

STATEQ: A Nonlinear Least-Squares Code for Obtaining Martin Thermodynamic Representations of Fluids in the Gaseous and Dense Gaseous Regions

S. L. Milora

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MARTIN THERMODYNAMIC REPRESENTATIONS OF FLUIDS
IN THE GASEOUS AND DENSE GASEOUS REGIONS

S. L. Milora

FEBRUARY 1976

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ABSTRACT

This report describes the use of the code NLIN (IBM Share Program No. 1428) to obtain empirical thermodynamic pressure-volume-temperature (P-V-T) relationships for substances in the gaseous and dense gaseous states. When sufficient experimental data exist, the code STATEQ will provide least-squares estimates for the 21 parameters of the Martin model. Another code, APPROX, is described which also obtains parameter estimates for the model by making use of the approximate generalized behavior of fluids.

Use of the codes is illustrated in obtaining thermodynamic representations for isobutane.

1. INTRODUCTION

This report describes the application of a nonlinear least-squares code to the estimation of the Martin-Hou equation-of-state parameters. The unmodified FORTRAN computer program NLIN (IBM Share Program No. 1428) and the algorithm upon which it is based are described in Ref. 1. The algorithm which was developed by Marquardt essentially interpolates between the Taylor series and the maximum descent methods by specifying at successive iterations the maximum neighborhood in which the Taylor series approximation to the nonlinear model is adequate. This approximation results in a marked reduction in computing time relative to the steepest descent method and assures convergence to the stationary point for any reasonable initial estimate of the parameters.

As presently comprised, the code NLIN can accommodate up to 50 independent parameters and as many as 1000 data points. In this application, 21 parameters are used although only 18 are varied independently.

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There are two strategies available for selecting the 21 equation-of-state parameters, and the method applicable in each case is dependent upon the quality and type of experimental pressure-volume-temperature data available. The two approaches are treated here, and a specific example is discussed, with isobutane being the test case.

To facilitate understanding and use of the code, a brief description of the nonlinear theory upon which the algorithm is based is presented first.

2. MATHEMATICAL DESCRIPTION OF NONLINEAR PARAMETER ESTIMATION

Let the n data points to which the model is to be applied be given by:

$$(P_i, T_{r_i}, v_{r_i}) \quad i = 1, n,$$

where P_i represents the pressure of the i th data point; and T_{r_i} and v_{r_i} , the corresponding values of reduced temperature and specific volume ($T_{r_i} = T_i/T_c$, $v_{r_i} = v_i/v_c$). The model which describes the pressure in terms of the independent variables T_r and v_r can be written in generalized form as follows:

$$E(P) = f(T_r, v_r, \vec{\beta}), \quad (2.1)$$

where the notation $E(P)$ has been introduced in order to distinguish between the expected and observed values of pressure. In the above formulation, $\vec{\beta}$ represents the vector of equation-of-state parameters whose components are $\beta_1, \beta_2, \dots, \beta_{21}$. In the Martin-Hou representation, a maximum of up to 18 parameters may be varied independently. The values of the remaining three parameters (chosen arbitrarily to be β_1, β_4 , and β_7) are prescribed by the three constraint relationships which describe the necessary conditions at the thermodynamic critical point. A brief description of the form of the equation of state and the methodology employed to handle critical point constraints is presented in Appendix A.

In the usual sense, specific values of the parameters $\vec{\beta}$ are chosen so as to minimize the sum of the squares of the residuals, or errors of prediction, for the available data. If the residual is defined on a

percentage error basis, then the quantity to be minimized will be:

$$\varphi = \sum_{i=1}^n (\text{RES}_i) = \sum_{i=1}^n \left[\frac{P_i - E(P_i)}{P_i} \right]^2, \quad (2.2)$$

and, hence, the necessary conditions for a stationary point are:

$$\varphi = \text{minimum} \Rightarrow \partial\varphi/\partial p_j = 0 \quad \text{for } j \neq 1, 4, 7. \quad (2.3)$$

Implicit in Eqs. (2.2) and (2.3) is the understanding that the dependent parameters β_1 , β_4 , and β_7 have been eliminated by the critical point constraints.

