38311	0.23200	1.06500
0.99999999999995					1E-10	0.37864	0.22781	1.06500
0.99999999999998					1E-10	0.37424	0.22369	1.06500
0.99999999999999					1E-10	0.36991	0.21964	1.06500
0.999999999999995					1E-10	0.36564	0.21566	1.06500
0.999999999999998					1E-10	0.36144	0.21174	1.06500
0.999999999999999					1E-10	0.35731	0.20787	1.06500
0.9999999999999995					1E-10	0.35324	0.20404	1.06500
0.9999999999999998					1E-10	0.34924	0.20026	1.06500
0.9999999999999999					1E-10	0.34531	0.19654	1.06500
0.99999999999999995					1E-10	0.34144	0.19287	1.06500
0.99999999999999998					1E-10	0.33764	0.18926	1.06500
0.99999999999999999					1E-10	0.33391	0.18571	1.06500
0.999999999999999995					1E-10	0.33024	0.18221	1.06500
0.999999999999999998					1E-10	0.32664	0.17876	1.06500
0.999999999999999999					1E-10	0.32311	0.17536	1.06500
0.9999999999999999995					1E-10	0.31964	0.17200	1.06500
0.9999999999999999998					1E-10	0.31624	0.16869	1.06500
0.9999999999999999999					1E-10	0.31291	0.16544	1.06500
0.99999999999999999995					1E-10	0.30964	0.16224	1.06500
0.99999999999999999998					1E-10	0.30644	0.15909	1.06500
0.99999999999999999999					1E-10	0.30331	0.15600	1.06500
0.999999999999999999995					1E-10	0.30024	0.15300	1.06500
0.999999999999999999998					1E-10	0.29724	0.15006	1.06500
0.999999999999999999999					1E-10	0.29431	0.14719	1.06500
0.9999999999999999999995					1E-10	0.29144	0.14439	1.06500
0.9999999999999999999998					1E-10	0.28864	0.14164	1.06500
0.9999999999999999999999					1E-10	0.28591	0.13894	1.06500
0.99999999999999999999995					1E-10	0.28324	0.13629	1.06500
0.99999999999999999999998					1E-10	0.28064	0.13369	1.06500
0.99999999999999999999999					1E-10	0.27811	0.13114	1.06500
0.999999999999999999999995					1E-10	0.27564	0.12864	1.06500
0.999999999999999999999998					1E-10	0.27324	0.12619	1.06500
0.999999999999999999999999					1E-10	0.27091	0.12379	1.06500
0.9999999999999999999999995					1E-10	0.26864	0.12144	1.06500
0.9999999999999999999999998					1E-10	0.26644	0.11914	1.06500
0.9999999999999999999999999					1E-10	0.26431	0.11689	1.06500
0.99999999999999999999999995					1E-10	0.26224	0.11469	1.06500
0.99999999999999999999999998					1E-10	0.26024	0.11254	1.06500
0.99999999999999999999999999					1E-10	0.25831	0.11044	1.06500
0.999999999999999999999999995					1E-10	0.25644	0.10839	1.06500
0.999999999999999999999999998					1E-10	0.25464	0.10639	1.06500
0.999999999999999999999999999					1E-10	0.25291	0.10444	1.06500
0.9999999999999999999999999995					1E-10	0.25124	0.10254	1.06500
0.9999999999999999999999999998					1E-10	0.24964	0.10069	1.06500
0.9999999999999999999999999999					1E-10	0.24811	0.09889	1.06500
0.99999999999999999999999999995					1E-10	0.24664	0.09714	1.06500
0.99999999999999999999999999998					1E-10	0.24524	0.09544	1.06500
0.99999999999999999999999999999					1E-10	0.24391	0.09379	1.06500

Fig. G4. Computed $u(x)$ curve fitted to the experimental data points with the use of FITLPS.

Fig. G5. Regenerated vanadium concentration profile determined from the computed $u(x)$ curve of Fig. G4.

Fig. G6. Regenerated titanium concentration profile determined from the computed $u(x)$ curve of Fig. G4.

Fig. G7. Interdiffusion coefficients in V-Ti alloys, determined experimentally and from the theories of Darken and Manning, as functions of vanadium composition.

The final sample problem presented in the following appendix demonstrates the manner in which MATANØ is used to output the corrected intensities of the particular set of alloy standards used for calibration of the electron microprobe. The actual least squares fit of the curves of $(1-K_i)/K_i$ versus $(1-C_i)/C_i$ or K_i versus C_i should be done separately on a desk computer. The sole purpose of this aspect of MATANØ is to portray conveniently the calibration curves for the user so he may then select the appropriate mathematical expression which best fits the individual data points. As in the two previous examples, the data used here is excerpted from a study of interdiffusion and intrinsic diffusion in the vanadium-titanium system;⁸ therefore, the intensities and concentrations tabulated on the following input and output sheets reflect the nine binary V-Ti alloy standards used in this investigation.

It is important to note in the following input sheet that since $N7=0$ and $N14=1$, cards 5 and 13-15 are not included (see section on Input Data Format). Also, the alloy compositions of V and Ti expressed in weight fraction are included in columns 56-60 and 66-70, respectively.

Card Column

1-9	10-19	20-29	30-39	40-49	50-59	60-69	70-79	80-89	90-99	100-109	110-119	120-129	130-139	140-149	150-159	160-169	170-179	180-189	190-199	200-209	210-219	220-229	230-239	240-249	250-259	260-269	270-279	280-289	290-299	300-309	310-319	320-329	330-339	340-349	350-359	360-369	370-379	380-389	390-399	400-409	410-419	420-429	430-439	440-449	450-459	460-469	470-479	480-489	490-499	500-509	510-519	520-529	530-539	540-549	550-559	560-569	570-579	580-589	590-599	600-609	610-619	620-629	630-639	640-649	650-659	660-669	670-679	680-689	690-699	700-709	710-719	720-729	730-739	740-749	750-759	760-769	770-779	780-789	790-799	800-809	810-819	820-829	830-839	840-849	850-859	860-869	870-879	880-889	890-899	900-909	910-919	920-929	930-939	940-949	950-959	960-969	970-979	980-989	990-999
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	

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Fig. H1. Microprobe calibration plot showing K_V versus C_V .

Fig. H2. Microprobe calibration plot showing K_{T1} versus C_{T1} .

Fig. H3. Microprobe calibration plot showing $\frac{(1-K_V)}{K_V}$ versus $(1-C_V)/C_V$.

Fig. H4. Microprobe calibration plot showing $(1-K_{Ti})/K_{Ti}$ versus $(1-C_{Ti})/C_{Ti}$.

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C
C   CARRY OUT MATRIX MULTIPLICATIONS FOR A-TRANSPOSE
C
15X 0150      500 D1 930  N=1,N5
15X 0159      D1 510  L=1,M1
15X 0160      V(L) = V*(N,L)
15X 0161      510 CONTINUE
15X 0162      D1 850  JJ=1,N5

C
C   FORM MATRIX (D,D,L,N) BY 4 SEPARATE TECHNIQUES
C
15X 0163      IF(N,NF,1) GO TO 550
15X 0165      NDUM=1
15X 0166      IF(JJ,NF,1) GO TO 530
15X 0168      JDDUM=1
15X 0169      SIGN = 1.00
15X 0170      GO TO 570
15X 0171      530 IF(JJ,NF,N5) GO TO 540
15X 0173      JDDUM=NS-1
15X 0174      SIGN = -1.00
15X 0175      GO TO 570
15X 0176      540 SIGN=1.00
15X 0177      GO TO 570
15X 0178      550 IF(N,NF,N5) GO TO 560
15X 0180      NDUM=NS-1
15X 0181      IF(JJ,NF,1) GO TO 560
15X 0183      JDDUM=1
15X 0184      SIGN = -1.00
15X 0185      GO TO 570
15X 0186      560 IF(JJ,NF,N5) GO TO 563
15X 0188      JDDUM=NS-1
15X 0189      SIGN = 1.00
15X 0190      GO TO 570
15X 0191      563 IF (JJ,NF,1) GO TO 562
15X 0193      JDDUM = 1
15X 0194      SIGN = 1.00
15X 0195      GO TO 610
15X 0196      562 IF (JJ,NF,N5) GO TO 680
15X 0198      JDDUM = NS-1
15X 0199      SIGN = -1.00
15X 0200      GO TO 610
15X 0201      564 SIGN = -1.00
15X 0202      GO TO 630

C
15X 0203      570 D1 590  L=1,M1
15X 0204      D1 590  J=1,M1
15X 0205      T(L,J) = 0.00
15X 0206      D1 590  K=1,M1
15X 0207      T(L,J) = T(L,J)+C(JDDUM,K,1)*N*(NDUM,K,J)
15X 0208      580 CONTINUE
15X 0209      590 CONTINUE

C
15X 0210      D1 610  L=1,M1
15X 0211      D1 605  J=1,M1
15X 0212      T(L,J) = 0.00
15X 0213      D1 600  K=1,M1
15X 0214      T(L,J) = T(L,J) + T(L,K)*C(NDUM,K,J)
15X 0215      600 CONTINUE

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1SN 0216      TT(I,J)= TT(I,J)*SIGN
1SN 0217      605 CONTINUE
1SN 0218      610 CONTINUE
1SN 0219      GO TO 800
C
1SN 0220      615 DO 617 I=1,MM
1SN 0221      DO 616 J=1,M1
1SN 0222      TT(I,J)= 0.00
1SN 0223      DO 616 K=1,MM
1SN 0224      TT(I,J)= TT(I,J)+BINV(JDUM,N,I,K)*C(N,K,J)-PINV(JDUM,N-I,I,K)*
1          C(N-I,K,J)
1SN 0225      616 CONTINUE
1SN 0226      617 CONTINUE
C
1SN 0227      DO 620 I=1,M1
1SN 0228      DO 619 J=1,M1
1SN 0229      TT(I,J)= 0.00
1SN 0230      DO 618 K=1,MM
1SN 0231      TT(I,J)= TT(I,J)+C(JDUM,K,I)*T(K,J)
1SN 0232      618 CONTINUE
1SN 0233      TT(I,J)= TT(I,J)*SIGN
1SN 0234      619 CONTINUE
1SN 0235      620 CONTINUE
1SN 0236      GO TO 800
C
1SN 0237      630 DO 650 I=1,M1
1SN 0238      DO 640 J=1,MM
1SN 0239      TT(I,J)= 0.00
1SN 0240      DO 640 K=1,MM
1SN 0241      TT(I,J)= TT(I,J)+C(IJ,J,K)*BINV(IJ,NDUM,K,J)-C(IJ-J-I,K,I)*
1          BINV(IJ-J-I,NDUM,K,J)
1SN 0242      640 CONTINUE
1SN 0243      650 CONTINUE
C
1SN 0244      DO 670 I=1,M1
1SN 0245      DO 665 J=1,M1
1SN 0246      TT(I,J)= 0.00
1SN 0247      DO 660 K=1,MM
1SN 0248      TT(I,J)= TT(I,J)+T(I,K)*C(NDUM,K,J)
1SN 0249      660 CONTINUE
1SN 0250      TT(I,J)= TT(I,J)*SIGN
1SN 0251      665 CONTINUE
1SN 0252      670 CONTINUE
1SN 0253      GO TO 800
C
1SN 0254      680 DO 700 I=1,M1
1SN 0255      DO 690 J=1,MM
1SN 0256      TT(I,J)= 0.00
1SN 0257      DO 690 K=1,MM
1SN 0258      TT(I,J)= TT(I,J)+C(IJ-J-I,K,I)*BINV(IJ-J-I,N-I,K,J)-C(IJ,K,I)*
1          BINV(IJ,N-I,K,J)
1SN 0259      690 CONTINUE
1SN 0260      700 CONTINUE
C
1SN 0261      DO 720 I=1,M1
1SN 0262      DO 710 J=1,M1
1SN 0263      TT(I,J)= 0.00
1SN 0264      DO 710 K=1,MM

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		TT(I,J)= TT(I,J)+T(I,K)*C(I,K,J)	319
15X 0265	710 CONTINUE		320
15X 0267	720 CONTINUE		321
			323
15X 0269	73 J=I,M1		324
15X 0270	74 J=J+1,M1		325
15X 0271	TT(I,J)= 0.0		326
15X 0273	75 J=K+1,M1		327
15X 0275	TT(I,J)= TT(I,J)+C(JJ,K,I)*INV(JJ,N,K,J)-C(JJ-1,K,I)*		328
		INV(JJ-1,N,K,J)	329
15X 0277	730 CONTINUE		330
15X 0279	740 CONTINUE		331
			333
15X 0279	75 J=I+1,M1		334
15X 0276	76 J=J+1,M1		335
15X 0277	77 J=K+1,M1		336
15X 0279	TT(I,J)= TT(I,J)+T(I,K)*C(N,K,J)		337
15X 0279	750 CONTINUE		338
15X 0280	760 CONTINUE		340
			341
		MATRIX D(JJ,N) IS STORED IN TT	342
			343
15X 0281	800 I=420 I+1,M1		344
15X 0282	VV(I)= 0.0		345
15X 0283	81 430 K=1,M1		346
15X 0284	VV(I)= VV(I)+VWX(JJ,K)*XWX(JJ,K,I)		347
15X 0285	410 CONTINUE		348
15X 0286	420 CONTINUE		349
15X 0287	81 840 I+1,M1		351
15X 0288	82 430 K=1,M1		352
15X 0289	VV(I)= VV(I)-VVK(K)*TT(K,I)		353
15X 0290	430 CONTINUE		354
15X 0291	440 CONTINUE		355
15X 0292	850 CONTINUE		357
			358
			359
15X 0293	860 I=420 I+1,M1		361
			360
15X 0294	AVN(I)= 0.0		362
15X 0295	87 410 K=1,M1		363
15X 0296	AVN(I)= AVN(I)+V(I)*XWX(N,K,I)		364
15X 0297	910 CONTINUE		365
15X 0298	920 CONTINUE		366
15X 0299	930 CONTINUE		369
			370
15X 0300	940 RETURN		371
15X 0301	END		372

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SUBROUTINE MINVAT(AIN,NM,DET ERR)
DOUBLE PRECISION AIN,A,AK,DET,ERR,ERR1
DIMENSION AIN(6,4),A(4,8)

C
C TRANSFER INPUT MATRIX (AIN) TO WORKING ARRAY (A) AND FILL
C REMAINDER OF WORKING ARRAY WITH UNIT MATRIX
C
      N=NM
      JMD=2*N
      DO 110 J=1,N
        DO 100 J1=1,N
          DO 100 J2=1,N
            A(J1,J2)=AIN(J1,J2)
          J2=J+N
        J1=J+N
      J=J+N
      A(J1,JN1)=0.00
      IF(1.EQ.J) A(J1,JN1)=1.00
      100 CONTINUE
      110 CONTINUE

C
C CALCULATE DETERMINANT AND ELIMINATE THE *BELOW THE DIAGONAL*
C ELEMENTS OF LEFT SIDE OF A
C
      DET=1.00
      DO 230 J=1,N
        DEF=DET*A(J,1)
        IF (A(J,1)).EQ.0.00) GO TO 400
        JST=1
        AK=A(J,1)
        DO 200 J1=JST,JND
          A(J1,J)=A(J1,J)/AK
          IF(1.EQ.N) GO TO 300
          KST=1+J
          DO 220 K=KST,N
            AK=A(K,1)
            DO 210 J1=JST,JND
              A(K,J1)=A(K,J1)-A(J,1)*AK
            220 CONTINUE
          230 CONTINUE
        200 A(J1,J)=A(K,J1)-A(J,1)*AK
        210 A(K,J1)=A(K,J1)-A(J,1)*AK
        220 CONTINUE
        230 CONTINUE

C
C ELIMINATE THE ABOVE THE DIAGONAL ELEMENTS OF LEFT SIDE OF A
C
      DO 300 J=1,N
        KND=1+J
        DO 320 J1=KND,N
          AK=A(J,1)
          JST=1
          DO 310 J2=JST,JND
            A(K,J2)=A(K,J2)-A(J,1)*AK
          310 CONTINUE
          320 CONTINUE
          330 CONTINUE
        300 DO 330 J1=KND,N
          KND=1+J1
          DO 320 J2=KND,N
            AK=A(J1,1)
            JST=1
            DO 310 J3=JST,JND
              A(K,J3)=A(K,J3)-A(J1,1)*AK
            310 CONTINUE
            320 CONTINUE
            330 CONTINUE
          300 CONTINUE
        300 CONTINUE

C
C INVERSE IS IN RIGHT SIDE OF A. MULTIPLY INPUT MATRIX BY
C THE INVERSE AND FIND THE MAXIMUM DEVIATION OF ELEMENTS
C OF THE PRODUCT MATRIX FROM THE UNIT MATRIX
C

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150 0044      (400=0.0)
150 0045      GO 420 1+1,N
150 0046      JN= JN
150 0047      JN= JN
150 0048      PR=10.000
150 0049      GO 400 K1,N
150 0050      400 FPR1= FPR1+AIN(1,M)*AIX,JN)
150 0051      400 L= DAMPER(1)
150 0052      IF(JL=0) FPR1= FPR1-1.00
150 0053      IF(L=1) FPR1= FPR1
150 0054      GO 410 1+JN,PRH
150 0055      410 CONTINUE
150 0056      420 CONTINUE
150 0057      C
150 0058      C TRANSFER INVERSE TO INPUT ARRAY
150 0059      C
150 0060      GO 430 1+1,N
150 0061      GO 430 1+1,N
150 0062      JN= JN
150 0063      AIN(1,JN)= AIN,JN)
150 0064      430 CONTINUE
150 0065      RETURN
150 0066      C
150 0067      C IN SINGULAR MATRIX, RETURN NULL MATRIX
150 0068      C
150 0069      GO 440 020 1+1,N
150 0070      GO 440 1+1,N
150 0071      440 AIN(1,JN)= 0.00
150 0072      440 CONTINUE
150 0073      RETURN
150 0074      C
150 0075      C

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134 0002 SUBROUTINE TRANSPIX,Y,X,M,NB,TRANX,TRANX,TRANX)
135 0003 DIMENSION X(1),Y(1),VC(1),XM(1)
136 0004 ONUMBE PRECISION VC
137 0005 LOGICAL TRANX,TRANX
138 0006 IF (-NOT.TRANX) GO TO 1
139 0007 DO 10 I=1,NX
140 0008 IF (X(I)-LE.O.) X(I)=1.E-30
141 0009 10 X(I) = ALOG10(X(I))
142 0010 IF(MB-LT-.0) GO TO 1
143 0011 IF (MB-EQ.O.) GO TO 4
144 0012 DO 11 I=1,M
145 0013 IF (X(I)-LE.O.) X(I)=1.E-30
146 0014 11 X(I) = ALOG10(X(I))
147 0015 4 XM(NB+1)=ALOG10(X(MB+1))
148 0016 XM(1)=ALOG10(XM(1))
149 0017 1 IF (-NOT.TRANX) GO TO 3
150 0018 DO 12 I=1,NX
151 0019 IF (Y(I)-LE.O.) Y(I)=1.E-30
152 0020 12 Y(I) = ALOG10(Y(I))
153 0021 GO TO 3
154 0022
155 0023
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15N 0002      SUBROUTINE DEXM(X,M,LOW,HIGH,IX,IXM,IL)
15N 0003      7(M,NS,M,X(IX),XM(IXM),LOW(IL),HIGH(IL)
15N 0004      RETURN
C
C      DIVIDE ACCORDING TO PRECHOSEN SPLINE JOINTS
C
15N 0005      ENTRY DEVM(X,M,LOW,HIGH,NR,NS,NB,M)
C
C      CHECK THAT SPLINE JOINTS MATCH THE RANGE OF X
C
15N 0006      300 GO 310 I=1,NB
15N 0007      IF (I.EQ.NB) GO TO 310
15N 0008      JI = I+1
15N 0009      DO 305 J=JI,NB
15N 0010      IF (XM(JI).LE. XM(J)) GO TO 305
15N 0011      T = XM(JI)
15N 0012      XM(JI) = XM(J)
15N 0013      XM(J) = T
15N 0014      305 CONTINUE
15N 0015      310 CONTINUE
C
15N 0016      311 GO 320 I=1,NB
15N 0017      IF (I.EQ.NB) GO TO 320
15N 0018      IF (XM(I).GE. XM(M+1)) GO TO 320
15N 0019      II = I+1
15N 0020      DO 315 J=II,NB
15N 0021      XM(J-1) = XM(J)
15N 0022      315 XM(J-1) = XM(J)
15N 0023      320 CONTINUE
C
15N 0024      320 CONTINUE
C
15N 0025      320 CONTINUE
C
15N 0026      320 CONTINUE
C
15N 0027      320 CONTINUE
C
15N 0028      320 CONTINUE
C
15N 0029      320 CONTINUE
C
15N 0030      320 CONTINUE
C
15N 0031      320 CONTINUE
C
15N 0032      320 CONTINUE
C
15N 0033      320 CONTINUE
C
15N 0034      320 CONTINUE
C
15N 0035      320 CONTINUE
C
15N 0036      320 CONTINUE
C
15N 0037      320 CONTINUE
C
15N 0038      320 CONTINUE
C
15N 0039      320 CONTINUE
C
15N 0040      320 CONTINUE
C
15N 0041      320 CONTINUE
C
15N 0042      320 CONTINUE
C
15N 0043      320 CONTINUE
C
15N 0044      320 CONTINUE
C
15N 0045      320 CONTINUE
C
15N 0046      320 CONTINUE
C
15N 0047      320 CONTINUE
C
15N 0048      320 CONTINUE
C
15N 0049      320 CONTINUE
C
15N 0050      320 CONTINUE
C
15N 0051      320 CONTINUE
C
15N 0052      320 CONTINUE
C
15N 0053      320 CONTINUE
C
15N 0054      320 CONTINUE

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15N 0055      LHIGH(NS) = NX
C             CHECK FOR SUFFICIENT POINTS IN EACH SUBSET
C
15N 0056      II = 0
15N 0057      ON 360 I=1,NS
15N 0058      IF (LHIGH(I)-LLOW(I)+1.GT.M) GO TO 360
15N 0059      II=I
15N 0060      WRITE (6,10) I
15N 0061      10 FORMAT(10,20HINSUFFICIENT POINTS IN SUBSET,15)
15N 0062      360 CONTINUE
15N 0063
C             IF ANY SUBSETS ARE DEFICIENT, COMBINE THEM WITH OTHER SUBSETS
C
15N 0064      IF (II.EQ.0) RETURN
15N 0065      NS5=NS
15N 0066      400 DO 470 I=1,NS5
15N 0067      NP2 = LHIGH(I)-LLOW(I)+1
15N 0068      IF (NP2.GT.M) GO TO 470
15N 0069      IF (I.NE.1) GO TO 410
15N 0070      LHIGH(1) = LHIGH(2)
15N 0071      LHIGH(2) = 0
15N 0072      LLOW(2) = 0
15N 0073      NM(1) = NM(2)
15N 0074      GO TO 480
15N 0075      410 IF (I.NE.NS5) GO TO 420
15N 0076      LHIGH(NS5-1) = NX
15N 0077      LHIGH(NS5) = 0
15N 0078      LLOW(NS5) = 0
15N 0079      NM(NS5) = 0
15N 0080      NM(NS5-1) = X(NX)
15N 0081      GO TO 480
15N 0082      420 NP2 = LHIGH(I+1)-LLOW(I+1)+1
15N 0083      IF (NP2.GT.M) GO TO 430
15N 0084      LHIGH(I+1) = LHIGH(I+1)
15N 0085      LLOW(I+1) = 0
15N 0086      NM(I) = NM(I+1)
15N 0087      GO TO 480
15N 0088      430 NP2 = (LHIGH(I)-LLOW(I)+1)/2
15N 0089      IF (NP2.GT.M) GO TO 460
15N 0090      LHIGH(I-1) = LHIGH(I-1) + NP2
15N 0091      LHIGH(I) = 0
15N 0092      LLOW(I+1) = LLOW(I+1)-NP2
15N 0093      IF (LLOW(I+1).LT.LHIGH(I-1)) LLOW(I+1) = LHIGH(I-1)
15N 0094      LLOW(I) = 0
15N 0095      440 IF (LLOW(I).NE.LHIGH(I-1)) GO TO 450
15N 0096      NP2 = LLOW(I+1)
15N 0097      NM(I-1) = X(NP2)
15N 0098      GO TO 480
15N 0099      450 NP2 = LLOW(I+1)
15N 0100      NM(I-1) = X(NP2)
15N 0101      NP2 = LHIGH(I-1)
15N 0102      4M(I-1) = -5*(NM(I-1)+X(NP2))
15N 0103      GO TO 480
15N 0104      460 LHIGH(I-1) = LHIGH(I-1) + NP2
15N 0105      LHIGH(I) = 0
15N 0106      LLOW(I+1) = LLOW(I+1)-NP2
15N 0107      LLOW(I) = 0
15N 0108
15N 0109
15N 0110
15N 0111
15N 0112
15N 0113
15N 0114
15N 0115

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APPENDIX C

Description of SIMRUL Subroutine

The subroutine SIMRUL is a relatively short subprogram which provides MATAN~~o~~ with the numerical integration tool necessary for the determination of the location of the Boltzmann-Mateno plane, interdiffusion coefficients, and intrinsic diffusion coefficients by the Heumann method. The mathematical basis of the subroutine is Simpson's rule for integration which approximates the curve by arcs of parabolas. A complete description of the mathematical arguments of Simpson's rule can be found in most textbooks on advanced calculus.²⁰

Definition of Variables Used by SIMRUL

The following section tabulates the variables used by SIMRUL in order of their appearance in the subroutine argument list.

<u>Symbol</u>	<u>Definition</u>
X(I)	Independent variable; distance coordinate of composition point I in units of microns
Y(I)	Dependent variable; composition of component 1 in atom fraction units corresponding to distance coordinate X(I).
MIN	Integer value of the FORTRAN subscript I corresponding to the lower limit of the definite integral.
MAX	Integer value of the FORTRAN subscript I corresponding to the upper limit of the definite integral.
NI	Total number of subintervals into which the interval to be integrated is regularly partitioned.
IS	Size of each subinterval within the partitioned interval to be integrated.
AREA	Value of the definite integral for the curve between the limits expressed by the values of MIN and MAX in units of atom fraction-microns.

Discussion of Program Operation of SIMRUL

The mathematical basis of Simpson's rule for numerical integration states that if a function $f(x)$ is continuous in the interval $[a,b]$, if n is an even integer, and if $r_n = [x_0, x_1, \dots, x_n]$ is the regular partition of $[a,b]$ into n subintervals, then the integral of $f(x)$ between the limits a and b may be approximated from the following expression:

$$\int_a^b f(x)dx \approx \frac{b-a}{3n} \left[f(x_0=a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \dots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n=b) \right] \quad (C1)$$

Some textbooks refer to this method as the parabolic rule since the basic idea is to approximate the curve $f(x)$ by arcs of parabolas. The reader should refer to an advanced calculus text for a detailed proof of Eq. (C1), as it is sufficient to note here that computation of this expression is the sole purpose of the SIMRUL subroutine.

The requirements of Simpson's rule that the number of subintervals (NI) be an even integer and that the sizes of the subintervals (IS) be equal give rise to certain limitations in the use of SIMRUL as it is currently written. These restrictions, however, should cause little difficulty in effective application of the subroutine. First, the necessity of a regular partition of the interval $[a,b]$ is satisfied by setting $IS = 1$ for all calls to SIMRUL; thereby, the equality of all subinterval sizes is assured. The second requirement that the number of subintervals, NI, be even makes necessary the proper choice of integration limits such that the quantity $(b-a)/IS$ will always be even. For determination of the integral used for the calculation of the Boltzmann-Matano plane location, this restriction is satisfied by forcing the maximum distance coordinate (XMAX) to be an even integer (since the lower limit is already $x=0$ and $IS=1$). For the remaining calls to SIMRUL used to determine interdiffusion and intrinsic diffusion coefficients, the upper and lower limits must likewise be even integer values. This

restriction is satisfied by simply computing the definite integral at even values of $X(I)$ only. The consequence of this limitation is that interdiffusion and intrinsic diffusion coefficients can be computed only at $x=0$ and $x=2n$ microns, where n is a positive integer. Except in cases of extreme curvature of the concentration profile, this restriction will not prevent the determination of diffusion coefficients at very closely spaced concentration increments. The implementation of the above limitations has already been incorporated into MATANØ, and the user need not concern himself further with it except when he inputs the value of the experimentally determined Kirkendall reference plane. The value of XK must likewise be an even integer. Once again, however, this should present little problem since the accuracy of such a determination is typically of the order of $\pm 1 \mu m$.

```

12  EVEN = EVEN + V(K)
11  CONTINUE
    AREA = (15/3.0)*(V(MIN) + 4.0*EVEN + 2.0*QDD + V(MAX))
    RETURN
    END
SUBROUTINE SIMULUX,V,MIN,MAX,N1,IS,AREA)
    DIMENSION X(4000), V(4000)
    QDD = 0.0
    EVEN = 0.0
    KMAX = N1 - 1
    MIN1 = MIN + 1
    KMAXM = KMAX + MIN
    DO 11 K = MIN1,KMAXM,2
        IF(K.EQ. KMAX+MIN) GO TO 12
        QDD = QDD + V(K+1)
        EVEN = EVEN + V(K)
12
11
    ISN 0002
    ISN 0003
    ISN 0004
    ISN 0005
    ISN 0006
    ISN 0007
    ISN 0008
    ISN 0009
    ISN 0010
    ISN 0012
    ISN 0013
    ISN 0014
    ISN 0015
    ISN 0016
    ISN 0017

```

APPENDIX D

Description of SELFD Subroutine

The subroutine SELFD provides MATAN~~6~~ with the tracer diffusion coefficient information for the two species at any temperature and composition within the range of interest for the determination of the theoretically predicted values of the diffusion parameters. It must be emphasized that SELFD as it is written is designed exclusively for use with the vanadium-titanium system and the mathematical expressions found in this subroutine reflect this particular binary. Experimental results of tracer and self diffusion investigations in binary alloys vary considerably throughout the literature in terms of their graphical and tabular representations; consequently, a subroutine designed to take into account all such contingencies would have been highly impractical. The user, therefore, will need to suitably alter SELFD to treat the particular experimental tracer diffusion data which is available for his chosen system. The vanadium-titanium data of Murdock and McHargue²¹ is presented as a series of Arrhenius plots; therefore, for this system SELFD was written to convert the diffusion coefficients to functions of concentration.

Description of Variables Used by SELFD

The following section tabulates the variables used by SELFD in order of their appearance in the argument list.

<u>Symbol</u>	<u>Definition</u>
T8	Temperature at which the tracer diffusion coefficients are to be determined in °C.
CPRITI(I)	Composition of component 2 in units of atom fraction.
CPRIV(I)	Composition of component 1 in units of atom fraction.
DVS(I)	Tracer diffusion coefficient of component 1 in units of cm^2/s .
DTS(I)	Tracer diffusion coefficient of component 2 in units of cm^2/s .

Symbol	Definition
MINC	Minimum FORTRAN subscript corresponding to the lower limit value of composition of the range of compositions over which DTS(I) and DTS(I) are to be computed.
MAXC	Maximum FORTRAN subscript corresponding to the upper limit value of composition of the range of compositions over which DTS(I) and DTS(I) are to be computed.

Discussion of Program Operation of SELFD

As has been implied throughout this report, the ability to use the theoretical prediction aspect of MATAN~~0~~ depends heavily on the availability of tracer diffusion coefficients covering a range of compositions. The results of tracer diffusion investigations in the literature are generally expressed either as functions of reciprocal temperature at one composition of the host material (Arrhenius plots) or as functions of composition at one particular temperature. The structure of MATAN~~0~~ requires that the representation of tracer coefficients be as functions of composition. The experimental results of Murdock and McHargue²¹ are presented as a series of Arrhenius diagrams where each such plot represents one particular host substance composition. The main purpose of SELFD, therefore, is to convert this type of representation to one in which the tracer coefficients are expressed as functions of composition at each temperature.

For the particular case of the vanadium-titanium system, the situation is further complicated by the fact that the Arrhenius plots are curved; consequently, the tracer diffusion coefficients of vanadium (component 1) and titanium (component 2) have been fitted to analytical expressions at each alloy composition with the following forms:

$$\ln[D_1^*(T)] = A + BT^{-1} + CT^{-2} \quad (D1)$$

$$\ln[D_2^*(T)] = D + ET^{-1} + FT^{-2} \quad (D2)$$

where the coefficients A through F have been determined outside the program structure and, of course, are different for each alloy composition. The temperature, T , is expressed in units of $^{\circ}\text{K}^{-1}$. The first statement in the $\text{D}\phi$ loop converts the atom fraction units of CPRITI (I) to weight fraction units $[\text{CONTI (I)}]$. This is necessary since the experimental data ²¹ has been represented as weight fraction increments of alloy composition. The remainder of SELF is simply interpolative in nature. SELF begins by testing the first concentration value, CONTI (MINC) , within the composition range to be treated to determine the two Arrhenius diagrams between which it lies. This is accomplished by means of the set of IF statements located at the beginning of the subroutine. Once the composition has been located, SELF interpolates between the appropriate sets of Eqs. (D1) and (D2) corresponding to the experimental tracer diffusion curves bounding CONTI (MINC) . This procedure results in tracer diffusion coefficients DVS (MINC) and DTS (MINC) corresponding to the tracer coefficients of components 1 and 2, respectively, at the composition CONTI (MINC) . The $\text{D}\phi$ loop continues to operate in this fashion until the composition CONTI (MAXC) is reached. The tracer diffusion coefficients, expressed now as functions of composition at the temperature T , are read into $\text{MATAN}\phi$ for further computations.

The above discussion is highly specialized, of course, as each individual binary system will be. The user is cautioned, therefore, to modify SELF to reflect the tracer data format available to him. If the tracer diffusion data is expressed as functions of composition at the temperature of the interdiffusion investigation, the subroutine can be simplified considerably and, in certain cases, deleted entirely.

PROGRAM Listing for BDRP

```

154 0002 SUMROUTINE SFLEN(TH,CPRIV,CPRIV,DVS,DVS,MIMC,MARC)
154 0003 DIMENSION CPRIV(4000), CUNT(4000), CPRIV(4000), DVS(4000),
154 0004 DVS(4000),DCUNT(4000)
154 0005 DO 50 I=MIMC,MARC
154 0006 CUNT(I) = (CPRIV(I)*47.90)/(CPRIV(I)*47.90 +
154 0007 (CPRIV(I)*50.942)
154 0008 IF (CUNT(I) .LE. 0.10) GO TO 9
154 0009 IF (CUNT(I) .GT. 0.10 .AND. CUNT(I) .LE. 0.20) GO TO 9
154 0010 IF (CUNT(I) .GT. 0.20 .AND. CUNT(I) .LE. 0.30) GO TO 10
154 0011 IF (CUNT(I) .GT. 0.30 .AND. CUNT(I) .LE. 0.40) GO TO 11
154 0012 IF (CUNT(I) .GT. 0.40 .AND. CUNT(I) .LE. 0.50) GO TO 12
154 0013 IF (CUNT(I) .GT. 0.50 .AND. CUNT(I) .LE. 0.60) GO TO 13
154 0014 IF (CUNT(I) .GT. 0.60 .AND. CUNT(I) .LE. 0.70) GO TO 14
154 0015 IF (CUNT(I) .GT. 0.70 .AND. CUNT(I) .LE. 0.80) GO TO 15
154 0016 IF (CUNT(I) .GT. 0.80 .AND. CUNT(I) .LE. 0.90) GO TO 16
154 0017 IF (CUNT(I) .GT. 0.90 .AND. CUNT(I) .LE. 1.00) GO TO 17
154 0018 IF (CUNT(I) .GT. 0.90 .AND. CUNT(I) .LE. 1.00) GO TO 17
154 0019 DVS = 1.0547171 - 6.891692E-04 + 2.110465E-07(19002)
154 0020 DVS = 1.2439161 - 7.716838E-04 + 3.120099E-07(19002)
154 0021 DVS = 1.3355641 - 7.448290E-04 + 3.329983E-07(19002)
154 0022 DVS = 1.414506 - 6.594904E-04 + 2.570717E-07(19002)
154 0023 DCUNT(I) = CUNT(I)
154 0024 IF (CUNT(I) .LE. 0.10) GO TO 20
154 0025 DVS = 5.244666 - 5.161633E-04 + 1.356457E-07(19002)
154 0026 DVS = 7.183604 - 5.867294E-04 + 2.137991E-07(19002)
154 0027 DCUNT(I) = CUNT(I) - 0.10
154 0028 IF (CUNT(I) .GT. 0.10 .AND. CUNT(I) .LE. 0.20) GO TO 23
154 0029 DVS = 9.311498 - 6.275361E-04 + 2.377810E-07(19002)
154 0030 DVS = 1.040942 - 3.780809E-04 + 6.176774E-07(19002)
154 0031 DCUNT(I) = CUNT(I) - 0.20
154 0032 IF (CUNT(I) .GT. 0.20 .AND. CUNT(I) .LE. 0.30) GO TO 23
154 0033 DVS = 1.2716461 - 7.231755E-04 + 3.234048E-07(19002)
154 0034 DVS = 5.608958 - 5.138070E-04 + 1.748564E-07(19002)
154 0035 DCUNT(I) = CUNT(I) - 0.30
154 0036 IF (CUNT(I) .GT. 0.30 .AND. CUNT(I) .LE. 0.40) GO TO 20
154 0037 DVS = 7.046167 - 5.473912E-04 + 2.052910E-07(19002)
154 0038 DVS = 5.197962 - 5.270367E-04 + 2.014617E-07(19002)
154 0039 DCUNT(I) = CUNT(I) - 0.40
154 0040 IF (CUNT(I) .GT. 0.40 .AND. CUNT(I) .LE. 0.50) GO TO 23
154 0041 DVS = 3.001068 - 4.142130E-04 + 1.142736E-07(19002)
154 0042 DVS = 4.95293 - 4.487045E-04 + 1.492614E-07(19002)
154 0043 DCUNT(I) = CUNT(I) - 0.50
154 0044 IF (CUNT(I) .GT. 0.50 .AND. CUNT(I) .LE. 0.60) GO TO 23
154 0045 DVS = 5.462342 - 4.881404E-04 + 1.797833E-07(19002)
154 0046 DVS = 3.430723 - 4.533433E-04 + 1.494272E-07(19002)
154 0047 DCUNT(I) = CUNT(I) - 0.60
154 0048 IF (CUNT(I) .GT. 0.60 .AND. CUNT(I) .LE. 0.70) GO TO 23
154 0049 DVS = 4.11062 - 4.394511E-04 + 1.508499E-07(19002)
154 0050 DVS = 0.590327 - 3.707950E-04 + 1.106923E-07(19002)
154 0051 DCUNT(I) = CUNT(I) - 0.70
154 0052 IF (CUNT(I) .GT. 0.70 .AND. CUNT(I) .LE. 0.80) GO TO 23
154 0053 DVS = 1.423495 - 3.765280E-04 + 1.171652E-07(19002)
154 0054 DVS = 0.8744271 - 3.495408E-04 + 1.441453E-07(19002)
154 0055 DCUNT(I) = CUNT(I) - 0.80
154 0056 IF (CUNT(I) .GT. 0.80 .AND. CUNT(I) .LE. 0.90) GO TO 20
154 0057 DVS = 3.373468 - 4.209883E-04 + 1.477700E-07(19002)

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134 0075      DT2 = 0.428147 - 3.7250054*DT9 + 1.38848087*(T9**2)
134 0076      DCMYI(I) = COMYI(I)-0.90
20      DV1 = EXP(DV1)
134 0077      DV2 = EXP(DV2)
134 0078      DT1 = EXP(DT1)
134 0079      DT2 = EXP(DT2)
134 0080      DVS(I) = AMINI(DV1,DV2) + (DCMYI(I)/0.10)*ABS(DV2-DV1)
134 0081      DTS(I) = AMINI(DT1,DT2) + (DCOMYI(I)/0.10)*ABS(DT2-DT1)
134 0082      CONTINUE
134 0083      RETURN
134 0084      END
134 0085

```

APPENDIX E

Description of ~~PL~~TR Subroutine

The sole purpose of ~~PL~~TR is to separate from MATAN~~0~~ all calls to the ~~OR~~GRAPH plotting subroutines which result in plots of the theoretically predicted diffusion and vacancy wind parameters. This is done to prevent the main program from being excessively long. The argument list contains the same variables as have been defined earlier in the main body of this report; consequently, the variables used by ~~PL~~TR are not listed here. The content of this subroutine can be seen from an examination of the program listing given below.

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PROGRAM PLOTTRAC 10-100878

```

1SN 0002 SUBROUTINE PLOTTRAC,TR,CVE,SM,VVM,VTM,DVS,NTS,DCDV,DVCM,DVCH,DCNT,
1SN 0003     DTCM,DRATD,DRATM)
1SN 0003     DIMENSION CVE(110),SM(110),VVM(110),VTM(110),DVS(4000),NTS(4000),
1SN 0003     DCDV(110),DVCM(110),DCNT(110),DTCM(110),DRATD(110),
2SN 0004     DRATM(110)
1SN 0004     CALL FIXPLT(0.0,1.0,0.1,0.1,2.0,LINEAR,IMFCH,20.20,0.0,HUFFR,10,
1SN 0004     'CARLSONS')
1SN 0005     CALL TITLE(0.2,5,FACTORS,ATOM FRACTION V%,58)
1SN 0005     CALL LIMPLTICVF,SM,101,-1,0)
1SN 0006     CALL QOOSYM(7.0,9.5,0.10,TRUNS,0.0,3)
1SN 0007     CALL QOQNUM(999.999,0.10,N7,0.0,(15))
1SN 0008     CALL QOOSYM(7.0,9.7,0.10,TEMPERATURES,0.0,11)
1SN 0009     CALL QOQNUM(999.999,0.10,TA,0.0,(F4,3))
1SN 0010     CALL QOQNUM(999.999,0.10,TA,0.0,(F4,3))
1SN 0011     CALL FIXPLT(0.0,1.0,0.0,0.2,0.0,LINEAR,IMFCH,20.20,0.0,HUFFR,10,
1SN 0011     'CARLSONS')
1SN 0012     CALL TITLE(0.2,1,0,1,AND 1-V2 FACTORS,ATOM FRACTION V%,
1SN 0012     '1,0,1,0 1-V2')
1SN 0013     CALL LIMPLTICVF,VVM,101,0,-1)
1SN 0013     CALL LIMPLTICVF,VTM,101,2,-1)
1SN 0014     CALL QOOSYM(7.0,9.5,0.10,TRUNS,0.0,3)
1SN 0015     CALL QOQNUM(999.999,0.10,N7,0.0,(15))
1SN 0016     CALL QOQNUM(999.999,0.10,N7,0.0,(15))
1SN 0017     CALL QOOSYM(7.0,9.3,0.10,TEMPERATURES,0.0,11)
1SN 0018     CALL QOQNUM(999.999,0.10,TA,0.0,(F4,3))
1SN 0019     CALL QOOSYM(7.0,9.9,0.10,1,0,0,0,-1)
1SN 0020     CALL QOQNUM(999.999,0.10,0,0,0,-1)
1SN 0021     CALL QOOSYM(7.0,8.7,0.10,1,0,0,0,-1)
1SN 0022     CALL QOQNUM(999.999,0.10,2,0,0,-1)
1SN 0023     CALL SETPLTICVF,DVS,101,'VLC',IMFCH,20.5,0.0,HUFFR,10,
1SN 0023     'CARLSONS')
1SN 0024     CALL TITLE(0.2,TRACER DIFFUSION COEFFICIENTS,
1SN 0024     'ATOM FRACTION V%,0 10 CM/SEC')
1SN 0025     CALL LIMPLTICVF,DVS,101,0,-1)
1SN 0026     CALL LIMPLTICVF,NTS,101,2,-1)
1SN 0027     CALL QOOSYM(7.0,9.5,0.10,TRUNS,0.0,3)
1SN 0028     CALL QOQNUM(999.999,0.10,N7,0.0,(15))
1SN 0029     CALL QOOSYM(7.0,9.3,0.10,TEMPERATURES,0.0,11)
1SN 0030     CALL QOQNUM(999.999,0.10,TA,0.0,(F4,3))
1SN 0031     CALL QOOSYM(7.0,9.0,0.10,VANADIUM,0.0,0,10)
1SN 0032     CALL QOQNUM(999.999,0.10,0,0,0,-1)
1SN 0033     CALL QOOSYM(7.0,8.7,0.10,TITANIUM,0.0,0,10)
1SN 0034     CALL QOQNUM(999.999,0.10,2,0,0,-1)
1SN 0035     CALL SETPLTICVF,DCDV,101,'VLC',IMFCH,20.5,0.0,HUFFR,10,
1SN 0035     'CARLSONS')
1SN 0036     CALL TITLE(0.2,INTRINSIC DIFFUSIVITIES,ATOM FRACTION V%,
1SN 0036     '0, 50 CM/SEC')
1SN 0037     CALL LIMPLTICVF,DCDV,101,0,-1)
1SN 0038     CALL LIMPLTICVF,DVCM,101,2,-1)
1SN 0039     CALL LIMPLTICVF,DCNT,101,4,-1)
1SN 0040     CALL LIMPLTICVF,DTCM,101,5,-1)
1SN 0041     CALL QOOSYM(7.0,9.5,0.10,TRUNS,0.0,3)
1SN 0042     CALL QOQNUM(999.999,0.10,N7,0.0,(15))
1SN 0043     CALL QOOSYM(7.0,9.3,0.10,TEMPERATURES,0.0,11)
1SN 0044     CALL QOQNUM(999.999,0.10,TA,0.0,(F4,3))
1SN 0045     CALL QOOSYM(7.0,8.9,0.10,V, MARRN,0.0,0,12)
1SN 0046     CALL QOQNUM(999.999,0.10,0,0,0,-1)
1SN 0047     CALL QOOSYM(7.0,8.7,0.10,V, MANNING,0.0,0,13)

```

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15N 0048      CALL QDOSVH(999.,999.,0.10,2.0,0.0,-1)
15N 0049      CALL QDOSVH(7.0,8.7,0.10,10.0,10.0,-1)
15N 0050      CALL QDOSVH(999.,999.,0.10,4.0,0.0,-1)
15N 0051      CALL QDOSVH(7.0,8.7,0.10,10.0,10.0,-1)
15N 0052      CALL QDOSVH(999.,999.,0.10,5.0,0.0,-1)
15N 0053      CALL SETPLTICV(,DRATM,101.,'LINEAR', 'MECH',20.,20.,RUEPFR,10.,
15N 0054      'CARLSINS')
15N 0055      CALL TITL(10,2,'INTRINSIC DIFFUSIVITY RATIO',PATOM FRACTION VS',
15N 0056      'DOV/VI')
15N 0057      CALL LIMPLTICV(,DRATM,101,0,-1)
15N 0058      CALL LIMPLTICV(,DRATM,101,2,-1)
15N 0059      CALL QDOSVH(7.0,8.7,0.10,10.0,10.0,-1)
15N 0060      CALL QDOSVH(999.,999.,0.10,7.0,0.0,115)
15N 0061      CALL QDOSVH(7.0,8.7,0.10,10.0,10.0,-1)
15N 0062      CALL QDOSVH(999.,999.,0.10,8.0,0.0,115)
15N 0063      CALL QDOSVH(7.0,8.7,0.10,10.0,10.0,-1)
15N 0064      CALL QDOSVH(999.,999.,0.10,9.0,0.0,115)
15N 0065      RETURN
15N 0066      END

```

APPENDIX F

Description of Sample Problem 1

The following appendix demonstrates the manner in which MATAN₂ may be used to determine the various interdiffusion, intrinsic diffusion, and vacancy wind parameters, theoretically predicted from the models of Darken and Manning. The output includes a tabulation of the tracer diffusion and thermodynamic information used in their determination. The vanadium-titanium system at 1350 °C has been chosen to illustrate this particular aspect of MATAN₂. The thermodynamic data are due to Rolinski *et al.*;²² the tracer diffusion coefficients have been determined by Murdock and McHargue²³ and have been incorporated into the SELF sub-routine (see Appendix D). As a result of this choice of sample system, the column headings and coordinate labels on the tables and plots, respectively, reflect the vanadium-titanium binary. As stated earlier, however, this labeling may be changed to conform with the particular system under investigation by altering the characters in the various Hollerith formats.

Computer Input for Sample Problem 1

When MATAN₂ is used to determine the theoretically predicted diffusion quantities in the absence of experimental data, only the first four cards tabulated in the section on Input Data Format are required. The entries on cards 1 and 2 have their usual significance, where N° now represents the number of different temperatures at which the theoretical parameters are to be computed. Card 3 is ignored in this application of MATAN₂; consequently, any set of nonnegative integers may be inserted on this card. Finally, the only nonzero quantities required on card 4 are N° and I° . The value of N° can be any nonzero

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integer chosen by the user to designate the particular run, while T^* is the temperature in °C. Accordingly, the input sheet for computation of theoretical diffusion parameters at 1350°C for the vanadium-titanium system would be:

ORNL-DWG 75-4290

COMPUTER INPUT FOR SAMPLE PROBLEM 1

Card Columns

1-5	6-10	11-15	16-20	21-25	26-30	31-35	36-40	41-45	46-50	51-55	56-60	61-65	66-70
1													
1													
2	6	6											
1350	1350	.000											

Computer Output for Sample Problem 1

The following pages present the computer generated output for this problem. In order that the calculated theoretical quantities will be smooth functions of composition, FITLQS is used to fit a least squares curve to the $\ln D_V^*$ versus N_V and $\ln D_{Ti}^*$ versus N_V data. The first six pages of tabular output result from this use of FITLQS. The remaining tabular and graphical output are self-explanatory.

Computer Output for Sample Problem 1

DATA DIVIDED AS EVENLY AS POSSIBLE AMONG THE NUMBER OF SUBSETS CHOSEN BY PROGRAMMER

DEGREE OF POLYNOMIAL = 2 NUMBER OF SECTIONS = 4

EQUATION FITTED IS $Y = A_0 + A_1 X + A_2 X^2$

SEGMENT COEFFICIENTS IN ASCENDING ORDER -

	A_0	A_1	A_2
-1.708318327642810D 01	-4.211444264333320D 01	-5.43454242410720D 00	
-1.74004315517520D 01	5.078759424032350D 01	-6.946019042748770D 00	

SPLINE JCTANTS ARE -

0.0 0.0 0.00000000 0.00000000

X	Y	Y'	Y''
0.0	-1.6955000E 01	-1.708318327642810D 01	-1.201204140171009D 01
0.0000000E 01	-1.6955000E 01	-1.708318327642810D 01	-1.201204140171009D 01
1.5955999E 02	-1.7023400E 01	-1.700258000000000D 01	-1.004229573598800D 01
2.5955999E 02	-1.7059400E 01	-1.710377444176000D 01	-0.000000000000000D 01
3.5955999E 02	-1.7096700E 01	-1.711574744176000D 01	-2.004243940000000D 01
4.5955999E 02	-1.7135400E 01	-1.714822000000000D 01	-3.100011000000000D 01
5.5955999E 02	-1.7175400E 01	-1.718420000000000D 01	-4.200000000000000D 01
6.5955999E 02	-1.7215400E 01	-1.721500000000000D 01	-5.300000000000000D 01
7.5955999E 02	-1.7255400E 01	-1.724500000000000D 01	-6.400000000000000D 01
8.5955999E 02	-1.7295400E 01	-1.727500000000000D 01	-7.500000000000000D 01
9.5955999E 02	-1.7335400E 01	-1.730500000000000D 01	-8.600000000000000D 01
1.0955999E 01	-1.7375400E 01	-1.733500000000000D 01	-9.700000000000000D 01
1.1955999E 01	-1.7415400E 01	-1.736500000000000D 01	-1.080000000000000D 01
1.2955999E 01	-1.7455400E 01	-1.739500000000000D 01	-1.190000000000000D 01
1.3955999E 01	-1.7495400E 01	-1.742500000000000D 01	-1.300000000000000D 01
1.4955999E 01	-1.7535400E 01	-1.745500000000000D 01	-1.410000000000000D 01
1.5955999E 01	-1.7575400E 01	-1.748500000000000D 01	-1.520000000000000D 01
1.6955999E 01	-1.7615400E 01	-1.751500000000000D 01	-1.630000000000000D 01
1.7955999E 01	-1.7655400E 01	-1.754500000000000D 01	-1.740000000000000D 01
1.8955999E 01	-1.7695400E 01	-1.757500000000000D 01	-1.850000000000000D 01
1.9955999E 01	-1.7735400E 01	-1.760500000000000D 01	-1.960000000000000D 01
2.0955999E 01	-1.7775400E 01	-1.763500000000000D 01	-2.070000000000000D 01
2.1955999E 01	-1.7815400E 01	-1.766500000000000D 01	-2.180000000000000D 01
2.2955999E 01	-1.7855400E 01	-1.769500000000000D 01	-2.290000000000000D 01
2.3955999E 01	-1.7895400E 01	-1.772500000000000D 01	-2.400000000000000D 01
2.4955999E 01	-1.7935400E 01	-1.775500000000000D 01	-2.510000000000000D 01
2.5955999E 01	-1.7975400E 01	-1.778500000000000D 01	-2.620000000000000D 01
2.6955999E 01	-1.8015400E 01	-1.781500000000000D 01	-2.730000000000000D 01
2.7955999E 01	-1.8055400E 01	-1.784500000000000D 01	-2.840000000000000D 01
2.8955999E 01	-1.8095400E 01	-1.787500000000000D 01	-2.950000000000000D 01
2.9955999E 01	-1.8135400E 01	-1.790500000000000D 01	-3.060000000000000D 01
3.0955999E 01	-1.8175400E 01	-1.793500000000000D 01	-3.170000000000000D 01
3.1955999E 01	-1.8215400E 01	-1.796500000000000D 01	-3.280000000000000D 01
3.2955999E 01	-1.8255400E 01	-1.799500000000000D 01	-3.390000000000000D 01
3.3955999E 01	-1.8295400E 01	-1.802500000000000D 01	-3.500000000000000D 01
3.4955999E 01	-1.8335400E 01	-1.805500000000000D 01	-3.610000000000000D 01
3.5955999E 01	-1.8375400E 01	-1.808500000000000D 01	-3.720000000000000D 01
3.6955999E 01	-1.8415400E 01	-1.811500000000000D 01	-3.830000000000000D 01
3.7955999E 01	-1.8455400E 01	-1.814500000000000D 01	-3.940000000000000D 01
3.8955999E 01	-1.8495400E 01	-1.817500000000000D 01	-4.050000000000000D 01
3.9955999E 01	-1.8535400E 01	-1.820500000000000D 01	-4.160000000000000D 01
4.0955999E 01	-1.8575400E 01	-1.823500000000000D 01	-4.270000000000000D 01

911

CORRELATION OF FITTED DATA TO ORIGINAL DATA

VARIANCE = 4.359732931702189E-03
STANDARD DEVIATION = 6.602827312453340E-02

CORRELATION INDEX = 0.979066701037000 CU
MAXIMUM CORRELATION = 0.9101500190819000 CU

41 FIT CHECK MADE

CORRELATION OF FITTED DATA TO ORIGINAL DATA

VARIANCE = 2.176529782502195E-03
 STANDARD DEVIATION = 5.056425561950033E-02

NO DEFIT CHECK MADE

CORRELATION INDEX =
 MAXIMUM CORRELATION =

U.S. NAVY
 U.S. NAVY

TRACER CUEFFICIENTS

INTERLUPPULION CUEFFICIENTS

AT PR Y	Y	T1	CVS/L13	GAPPA Y	GAPPA T1	WPI	S	WAPPA	WAPPA
0.0	0.3009M-07	0.3023E-07	1.2580E-07	1.71437	1.00000	1.00000	1.00000	1.00000	1.00000
0.01000	0.3772E-07	0.29570E-07	1.27745	1.71471	1.00000	1.00000	1.00000	1.00000	1.00000
0.02000	0.3772E-07	0.28909E-07	1.27914	1.71491	1.00000	1.00000	1.00000	1.00000	1.00000
0.03000	0.36070E-07	0.28213E-07	1.30604	1.71009	1.00000	1.00000	1.00000	1.00000	1.00000
0.04000	0.36070E-07	0.27570E-07	1.34028	1.68460	1.00000	1.00000	1.00000	1.00000	1.00000
0.05000	0.35000E-07	0.26912E-07	1.33303	1.68424	1.00000	1.00000	1.00000	1.00000	1.00000
0.06000	0.3534E-07	0.26250E-07	1.34640	1.68057	1.00000	1.00000	1.00000	1.00000	1.00000
0.07000	0.3477E-07	0.25612E-07	1.33750	1.67727	1.00000	1.00000	1.00000	1.00000	1.00000
0.08000	0.34180E-07	0.24972E-07	1.33072	1.67418	1.00000	1.00000	1.00000	1.00000	1.00000
0.09000	0.3355E-07	0.24344E-07	1.31601	1.66979	1.00000	1.00000	1.00000	1.00000	1.00000
0.10000	0.3290E-07	0.23714E-07	1.30704	1.66569	1.00000	1.00000	1.00000	1.00000	1.00000
0.11000	0.3223E-07	0.23090E-07	1.29907	1.66189	1.00000	1.00000	1.00000	1.00000	1.00000
0.12000	0.3154E-07	0.22480E-07	1.29216	1.65815	1.00000	1.00000	1.00000	1.00000	1.00000
0.13000	0.3083E-07	0.21880E-07	1.28604	1.65449	1.00000	1.00000	1.00000	1.00000	1.00000
0.14000	0.3010E-07	0.21280E-07	1.28004	1.65112	1.00000	1.00000	1.00000	1.00000	1.00000
0.15000	0.2936E-07	0.20670E-07	1.27413	1.64780	1.00000	1.00000	1.00000	1.00000	1.00000
0.16000	0.2860E-07	0.20070E-07	1.26831	1.64452	1.00000	1.00000	1.00000	1.00000	1.00000
0.17000	0.2784E-07	0.19480E-07	1.26261	1.64128	1.00000	1.00000	1.00000	1.00000	1.00000
0.18000	0.2706E-07	0.18900E-07	1.25704	1.63805	1.00000	1.00000	1.00000	1.00000	1.00000
0.19000	0.2628E-07	0.18330E-07	1.25151	1.63484	1.00000	1.00000	1.00000	1.00000	1.00000
0.20000	0.2549E-07	0.17770E-07	1.24604	1.63164	1.00000	1.00000	1.00000	1.00000	1.00000
0.21000	0.2470E-07	0.17220E-07	1.24071	1.62844	1.00000	1.00000	1.00000	1.00000	1.00000
0.22000	0.2391E-07	0.16670E-07	1.23541	1.62524	1.00000	1.00000	1.00000	1.00000	1.00000
0.23000	0.2312E-07	0.16130E-07	1.23014	1.62204	1.00000	1.00000	1.00000	1.00000	1.00000
0.24000	0.2233E-07	0.15590E-07	1.22491	1.61884	1.00000	1.00000	1.00000	1.00000	1.00000
0.25000	0.2154E-07	0.15060E-07	1.21971	1.61564	1.00000	1.00000	1.00000	1.00000	1.00000
0.26000	0.2075E-07	0.14530E-07	1.21451	1.61244	1.00000	1.00000	1.00000	1.00000	1.00000
0.27000	0.1996E-07	0.14000E-07	1.20931	1.60924	1.00000	1.00000	1.00000	1.00000	1.00000
0.28000	0.1917E-07	0.13470E-07	1.20411	1.60604	1.00000	1.00000	1.00000	1.00000	1.00000
0.29000	0.1838E-07	0.12940E-07	1.19891	1.60284	1.00000	1.00000	1.00000	1.00000	1.00000
0.30000	0.1759E-07	0.12410E-07	1.19371	1.59964	1.00000	1.00000	1.00000	1.00000	1.00000
0.31000	0.1680E-07	0.11880E-07	1.18851	1.59644	1.00000	1.00000	1.00000	1.00000	1.00000
0.32000	0.1601E-07	0.11350E-07	1.18331	1.59324	1.00000	1.00000	1.00000	1.00000	1.00000
0.33000	0.1522E-07	0.10820E-07	1.17811	1.59004	1.00000	1.00000	1.00000	1.00000	1.00000
0.34000	0.1443E-07	0.10290E-07	1.17291	1.58684	1.00000	1.00000	1.00000	1.00000	1.00000
0.35000	0.1364E-07	0.09760E-07	1.16771	1.58364	1.00000	1.00000	1.00000	1.00000	1.00000
0.36000	0.1285E-07	0.09230E-07	1.16251	1.58044	1.00000	1.00000	1.00000	1.00000	1.00000
0.37000	0.1206E-07	0.08700E-07	1.15731	1.57724	1.00000	1.00000	1.00000	1.00000	1.00000
0.38000	0.1127E-07	0.08170E-07	1.15211	1.57404	1.00000	1.00000	1.00000	1.00000	1.00000
0.39000	0.1048E-07	0.07640E-07	1.14691	1.57084	1.00000	1.00000	1.00000	1.00000	1.00000
0.40000	0.0969E-07	0.07110E-07	1.14171	1.56764	1.00000	1.00000	1.00000	1.00000	1.00000
0.41000	0.0890E-07	0.06580E-07	1.13651	1.56444	1.00000	1.00000	1.00000	1.00000	1.00000
0.42000	0.0811E-07	0.06050E-07	1.13131	1.56124	1.00000	1.00000	1.00000	1.00000	1.00000
0.43000	0.0732E-07	0.05520E-07	1.12611	1.55804	1.00000	1.00000	1.00000	1.00000	1.00000
0.44000	0.0653E-07	0.04990E-07	1.12091	1.55484	1.00000	1.00000	1.00000	1.00000	1.00000
0.45000	0.0574E-07	0.04460E-07	1.11571	1.55164	1.00000	1.00000	1.00000	1.00000	1.00000
0.46000	0.0495E-07	0.03930E-07	1.11051	1.54844	1.00000	1.00000	1.00000	1.00000	1.00000
0.47000	0.0416E-07	0.03400E-07	1.10531	1.54524	1.00000	1.00000	1.00000	1.00000	1.00000
0.48000	0.0337E-07	0.02870E-07	1.10011	1.54204	1.00000	1.00000	1.00000	1.00000	1.00000
0.49000	0.0258E-07	0.02340E-07	1.09491	1.53884	1.00000	1.00000	1.00000	1.00000	1.00000
0.50000	0.0179E-07	0.01810E-07	1.08971	1.53564	1.00000	1.00000	1.00000	1.00000	1.00000
0.51000	0.0100E-07	0.01280E-07	1.08451	1.53244	1.00000	1.00000	1.00000	1.00000	1.00000
0.52000	0.0021E-07	0.00750E-07	1.07931	1.52924	1.00000	1.00000	1.00000	1.00000	1.00000
0.53000	0.0000E-07	0.0000E-07	1.07411	1.52604	1.00000	1.00000	1.00000	1.00000	1.00000
0.54000	0.0000E-07	0.0000E-07	1.06891	1.52284	1.00000	1.00000	1.00000	1.00000	1.00000
0.55000	0.0000E-07	0.0000E-07	1.06371	1.51964	1.00000	1.00000	1.00000	1.00000	1.00000
0.56000	0.0000E-07	0.0000E-07	1.05851	1.51644	1.00000	1.00000	1.00000	1.00000	1.00000
0.57000	0.0000E-07	0.0000E-07	1.05331	1.51324	1.00000	1.00000	1.00000	1.00000	1.00000
0.58000	0.0000E-07	0.0000E-07	1.04811	1.51004	1.00000	1.00000	1.00000	1.00000	1.00000
0.59000	0.0000E-07	0.0000E-07	1.04291	1.50684	1.00000	1.00000	1.00000	1.00000	1.00000
0.60000	0.0000E-07	0.0000E-07	1.03771	1.50364	1.00000	1.00000	1.00000	1.00000	1.00000
0.61000	0.0000E-07	0.0000E-07	1.03251	1.50044	1.00000	1.00000	1.00000	1.00000	1.00000
0.62000	0.0000E-07	0.0000E-07	1.02731	1.49724	1.00000	1.00000	1.00000	1.00000	1.00000
0.63000	0.0000E-07	0.0000E-07	1.02211	1.49404	1.00000	1.00000	1.00000	1.00000	1.00000
0.64000	0.0000E-07	0.0000E-07	1.01691	1.49084	1.00000	1.00000	1.00000	1.00000	1.00000
0.65000	0.0000E-07	0.0000E-07	1.01171	1.48764	1.00000	1.00000	1.00000	1.00000	1.00000
0.66000	0.0000E-07	0.0000E-07	1.00651	1.48444	1.00000	1.00000	1.00000	1.00000	1.00000
 			

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S FACTOR

Fig. F1. Vacancy wind factor, S , for interdiffusion coefficients in V-Ti alloys as a function of vanadium composition.

1+V1 AND 1-V2 FACTORS

Fig. F2. Vacancy wind factors, $1 + V_1$ and $1 - V_2$, for intrinsic diffusion coefficients in V-Ti alloys as functions of vanadium composition.

Fig. P3. Tracer diffusion coefficients of V and Ti in V-Ti alloys as functions of vanadium composition.

INTRINSIC DIFFUSIVITIES

Fig. P4. Intrinsic diffusivities of V and Ti in V-Ti alloys, calculated from the analyses of Manning and Darken as functions of vanadium composition.

Fig. F5. Intrinsic diffusivity ratios, D_v/D_{Ti} , calculated from the analyses of Manning and Darken as functions of vanadium composition.

APPENDIX G

Description of Sample Problem 2

The following appendix demonstrates the use of MATAN⁸ for the determination of interdiffusion, intrinsic diffusion and vacancy wind parameters from experimental intensity-penetration profiles obtained from electron probe microanalysis. The problem has been divided into two parts to illustrate the manner in which such experimental data might typically be treated. Part 1 presents the computer input and output for the case in which only the experimental points, corrected for background, are outputted. Generally, this information is necessary prior to fitting a curve to the experimental data since the number of segments into which the curve is to be divided and the location of the spline joints of these segments are rarely known in advance. Part 2 gives the input and output for a least squares fit of the experimental data presented in Part 1 with subsequent computation to produce the various diffusion quantities.

When reading the computer input sheets that follow, the user should consult the tables of variables and constants presented earlier as well as the section on Input Data Format. The experimental data presented here reflect the analysis⁸ of a V/Ti/V diffusion couple annealed at 1352.94°C for 1 day (8.64×10^4 s).

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COMPUTER DEPT FOR SAMPLE PROBLEM 4, PART 1

Core Columns												
1-5	6-10	11-15	16-20	21-25	26-30	31-35	36-40	41-45	46-50	51-55	56-60	61-65
1	130	130	130	130	130	130	130	130	130	130	130	130
2	130	130	130	130	130	130	130	130	130	130	130	130
3	130	130	130	130	130	130	130	130	130	130	130	130
4	130	130	130	130	130	130	130	130	130	130	130	130
5	130	130	130	130	130	130	130	130	130	130	130	130
6	130	130	130	130	130	130	130	130	130	130	130	130
7	130	130	130	130	130	130	130	130	130	130	130	130
8	130	130	130	130	130	130	130	130	130	130	130	130
9	130	130	130	130	130	130	130	130	130	130	130	130
10	130	130	130	130	130	130	130	130	130	130	130	130
11	130	130	130	130	130	130	130	130	130	130	130	130
12	130	130	130	130	130	130	130	130	130	130	130	130
13	130	130	130	130	130	130	130	130	130	130	130	130
14	130	130	130	130	130	130	130	130	130	130	130	130
15	130	130	130	130	130	130	130	130	130	130	130	130
16	130	130	130	130	130	130	130	130	130	130	130	130
17	130	130	130	130	130	130	130	130	130	130	130	130
18	130	130	130	130	130	130	130	130	130	130	130	130
19	130	130	130	130	130	130	130	130	130	130	130	130
20	130	130	130	130	130	130	130	130	130	130	130	130
21	130	130	130	130	130	130	130	130	130	130	130	130
22	130	130	130	130	130	130	130	130	130	130	130	130
23	130	130	130	130	130	130	130	130	130	130	130	130
24	130	130	130	130	130	130	130	130	130	130	130	130
25	130	130	130	130	130	130	130	130	130	130	130	130
26	130	130	130	130	130	130	130	130	130	130	130	130
 									

DIFFUSION RUN 1

NOMINAL TEMPERATURE 1352.940

DIFFUSION TIME IN SEC 3.86400E 05

NOMINAL WT PERCENT V IN A 100
NOMINAL WT PERCENT TI IN A 0
NOMINAL WT PERCENT V IN W 0
NOMINAL WT PERCENT TI IN W 100

PROB FILE NUMBER 1

DISTANCE	INT DATE V	INT DATE TI	INT RATIO TI	WT FRAC V	WT FRAC TI	AT FRAC V	AT FRAC TI
0.0	1.10000		0.00005	1.01742	0.00001	0.99999	0.00002
20.00000	0.99402		0.00001	1.01450	0.00000	1.00000	0.00000
40.00000	0.99481		-0.00006	1.01724	0.00002	0.99998	0.00002
60.00000	0.99710		-0.00039	1.01544	0.00015	0.99984	0.00016
80.00000	0.99468		0.00004	1.01337	0.00002	0.99997	0.00002
100.00000	0.99419		-0.00027	1.00950	0.00010	0.99989	0.00011
120.00000	0.99566		-0.00038	1.01424	0.00015	0.99984	0.00016
140.00000	0.99481		-0.00023	1.00191	0.00009	0.99991	0.00009
160.00000	0.99462		-0.00014	1.01480	0.00007	0.99993	0.00007
180.00000	0.99088		0.00006	1.01074	0.00002	0.99998	0.00002
200.00000	0.99747		0.00023	1.01190	0.00004	0.99996	0.00004
220.00000	0.99674		0.00043	1.00769	0.00016	0.99814	0.00044
240.00000	0.99207		0.00047	1.00426	0.00016	0.99152	0.00068
260.00000	0.99562		0.00146	0.99514	0.00214	0.97720	0.02290
280.00000	0.99491		0.00646	0.99131	0.00661	0.92929	0.07071
300.00000	0.99765		0.00991	0.97626	0.02701	0.91976	0.08124
320.00000	0.99324		0.01659	0.87484	0.12040	0.97220	0.12180
340.00000	0.99570		0.02101	0.97387	0.11974	0.81163	0.18837
360.00000	0.99791		0.02767	0.76344	0.26501	0.74544	0.25646
380.00000	0.99791		0.02311	0.71340	0.29164	0.69674	0.30320
400.00000	0.99785		0.03654	0.64454	0.31424	0.67250	0.32741
420.00000	0.99509		0.03902	0.63133	0.34873	0.61685	0.38315
440.00000	0.99405		0.05501	0.58160	0.42861	0.56065	0.43043
460.00000	0.99137		0.05673	0.53174	0.48271	0.51207	0.48793
480.00000	0.99006		0.05210	0.52281	0.50312	0.49550	0.50450
500.00000	0.99113		0.05266	0.49403	0.53339	0.46620	0.53703
520.00000	0.99336		0.05266	0.46272	0.56597	0.44386	0.54614
540.00000	0.99367		0.05266	0.43574	0.59377	0.42374	0.57626
560.00000	0.99485		0.05047	0.41229	0.59162	0.39083	0.60117
580.00000	0.99400		0.04022	0.41334	0.58297	0.36420	0.60579
600.00000	0.99637		0.02246	0.39287	0.60962	0.33730	0.62270
620.00000	0.99485		0.02173	0.40351	0.60892	0.31830	0.61611
640.00000	0.99533		0.01954	0.41445	0.62642	0.30434	0.61566
660.00000	0.99577		0.01647	0.37403	0.63005	0.28420	0.64177
680.00000	0.99337		0.01500	0.34574	0.64570	0.26420	0.65171
700.00000	0.99337		0.01691	0.33133	0.63704	0.23022	0.66078
720.00000	0.99337		0.01661	0.33667	0.64197	0.21600	0.68310

720.00000	0.20355	0.69701	0.42377	0.60247	0.30938	0.66662
740.00000	0.19798	0.70816	0.31737	0.70494	0.29749	0.70257
760.00000	0.18720	0.72603	0.29685	0.72497	0.28335	0.71665
780.00000	0.18146	0.74232	0.29068	0.72130	0.28013	0.71987
800.00000	0.17301	0.75966	0.28006	0.74030	0.26786	0.73216
850.00000	0.16627	0.75191	0.27746	0.73999	0.25706	0.74295
900.00000	0.15977	0.74358	0.26706	0.73992	0.24726	0.77274
950.00000	0.15206	0.80008	0.25617	0.80466	0.20960	0.79040
1000.00000	0.14412	0.81286	0.21353	0.82320	0.19608	0.80192
1050.00000	0.13748	0.82366	0.20853	0.83549	0.18711	0.81289
1100.00000	0.08866	0.83396	0.17807	0.84728	0.16501	0.83499
1150.00000	0.08540	0.83471	0.17335	0.85385	0.16030	0.83970
1200.00000	0.08982	0.86976	0.14986	0.88829	0.13700	0.86300
1250.00000	0.08335	0.86913	0.13984	0.88756	0.12903	0.87097
1300.00000	0.08478	0.89176	0.12366	0.91360	0.11476	0.88524
1350.00000	0.08834	0.90372	0.11512	0.92971	0.10429	0.89571
1400.00000	0.08253	0.90811	0.10599	0.93246	0.09573	0.90427
1450.00000	0.08291	0.92106	0.09712	0.94745	0.07958	0.92062
1500.00000	0.02488	0.93083	0.07368	0.95874	0.05723	0.93769
1550.00000	0.02280	0.94305	0.06704	0.97291	0.06085	0.93915
1600.00000	0.01866	0.95039	0.05760	0.98146	0.05229	0.94771
1650.00000	0.01606	0.95696	0.04737	0.98896	0.04309	0.95491
1700.00000	0.01027	0.97178	0.03775	1.00631	0.03340	0.96590
1750.00000	0.00942	0.97468	0.03551	1.00947	0.03207	0.96794
1800.00000	0.00807	0.97359	0.02769	1.00838	0.02517	0.97483
1850.00000	0.00438	0.98656	0.01963	1.03119	0.01758	0.98242
1900.00000	0.00219	0.98801	0.01266	1.01608	0.01138	0.98862
1950.00000	0.00096	0.99332	0.00889	1.03164	0.00624	0.99376
2000.00000	0.00155	0.99928	0.00924	1.03860	0.00887	0.99113
2100.00000	0.00017	0.99693	0.00700	1.03565	0.00181	0.79819

DISTANCE	K RATIO V	K RATIO TI	LAMBDA	AT PRAC V	AT PRAC TI
0.0	0.0	20129.22764	0.0	0.99998	0.00002
20.00000	0.00400	80519.12500	0.64041P-01	1.00000	0.00000
40.00000	0.00019	-1.6105.26172	0.13608P 00	0.99998	0.00002
60.00000	0.00211	-2565.34694	0.20412P 00	0.99994	0.00016
100.00000	0.00535	17503.54688	0.34031E 00	0.99997	0.00002
120.00000	0.01093	-3694.62964	0.40825E 00	0.99989	0.00011
140.00000	0.00436	-2615.32300	0.47629E 00	0.99984	0.00016
160.00000	0.02138	-4284.05514	0.54433E 00	0.99981	0.00009
180.00000	0.00359	-5298.44141	0.61237E 00	0.99993	0.00007
200.00000	0.00920	17503.54688	0.68041E 00	0.99988	0.00002
220.00000	0.00759	4375.14453	0.74846P 00	0.99991	0.00009
240.00000	0.01344	290.32080	0.81650P 00	0.99915	0.00184
260.00000	0.01824	94.63206	0.88454E 00	0.99352	0.00648
280.00000	0.04578	10.29221	0.95258P 00	0.97720	0.02280
300.00000	0.13082	10.50007	0.10206E 01	0.92824	0.07071
320.00000	0.13440	9.11039	0.16487P 01	0.91976	0.08126
340.00000	0.27044	5.77554	0.1937E 01	0.97220	0.12780
360.00000	0.14155	3.75815	0.1247P 01	0.81163	0.18837
380.00000	0.49074	2.61344	0.12928E 01	0.74554	0.25444
400.00000	0.64066	2.09494	0.13608P 01	0.64674	0.35326
420.00000	0.72745	1.89425	0.14289P 01	0.67259	0.32741
440.00000	0.94143	1.51241	0.14969P 01	0.61689	0.38314
460.00000	1.17555	1.19777	0.15650P 01	0.54369	0.45694
480.00000	1.42011	0.97735	0.16330P 01	0.41207	0.58794
500.00000	1.52484	0.91535	0.17010P 01	0.49550	0.50450
520.00000	1.74008	0.80944	0.17691E 01	0.46297	0.53703
540.00000	1.99937	0.77804	0.18371E 01	0.44386	0.55619
560.00000	2.25027	0.74031	0.19052E 01	0.42374	0.57626
580.00000	2.45239	0.65067	0.19732P 01	0.39643	0.60117
590.00000	2.53561	0.64684	0.20712P 01	0.39420	0.60579
600.00000	2.75488	0.60679	0.20412P 01	0.37730	0.62270
610.00000	2.61735	0.60843	0.20753P 01	0.38384	0.61511
620.00000	2.90577	0.56541	0.21093P 01	0.36614	0.63464
640.00000	3.01975	0.56078	0.21731E 01	0.35821	0.64177
660.00000	3.28237	0.52471	0.22468P 01	0.34224	0.64771
680.00000	3.38538	0.47750	0.23149P 01	0.33522	0.64974
700.00000	3.45481	0.45431	0.23814P 01	0.31540	0.64810
720.00000	3.51280	0.43449	0.24495E 01	0.30538	0.64462
740.00000	4.54096	0.41212	0.25175P 01	0.29743	0.63957
760.00000	4.34182	0.37735	0.25856E 01	0.28315	0.61649
780.00000	4.49565	0.38290	0.26536E 01	0.28313	0.61787
800.00000	4.78000	0.35197	0.27217P 01	0.26786	0.73516
850.00000	5.08930	0.33012	0.28418P 01	0.25705	0.74295
900.00000	6.15465	0.27420	0.30619E 01	0.27224	0.77774
950.00000	6.99622	0.24987	0.32320P 01	0.20940	0.79140
1000.00000	7.74308	0.23022	0.34021E 01	0.19608	0.80192
1050.00000	8.30377	0.21413	0.35722E 01	0.18711	0.81289
1100.00000	10.28004	0.19909	0.37423P 01	0.16501	0.83490
1150.00000	10.75089	0.19089	0.39124E 01	0.16310	0.83970
1200.00000	13.32235	0.14974	0.40825P 01	0.13700	0.86100
1250.00000	16.78462	0.13059	0.42526E 01	0.12903	0.87037
1300.00000	17.25377	0.12138	0.44227P 01	0.11674	0.88524
1350.00000	19.68573	0.10409	0.45928E 01	0.10429	0.89571
1400.00000	22.51314	0.10119	0.47629P 01	0.09973	0.90427
1450.00000	29.47517	0.08571	0.49330E 01	0.07854	0.92042
1500.00000	33.62172	0.07431	0.51031E 01	0.07231	0.92749

1550.00000	42.46932	0.06030	0.527321 01	0.06749	0.03119
1600.00000	43.17642	0.05270	0.564337 01	0.06229	0.04771
1650.00000	70.10217	0.04504	0.561345 01	0.06304	0.04691
1700.00000	96.18398	0.02904	0.574345 01	0.03410	0.04490
1750.00000	105.10419	0.02618	0.595367 01	0.03702	0.04799
1800.00000	148.46449	0.02717	0.612372 01	0.02517	0.07493
1850.00000	148.46449	0.02717	0.629387 01	0.01798	0.08242
1900.00000	246.14901	0.01970	0.646395 01	0.01114	0.08462
1950.00000	445.11499	0.02724	0.660610 01	0.00524	0.09376
2000.00000	1036.01616	0.00672	0.697425 01	0.00887	0.09113
2050.00000	627.13525	0.00073	0.714435 01	0.00181	0.09419
2100.00000	9784.12422	0.00308			

DISTANCE	UMSW	NORMALIZED CONC. V	
		EXPERIMENTAL	COMPUTED FROM UMSW
0.0	-2.946725	0.99984	0.99984
20.000000	-3.203323	0.99997	0.99997
40.000000	-2.513744	0.99980	0.99980
60.000000	-2.545626	0.99941	0.99941
100.000000	-2.918544	0.99982	0.99981
120.000000	-2.618914	0.99984	0.99984
140.000000	-2.549034	0.99984	0.99984
160.000000	-2.647443	0.99989	0.99989
180.000000	-2.691332	0.99929	0.99929
200.000000	-2.916820	0.99987	0.99981
220.000000	-2.633426	0.99912	0.99912
240.000000	-2.032398	0.99814	0.99814
260.000000	-1.796890	0.99316	0.99315
280.000000	-1.413598	0.977203	0.977202
300.000000	-1.039833	0.92923	0.92923
320.000000	-0.967661	0.918737	0.918737
340.000000	-0.803887	0.872203	0.872203
360.000000	-0.625024	0.811630	0.811630
380.000000	-0.467061	0.745541	0.745541
400.000000	-0.314194	0.667451	0.667451
420.000000	-0.161140	0.672594	0.672594
440.000000	-0.210165	0.618850	0.618850
460.000000	-0.167923	0.560633	0.560633
480.000000	-0.021403	0.512075	0.512075
500.000000	0.007934	0.495501	0.495501
520.000000	0.065378	0.462970	0.462970
540.000000	0.099839	0.443858	0.443858
560.000000	0.136064	0.423737	0.423737
580.000000	0.161280	0.408833	0.408833
590.000000	0.189770	0.394785	0.394785
600.000000	0.221036	0.377295	0.377295
610.000000	0.250790	0.363892	0.363892
620.000000	0.245264	0.343319	0.343319
640.000000	0.256889	0.358214	0.358214
660.000000	0.287238	0.342792	0.342792
680.000000	0.310641	0.330218	0.330218
700.000000	0.336947	0.316904	0.316904
720.000000	0.359509	0.305360	0.305360
740.000000	0.376094	0.297425	0.297425
760.000000	0.405113	0.283351	0.283351
780.000000	0.411891	0.280177	0.280177
800.000000	0.437918	0.267854	0.267854
850.000000	0.441362	0.257051	0.257051
900.000000	0.528836	0.227256	0.227256
950.000000	0.571194	0.209605	0.209605
1000.000000	0.609087	0.196074	0.196074
1050.000000	0.628325	0.187113	0.187113
1100.000000	0.668785	0.165086	0.165086
1150.000000	0.702321	0.160798	0.160798
1200.000000	0.713517	0.136954	0.136954

1250.0000000	0.129024	0.129024	0.129024
1300.0000000	0.116759	0.116759	0.116759
1350.0000000	0.106284	0.106284	0.106284
1400.0000000	0.099732	0.099732	0.099732
1450.0000000	0.079581	0.079581	0.079581
1500.0000000	0.072214	0.072214	0.072214
1550.0000000	0.060951	0.060951	0.060951
1600.0000000	0.052299	0.052299	0.052299
1650.0000000	0.043293	0.043293	0.043293
1700.0000000	0.034594	0.034594	0.034594
1750.0000000	0.032022	0.032022	0.032022
1800.0000000	0.029171	0.029171	0.029171
1850.0000000	0.017918	0.017918	0.017918
1900.0000000	0.011302	0.011302	0.011302
1950.0000000	0.006243	0.006243	0.006243
2000.0000000	0.000870	0.000870	0.000870
2100.0000000	0.001014	0.001014	0.001014

0.749715
 0.849641
 0.849152
 0.823617
 0.749513
 0.711208
 0.649184
 0.572415
 0.513277
 0.449501
 0.409415
 0.383461
 0.349551
 0.310146
 0.249418
 0.176518
 2.049895

Fig. G1. Variable $u(x)$, determined from experimental vanadium compositions by the Newton-Raphson method, as a function of penetration distance.

Fig. Q2. Experimental concentration profile of vanadium as determined from electron microprobe analysis.

Fig. G3. Experimental concentration profile of titanium as determined by electron microprobe analysis.

Computer Output for Sample Problem 9, Part 1

DIFFUSION RUN 1

NOMINAL TEMPERATURE 1352.960

DIFFUSION TIME IN SEC 0.3640E 05

NOMINAL WT PERCENT V IN A 1.00
 NOMINAL WT PERCENT TI IN A 0
 NOMINAL WT PERCENT V IN B 0
 NOMINAL WT PERCENT TI IN B 100

PROFILE NUMBER 1

DISTANCE	INT RATIO V	INT RATIO TI	WT FRAC V	WT FRAC TI	AT FRAC V	AT FRAC TI
0.0	1.00000	0.00005	1.01747	0.00001	0.99999	0.00002
20.00000	0.93602	0.00001	1.01450	0.00000	1.00000	0.00000
40.00000	0.19981	-0.00006	1.01128	0.00002	0.99998	0.00002
60.00000	0.99730	-0.00039	1.01444	0.00015	0.99984	0.00016
100.00000	0.95664	0.00006	1.01357	0.00007	0.99993	0.00002
120.00000	0.94719	-0.00027	1.00950	0.00010	0.99990	0.00011
140.00000	0.99506	-0.00034	1.01474	0.00015	0.99984	0.00016
160.00000	0.97484	-0.00023	1.01491	0.00009	0.99991	0.00009
180.00000	0.99642	-0.00019	1.01490	0.00007	0.99993	0.00007
200.00000	0.99084	0.00006	1.01374	0.00002	0.99998	0.00002
220.00000	0.99247	0.00023	1.01190	0.00008	0.99991	0.00009
240.00000	0.98674	0.00043	1.00769	0.00176	0.99815	0.00145
260.00000	0.97407	0.01047	1.00426	0.00616	0.99352	0.00648
280.00000	0.97527	0.03196	0.98518	0.02161	0.97770	0.02280
300.00000	0.94431	0.08606	0.93131	0.06663	0.92929	0.07071
320.00000	0.97765	0.09891	0.92670	0.07701	0.91876	0.08124
340.00000	0.91324	0.14759	0.87044	0.12080	0.87720	0.12780
360.00000	0.74570	0.21017	0.82312	0.17978	0.81163	0.18837
380.00000	0.67011	0.27674	0.76344	0.24501	0.74554	0.25446
400.00000	0.60951	0.32311	0.71259	0.29164	0.69674	0.30326
420.00000	0.57875	0.34520	0.68554	0.31424	0.67259	0.32741
440.00000	0.51508	0.31902	0.63133	0.36871	0.61685	0.38315
460.00000	0.45965	0.45501	0.58164	0.42861	0.56085	0.43945
480.00000	0.41120	0.50573	0.53878	0.48271	0.51207	0.48793
500.00000	0.39606	0.52210	0.52261	0.50032	0.49550	0.50450
520.00000	0.36113	0.55266	0.48403	0.53338	0.44297	0.53703
540.00000	0.33340	0.56240	0.46172	0.54397	0.44386	0.55614
560.00000	0.30767	0.57461	0.43379	0.55727	0.42774	0.57626
580.00000	0.28465	0.60592	0.41124	0.59142	0.39883	0.60117
600.00000	0.29300	0.60727	0.41036	0.59297	0.39420	0.60579
620.00000	0.26632	0.62236	0.39282	0.60967	0.37730	0.62270
640.00000	0.27645	0.62173	0.40351	0.60492	0.38489	0.61611
660.00000	0.25603	0.63759	0.38195	0.62647	0.36434	0.63566
680.00000	0.24477	0.64087	0.37403	0.63005	0.35823	0.64177
700.00000	0.22352	0.65500	0.35358	0.64570	0.34229	0.64771
720.00000	0.22403	0.67691	0.35133	0.67006	0.33027	0.66978
740.00000	0.21474	0.68761	0.33647	0.68197	0.31690	0.68310

720.00000	0.20355	0.69701	0.52377	0.64247	0.30598	0.00867
740.00000	0.19798	0.70815	0.31737	0.70493	0.29745	0.70257
760.00000	0.18720	0.72603	0.30485	0.72497	0.28335	0.71665
780.00000	0.18196	0.72312	0.29668	0.72170	0.28013	0.71987
800.00000	0.17301	0.73966	0.28904	0.74030	0.26786	0.74214
850.00000	0.16422	0.75181	0.27744	0.75399	0.25705	0.74595
900.00000	0.15977	0.78358	0.26706	0.78992	0.27726	0.77274
950.00000	0.15506	0.80008	0.22307	0.80866	0.20960	0.79040
1000.00000	0.15412	0.81286	0.21353	0.82320	0.19608	0.80592
1050.00000	0.10748	0.82364	0.20553	0.83549	0.18711	0.81284
1100.00000	0.08865	0.83396	0.17807	0.84728	0.16501	0.83499
1150.00000	0.08540	0.83971	0.17335	0.85385	0.16030	0.83970
1200.00000	0.08982	0.86976	0.14996	0.88829	0.13700	0.86300
1250.00000	0.06335	0.86913	0.13936	0.88756	0.12903	0.87097
1300.00000	0.05478	0.89176	0.12596	0.91360	0.11476	0.88524
1350.00000	0.04834	0.90572	0.11512	0.92971	0.10429	0.89571
1400.00000	0.04253	0.90811	0.10499	0.93246	0.09573	0.90427
1450.00000	0.03281	0.92106	0.08712	0.94743	0.07958	0.92042
1500.00000	0.02880	0.93083	0.07948	0.95874	0.07231	0.92769
1550.00000	0.02280	0.94305	0.06704	0.97291	0.06085	0.93915
1600.00000	0.01844	0.95039	0.05760	0.98144	0.05229	0.94171
1650.00000	0.01406	0.95686	0.04737	0.98996	0.04309	0.94691
1700.00000	0.11027	0.97178	0.03778	1.00631	0.03410	0.96590
1750.00000	0.00942	0.97468	0.03551	1.00947	0.03207	0.96798
1800.00000	0.00667	0.97355	0.02769	1.00838	0.02517	0.97483
1850.00000	0.00408	0.98456	0.01943	1.02119	0.01748	0.98242
1900.00000	0.00219	0.98015	0.01246	1.01608	0.01138	0.98862
2000.00000	0.00094	0.99332	0.00489	1.03146	0.00624	0.99376
2050.00000	0.00159	0.99928	0.00988	1.03840	0.00987	0.99113
2100.00000	0.00017	0.99693	0.00700	1.03565	0.00181	0.99819

1550.00000	42.14432	0.36039	0.52722F 01	0.06085	0.93915
1600.00000	53.17642	0.05220	0.56433F 01	0.05224	0.94771
1650.00000	70.10217	0.04508	0.56136F 01	0.04309	0.94491
1700.00000	96.16198	0.02906	0.57436E 01	0.03410	0.96590
1750.00000	105.10419	0.02618	0.59536E 01	0.03222	0.94794
1800.00000	146.46465	0.02717	0.61237F 01	0.02517	0.97483
1850.00000	246.16521	0.01570	0.62438F 01	0.01754	0.92742
1900.00000	435.11498	0.02025	0.64639E 01	0.01134	0.98862
1950.00000	1036.01616	0.00672	0.66041F 01	0.00674	0.99376
2000.00000	427.11925	0.00073	0.69742F 01	0.00887	0.99113
2050.00000	5786.32422	0.00108	0.71431F 01	0.00101	0.99819
2100.00000					

MAXIMUM ATOM FRACTION VANADIUM			0.9999	NORMALIZED CONC V		NORMALIZED CONC V	
MINIMUM ATOM FRACTION VANADIUM			0.00181	EXPERIMENTAL		COMPUTED FROM LINE#	
MAXIMUM VANADIUM PENETRATION (MICRONS)			2100.00000				
DISTANCE	LINE#						
0.0	-2.946725		0.999984	0.999984	0.999984		
20.000000	-3.203533		0.999997	0.999997	0.999997		
40.000000	-2.903744		0.999980	0.999980	0.999980		
60.000000	-2.545636		0.999941	0.999941	0.999941		
100.000000	-2.918548		0.999982	0.999982	0.999981		
120.000000	-2.618914		0.999844	0.999844	0.999844		
140.000000	-2.549034		0.999844	0.999844	0.999844		
160.000000	-2.647443		0.999909	0.999909	0.999909		
180.000000	-2.691332		0.999929	0.999929	0.999929		
200.000000	-2.916820		0.999982	0.999982	0.999981		
220.000000	-2.633426		0.999912	0.999912	0.999912		
240.000000	-2.052398		0.998149	0.998149	0.998149		
260.000000	-1.756890		0.993516	0.993516	0.993515		
280.000000	-1.413598		0.977203	0.977203	0.977202		
300.000000	-1.039835		0.929243	0.929243	0.929243		
320.000000	-0.987661		0.918757	0.918757	0.918757		
340.000000	-0.803887		0.872203	0.872203	0.872203		
360.000000	-0.625024		0.811630	0.811630	0.811630		
380.000000	-0.467061		0.745541	0.745541	0.745541		
400.000000	-0.364196		0.696741	0.696741	0.696741		
420.000000	-0.316140		0.672595	0.672595	0.672595		
440.000000	-0.210165		0.616850	0.616850	0.616850		
460.000000	-0.107923		0.540653	0.540653	0.540653		
480.000000	-0.021405		0.516775	0.516775	0.516774		
500.000000	0.007974		0.495501	0.495501	0.495501		
520.000000	0.065728		0.462970	0.462970	0.462970		
540.000000	0.099839		0.443058	0.443058	0.443058		
560.000000	0.136006		0.423737	0.423737	0.423737		
580.000000	0.181280		0.398833	0.398833	0.398833		
590.000000	0.189770		0.394205	0.394205	0.394205		
600.000000	0.21036		0.377295	0.377295	0.377295		
610.000000	0.25790		0.383892	0.383892	0.383892		
620.000000	0.245244		0.364739	0.364739	0.364739		
640.000000	0.256809		0.358234	0.358234	0.358234		
660.000000	0.287238		0.342292	0.342292	0.342292		
680.000000	0.310641		0.330214	0.330214	0.330214		
700.000000	0.348847		0.316904	0.316904	0.316904		
720.000000	0.399909		0.303380	0.303380	0.303380		
740.000000	0.376054		0.297425	0.297425	0.297425		
760.000000	0.405113		0.283341	0.283341	0.283341		
780.000000	0.41891		0.280133	0.280133	0.280133		
800.000000	0.437918		0.267856	0.267856	0.267856		
850.000000	0.461362		0.257051	0.257051	0.257051		
900.000000	0.528456		0.227254	0.227254	0.227254		
950.000000	0.571196		0.209605	0.209605	0.209605		
1000.000000	0.605087		0.196076	0.196076	0.196076		
1050.000000	0.628325		0.187113	0.187113	0.187113		
1100.000000	0.688785		0.169006	0.169006	0.169006		
1150.000000	0.702321		0.160298	0.160298	0.160298		
1200.000000	0.773517		0.136995	0.136995	0.136995		

1250.-000000	0.799735	0.129024	0.129724
1300.-000000	0.849661	0.114759	0.114759
1350.-000000	0.889187	0.104244	0.104244
1400.-000000	0.923667	0.095732	0.095732
1450.-000000	0.995333	0.079581	0.079581
1500.-000000	1.031508	0.072314	0.072314
1550.-000000	1.094368	0.060851	0.060851
1600.-000000	1.147635	0.052295	0.052295
1650.-000000	1.213299	0.043093	0.043093
1700.-000000	1.289561	0.034094	0.034094
1750.-000000	1.369475	0.032022	0.032022
1800.-000000	1.383843	0.025171	0.025171
1850.-000000	1.489353	0.017474	0.017514
1900.-000000	1.610346	0.011382	0.011342
2000.-000000	1.766434	0.006243	0.006243
2050.-000000	1.676556	0.008470	0.008470
2100.-000000	2.056885	0.001414	0.001814

DEGREE OF POLYNOMIAL = 3 NUMBER OF SEGMENTS = 3

EQUATION FITTED IS

SEGMENT COEFFICIENTS IN ASCENDING ORDER -

A0	A1	A2	A3
-3.079202857178600	2.073218017462510-02	-0.703206316319770-05	1.044882220157600-09
1.000202857178600	4.8926941686402270-03	-5.298985615701530-06	2.221147943030940-09
-3.351108827323200-01	-3.4204907614251510-04	7.18040402510251940-07	-8.4594925427076130-11

SPLINE JOINTS ARE -

0.0	340.0000	070.0000	1070.000
0.0	340.0000	070.0000	1070.000

X	Y	Y ²	DY	H-10P
0.0	-2.491331W	00	-3.96870505927663700-01	0.14746249476474420-01
2.000000E	-2.9168194E	01	-2.25177347607482720-01	-0.27196614859546730-01
4.000000E	-2.533422E	01	-3.2527835279722400-01	-0.12154729518140000-01
6.000000E	-2.0523497E	00	-4.84625984566571200-02	-0.23629279462264700-01
8.000000E	-1.7568937E	00	-4.7790116154614900-02	-0.27201562666401290-01
1.000000E	-1.4133591E	00	-3.08207520500681800-02	-0.21816213174277700-01
2.000000E	-1.03980350E	01	-1.68821216162006870-01	-0.161768117174277700-01
3.000000E	-8.764112E-01	-01	-1.045496345034104100-02	-0.10646601871110300-01
4.000000E	-8.0127663E-01	-01	-8.84010412779647300-01	-0.11059496116776630-01
5.000000E	-6.2502644E-01	-01	-2.51257570277111300-02	-0.40149445494360000-01
6.000000E	-4.6704110E-01	-01	-4.13135361330450400-02	-0.48459411752650000-01
7.000000E	-3.6419545E-01	-01	-2.13462143041861300-02	-0.74059496849410400-01
8.000000E	-3.1613988E-01	-01	-1.62055209427067400-02	-0.11457167636314500-01
9.000000E	-2.1016528E-01	-01	-2.06273387305132400-02	-0.4848171602065574800-01
1.000000E	-1.079237E-01	-01	-4.61449732027607100-03	-0.42761492774064000-01
2.000000E	-7.1505334E-02	-02	-5.4649660519639000-04	-0.11900484968444700-01
3.000000E	7.9733615E-03	-03	-7.50187858641491100-04	-0.96079687400170270-01
4.000000E	6.9128088E-02	-02	-9.01242231363140800-03	-0.13172749329268300-01
5.000000E	9.4939032E-02	-02	-1.07460511932758940-03	-0.10755248764643300-01
6.000000E	1.3406012E-01	-01	-7.31233415368771100-04	-0.153766217327864400-02
7.000000E	1.8127990E-01	-01	-9.07635664064271900-03	-0.4008415545424000-01
8.000000E	1.8977046E-01	-01	-6.30501867688976300-04	-0.332724790392116600-02
9.000000E	2.2103366E-01	-01	-1.63726420194765200-02	-0.70246464927601400-01
1.000000E	2.214860631E-02	-02	-1.26491491466171300-03	-0.60849402272831300-01
2.000000E	2.36422371E-02	-02	-8.31611273453775500-03	-0.16087415490736600-01
3.000000E	2.6638388502864500-01	-01	9.5790003317256600-03	-0.17020907537164900-01
4.000000E	2.9640675259284400-01	-01	6.82959572016213100-03	-0.23775684160943300-01
5.000000E	3.2006647109856400-01	-01	9.4259572016213100-03	-0.10316161609433300-01
6.000000E	3.4649184526451200-01	-01	7.6649679257824700-03	-0.2249542366001100-01
7.000000E	3.67450237114205500-01	-01	7.54394770784349260-03	-0.2094243763711400-01
8.000000E	3.89048379356781400-01	-01	1.279633042119427100-02	-0.36456498787644100-01
9.000000E	4.28590125807670500-01	-01	4.2779469261136136700-03	-0.105645581627774900-01
1.000000E	4.46747015622554600-01	-01	1.67338651056136700-03	-0.29310110924907700-01
2.000000E	4.88287006421748000-01	-01	8.2828498440009994100-03	-0.58435941001129400-01
3.000000E	5.2885610E-01	-01	2.69245847068162900-02	-0.60409814617614900-02
4.000000E	5.60521895402323700-01	-01	-1.06760467466927600-02	-0.18461191371063300-01
5.000000E	5.9454637729647832700-01	-01	-1.05737724663032700-02	-0.1745115611049500-01
6.000000E	6.29603263165688500-01	-01	-1.078039242994901600-03	-0.17157344646666600-02
7.000000E	6.7023523E-01	-01	-2.22195223645086700-02	-0.13607178656461100-01
8.000000E	6.8878540E-01	-01	3.63720622536356300-03	-0.71715116464641000-01
9.000000E	7.0232141E-01			

1.0200000F 03	7.7351671E-01	7.4781111720489480-01	-2.5705597368011660-02	-0.3323211623649420-01
1.0700000F 03	7.9973507E-01	7.9197247714347970-01	-7.7674921314226070-03	-0.9706454548641030-02
1.1200000F 03	8.4966081E-01	8.1837442845445780-01	-1.1286385253483330-02	-0.1378350094136430-01
1.1700000F 03	8.8918269E-01	8.4649370376337570-01	-2.2283870155194450-03	-0.3906108747215790-02
1.2200000F 03	9.2366707E-01	9.3764703501730820-01	1.3979951767492270-02	0.1913528215129010-01
1.2700000F 03	9.553259E-01	9.9039115468104060-01	-5.1418368709124880-03	-0.514996512754370-02
1.3200000F 03	1.0315084E 00	1.0451227950408810 00	1.3616339301135140-02	0.1319849555578410-01
1.3700000F 03	1.0943680E 00	1.1017786886027800 00	7.4107074457288530-03	0.67771477874803440-02
1.4200000F 03	1.1476345E 00	1.1602955470726040 00	1.2481040847020120-02	0.1101231105228840-01
1.4700000F 03	1.2132488E 00	1.2206101633563480 00	7.3113637489245480-03	0.6026022413723870-02
1.5200000F 03	1.2795613E 00	1.2824592095599160 00	-6.9020621075643880-03	-0.5192256041808190-02
1.5700000F 03	1.3594749E 00	1.3463794379842380 00	3.4904492920878380-02	0.2818766740290830-01
1.6200000F 03	1.4388434E 00	1.4117075409502430 00	2.7844359014207510-02	0.2013536087203680-01
1.6700000F 03	1.4995535E 00	1.4785803707488600 00	-1.0073304078922540-02	-0.7366691826171700-02
1.7200000F 03	1.6103458E 00	1.6464365396910190 00	-6.39411370763083100-02	-0.4937744251987680-01
1.7700000F 03	1.7664375E 00	1.8878339442796770 00	-7.8603366287901100-02	-0.4449816743723950-01
1.8200000F 03	1.8765556E 00	1.760252444380340 00	8.3697010893112100-02	0.4992700033120430-01

CORRELATION OF FITTED DATA TO ORIGINAL DATA

STANDARD DEVIATION =	7.2227372862429770-03	CORRELATION INDEX =	0.8938927648750550 00
	8.4986688762057000-02	MAXIMUM CORRELATION =	0.8965517261379310 00

NO. REF IT CHECK MADE

DISTANCE	UNEM ITERATED	UF COMPUTED	AT PRAC V EXPERIMENTAL	AT PRAC V COMPUTED	DIFFERENCE	PERCENT DIFFERENCE
0.0	-0.269133E 01	-0.308820E 01	0.999927	0.999996	0.64194E-04	0.64199E-03
20.000000	-0.291682E 01	-0.269144E 01	0.999982	0.999929	-0.57096E-04	-0.57099E-03
40.000000	-0.265343E 01	-0.233089E 01	0.999912	0.999910	-0.40221E-03	-0.40223E-01
60.000000	-0.205240E 01	-0.200396E 01	0.998149	0.997702	-0.44718E-03	-0.44816E-01
80.000000	-0.174896E 01	-0.170910E 01	0.993515	0.992174	-0.13397E-02	-0.13488E-01
100.000000	-0.141386E 01	-0.144442E 01	0.977293	0.979463	0.22511E-02	0.23094E-01
120.000000	-0.103983E 01	-0.120805E 01	0.929293	0.946222	0.26922E-01	0.28078E-01
140.000000	-0.687681E 00	-0.998121E 00	0.918737	0.927963	0.22022E-02	0.23973E-01
160.000000	-0.803887E 00	-0.812770E 00	0.872203	0.874815	0.26049E-02	0.29412E-01
180.000000	-0.25024E 00	-0.450150E 00	0.811630	0.821072	0.94602E-02	0.11631E-01
200.000000	-0.467081E 00	-0.508376E 00	0.745541	0.743414	-0.18374E-01	0.24643E-01
220.000000	-0.364196E 00	-0.385591E 00	0.696747	0.707235	0.10647E-01	0.15444E-01
240.000000	-0.316140E 00	-0.279934E 00	0.672594	0.651905	-0.18837E-01	-0.27780E-01
260.000000	-0.21016E 00	-0.189538E 00	0.616850	0.605644	-0.11122E-01	-0.18128E-01
280.000000	-0.107923E 00	-0.112538E 00	0.560653	0.563226	0.25724E-02	0.45882E-01
300.000000	-0.216034E-01	-0.470723E-01	0.512074	0.526534	0.14661E-01	0.28246E-01
320.000000	0.797394E-02	0.872415E-02	0.495501	0.495079	-0.42334E-03	-0.87610E-01
340.000000	0.657281E-01	0.547152E-01	0.462970	0.468035	0.50699E-02	0.11442E-01
360.000000	0.998347E-01	0.987650E-01	0.441848	0.444439	0.25989E-03	0.11917E-01
380.000000	0.136006E 00	0.136737E 00	0.423337	0.423337	-0.40501E-03	-0.41941E-01
400.000000	0.181280E 00	0.172206E 00	0.398813	0.403796	0.49622E-02	0.12646E-01
410.000000	0.18970E 00	0.189140E 00	0.394205	0.394548	0.34314E-03	0.87047E-01
420.000000	0.221036E 00	0.205563E 00	0.377795	0.385637	0.78411E-02	0.2179E-01
430.000000	0.208790E 00	0.221486E 00	0.343897	0.377051	0.46390E-02	0.17615E-01
440.000000	0.245284E 00	0.236922E 00	0.364339	0.368797	0.44508E-02	0.12716E-01
460.000000	0.254809E 00	0.266388E 00	0.358234	0.351187	-0.50471E-02	-0.14289E-01
480.000000	0.287238E 00	0.294068E 00	0.342282	0.338791	-0.3409E-02	-0.10349E-01
500.000000	0.710641E 00	0.520366E 00	0.330218	0.325403	-0.48146E-02	-0.14589E-01
520.000000	0.336847E 00	0.344492E 00	0.316404	0.313066	-0.33849E-02	-0.12119E-01

540.000000	0.359404E 00	0.347450D 00	0.105340	0.301653	-0.17275E-02	-0.12206F 01
560.000000	0.376054E 00	0.349044D 00	0.297425	0.291092	-0.63332E-02	-0.21293F 01
580.000000	0.405113E 00	0.439390D 00	0.283351	0.281305	-0.20459E-02	-0.72188F 00
600.000000	0.431651E 00	0.428590D 00	0.280133	0.272218	-0.79190E-02	-0.78234F 01
620.000000	0.437918E 00	0.446747D 00	0.267856	0.263760	-0.40960E-02	-0.19202F 01
640.000000	0.461362E 00	0.488287D 00	0.257051	0.244927	-0.13124E-01	-0.47166F 01
670.000000	0.528856E 00	0.523657D 00	0.227756	0.228623	0.13670E-02	0.60131F 00
720.000000	0.571196F 00	0.560522D 00	0.209605	0.213977	0.43721E-02	0.20849F 01
820.000000	0.605087E 00	0.594549D 00	0.196076	0.200225	0.41488E-02	0.21139F 01
870.000000	0.628325E 00	0.629403D 00	0.187113	0.184703	-0.40954E-03	-0.21898F 00
920.000000	0.688745F 00	0.665763D 00	0.165006	0.172963	0.79564E-02	0.48221E 01
970.000000	0.707321E 00	0.705954D 00	0.160298	0.159050	-0.12481E-02	-0.27867F 00
1020.000000	0.771517E 00	0.747811D 00	0.136993	0.145127	0.81314E-02	0.99356F 01
1070.000000	0.799735E 00	0.791972D 00	0.129028	0.131353	0.23240E-02	0.18017F 01
1120.000000	0.849661E 00	0.838374D 00	0.114759	0.117882	0.31232E-02	0.27216F 01
1170.000000	0.889182E 00	0.886954D 00	0.104288	0.104859	0.57171E-03	0.54782F 00
1220.000000	0.927667E 00	0.937647D 00	0.094732	0.092416	-0.33171E-02	-0.37663F 01
1270.000000	0.995513E 00	0.990391D 00	0.079541	0.080663	0.13822E-02	0.13599F 01
1320.000000	0.103151E 01	0.104512D 01	0.072314	0.069702	-0.26136E-02	-0.36140F 01
1370.000000	0.109437E 01	0.110178D 01	0.060851	0.059399	-0.19520E-02	-0.20974F 01
1420.000000	0.114763E 01	0.116030D 01	0.052294	0.050408	-0.18960E-02	-0.36064F 01
1470.000000	0.121330E 01	0.122061D 01	0.043093	0.042194	-0.93797E-03	-0.21766F 01
1520.000000	0.128956E 01	0.129766D 01	0.034094	0.034462	0.74483E-03	0.21849F 01
1570.000000	0.130947E 01	0.134638D 01	0.032022	0.028451	-0.33710E-02	-0.11132F 02
1620.000000	0.138346E 01	0.141171D 01	0.025171	0.022942	-0.27286E-02	-0.88499F 01
1670.000000	0.148455E 01	0.147854D 01	0.017578	0.018263	0.68437E-03	0.38932F 01
1720.000000	0.161015E 01	0.154693D 01	0.011382	0.014365	0.29440E-02	0.24041F 02
1820.000000	0.174646F 01	0.169783D 01	0.006243	0.008494	0.22515E-02	0.36037F 02
1870.000000	0.187646E 01	0.176024D 01	0.008670	0.006199	-0.26714E-02	-0.27867F 02

BOLTZMANN-MATANO INTERFACE = 488.9976

DISTANCE	AT FPAC V	AT FRAC TI	SLOPE	AREA	INTERDISPERSSION D-VALUE VS MATANO CURVE
2.00000	0.99999	0.00001	-0.107847-04	0.911749-03	0.49999W-14
4.00000	0.99999	0.00001	-0.122867-05	0.947666-02	0.11619W-09
6.00000	0.99999	0.00002	-0.211057-05	0.784208-02	0.16743W-09
10.00000	0.99996	0.00004	-1.41610E-05	0.14213E-01	0.19743W-09
14.00000	0.99994	0.00006	-0.62584E-05	0.23318E-01	0.22116E-09
18.00000	0.99991	0.00009	-0.92299E-05	0.28278E-01	0.23969W-09
22.00000	0.99987	0.00013	-0.13356E-04	0.39355E-01	0.25589W-09
26.00000	0.99980	0.00020	-0.14978E-04	0.48277E-01	0.27036W-09
30.00000	0.99971	0.00029	-0.24496E-04	0.12092E-01	0.28376W-09
34.00000	0.99959	0.00041	-0.34371E-04	0.18452E-01	0.29614W-09
38.00000	0.99942	0.00054	-0.4126E-04	0.26273E-01	0.30949W-09
42.00000	0.99919	0.00081	-0.63233E-04	0.36618E-01	0.32242W-09
46.00000	0.99889	0.00111	-0.89565E-04	0.49667E-01	0.33479W-09
50.00000	0.99850	0.00150	-0.11047E-03	0.66713E-01	0.34943W-09
54.00000	0.99800	0.00200	-0.14067E-03	0.88390E-01	0.36363W-09
58.00000	0.99737	0.00263	-0.17675E-03	0.11551E-01	0.37927E-09
62.00000	0.99658	0.00342	-0.21977E-03	0.14909E-01	0.39469W-09
66.00000	0.99560	0.00440	-0.26970E-03	0.19308E-01	0.40919W-09
70.00000	0.99442	0.00558	-0.32543E-03	0.23533E-01	0.42494E-04
74.00000	0.99299	0.00701	-0.38972E-03	0.27848E-01	0.44123W-09
78.00000	0.99129	0.00871	-0.46169E-03	0.36803E-01	0.46110W-09
82.00000	0.98929	0.01071	-0.54133E-03	0.49813E-01	0.48016W-09
86.00000	0.98695	0.01305	-0.62844E-03	0.64286E-01	0.49889W-09
90.00000	0.98425	0.01575	-0.72248E-03	0.83205E-01	0.52049E-03
94.00000	0.98116	0.01884	-0.82353E-03	0.17148E-01	0.54213W-09
98.00000	0.97764	0.02235	-0.93035E-03	0.30789E-01	0.56471E-09
102.00000	0.97371	0.02629	-0.10423E-02	0.10497E-02	0.58834E-09
106.00000	0.96931	0.03049	-0.11985E-02	0.12273E-02	0.61306W-09
110.00000	0.96444	0.03556	-0.12780E-02	0.14110E-02	0.63893E-09
114.00000	0.95908	0.04097	-0.13996E-02	0.16107E-02	0.66601E-09
118.00000	0.95324	0.04676	-0.15221E-02	0.18263E-02	0.69434E-09
122.00000	0.94691	0.05309	-0.16445E-02	0.20574E-02	0.72400W-09
126.00000	0.94008	0.05992	-0.17657E-02	0.23037E-02	0.75504W-09
130.00000	0.93278	0.06727	-0.18843E-02	0.25643E-02	0.78733W-09
134.00000	0.92501	0.07499	-0.19994E-02	0.28385E-02	0.82194W-09
138.00000	0.91679	0.08321	-0.21102E-02	0.31244E-02	0.85713W-09
142.00000	0.90814	0.09184	-0.22155E-02	0.34240E-02	0.89417E-09
146.00000	0.89908	0.10092	-0.23145E-02	0.37310E-02	0.93114W-09
150.00000	0.88963	0.11037	-0.24067E-02	0.40513E-02	0.97416E-09
154.00000	0.87983	0.12017	-0.24913E-02	0.43775E-02	0.10149W-09
158.00000	0.86971	0.13029	-0.25680E-02	0.47104E-02	0.10614W-09
162.00000	0.85930	0.14070	-0.26363E-02	0.50489E-02	0.11083W-09
166.00000	0.84866	0.15137	-0.26961E-02	0.53913E-02	0.11537E-09
170.00000	0.83774	0.16224	-0.27473E-02	0.57363E-02	0.12044E-09
174.00000	0.82667	0.17333	-0.27975E-02	0.60832E-02	0.12419W-09
178.00000	0.81544	0.18456	-0.28433E-02	0.64302E-02	0.12799W-09
182.00000	0.80409	0.19591	-0.28840E-02	0.67763E-02	0.13176W-09
186.00000	0.79266	0.20734	-0.29260E-02	0.71204E-02	0.13479W-09
190.00000	0.78117	0.21883	-0.29752E-02	0.74615E-02	0.13814W-09
194.00000	0.76967	0.23033	-0.29768E-02	0.77987E-02	0.14184W-09
198.00000	0.75817	0.24183	-0.29712E-02	0.81307E-02	0.14584W-09
202.00000	0.74671	0.25329	-0.29589E-02	0.84576E-02	0.14979W-09
206.00000					

210.00000	0.73530	0.26470	-0.28403E-02	0.87800E 02	0.17884E-08
214.00000	0.73399	0.27601	-0.28159E-02	0.90914E 02	0.18484E-08
218.00000	0.73279	0.28721	-0.27461E-02	0.93973E 02	0.19141E-08
222.00000	0.73171	0.29829	-0.27915E-02	0.96953E 02	0.20191E-08
226.00000	0.73078	0.30422	-0.27126E-02	0.99849E 02	0.21302E-08
230.00000	0.68001	0.31994	-0.26698E-02	0.10266E 03	0.22253E-08
234.00000	0.66434	0.33057	-0.26235E-02	0.10538E 03	0.23245E-08
238.00000	0.64903	0.34097	-0.25743E-02	0.10801E 03	0.24280E-08
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442.00000	0.36718	0.63282	-0.80442E-03	0.15764E 03	0.11340E-07
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