If the individual components of $\vec{p}$ appear linearly in the equation-of-state representation, then the surfaces of constant φ would be ellipsoids in the multidimensional parameter space; and Eq. (2.3) would reduce to a system of 18 linear equations (normal equations) with 18 unknowns, the solution of which would be straightforward. If, as in the case here, the P-V-T representation is nonlinear in some or all of the parameters $\vec{\beta}$, then an iterative technique is required which proceeds from some initial estimate, $\vec{\beta}_0$, to the value $\vec{\beta}$ which minimizes φ .

In practice, two methods are commonly employed to obtain the least-squares estimates of $\vec{\beta}$. In the Taylor series method, the function $f(T_r, v_r, \vec{\beta})$ is expanded about a point $\vec{\beta}_0$ to first order in a small correction vector $\vec{\delta}_t$, and the following linearized (approximate) model results:

$$f_t(v_r, T_r, \vec{\beta}_0 + \vec{\delta}) \approx f(v_r, T_r, \vec{\beta}_0) + \sum_i \frac{\partial f(v_r, T_r, \vec{\beta})}{\partial \beta_i} \delta t_i, \quad (2.4)$$

where it is understood that the multidimensional gradient operator, $\partial/\partial \vec{\beta}$, does not operate on dependent parameters (or any other parameters whose values are to remain constant). When Eq. (2.4) is substituted into Eq. (2.3), a system of linear equations results which, when solved, gives that value of the correction vector $\vec{\delta}_t$ which minimizes φ_t , the sum of the squares of the residuals for the approximate linearized model. By adding this value of $\vec{\delta}_t$ to the original vector and by repeating the process at the new point, $\vec{\beta}_0 + \vec{\delta}_t$, a second approximation to the least-

squares estimate of $\vec{\beta}$ is obtained. Successive iterations are performed until a true minimum in φ is obtained which yields the desired result $\vec{\beta}$.

This method is certain to converge only if the original estimate, $\vec{\beta}_0$, is sufficiently close to the true minimum such that the truncated Taylor series represents, reasonably well, the nonlinear model in the interval between $\vec{\beta}_0$ and $\vec{\beta}$. If this condition is not satisfied, then the iterations will most likely diverge.

In the method of steepest descent, convergence is practically assured; however, machine calculation times are frequently prohibitively large. The stationary point is reached by taking a succession of incremental steps that are parallel, locally, to the normal of the surfaces of constant φ ; that is,

$$\vec{\delta}_i \text{ (} i\text{th iteration)} = \kappa \frac{\vec{\nabla} \varphi}{|\vec{\nabla} \varphi|} \bigg|_{\vec{\beta}=\vec{\beta}_i}$$

and

$$\vec{\beta}_{i+1} = \vec{\beta}_i + \vec{\delta}_i.$$

To accelerate convergence, the constant κ is adjusted so that the angle between any two successive correction vectors is greater than zero but less than $\pi/2$. Still, if the model is highly nonlinear, the direction of the initial correction vector may not be optimum although convergence will eventually occur.

As described by Marquardt,¹ the method upon which NLIN is based interpolates between the two methods. This is accomplished by introducing into the approximate Taylor series method a constraint condition which minimizes φ for the approximate linearized model in the spherical region $|\vec{\delta}| \leq |\vec{\delta}_0|$, where $\vec{\delta}_0$ is of arbitrary size. The region $|\vec{\delta}_0|$ may be increased (or decreased) by decreasing (or increasing) the Lagrange multiplier λ . If the maximum neighborhood $|\vec{\delta}_0|$ is made too large, then the modified Taylor series method may diverge. On the other hand, if the region $|\vec{\delta}_0|$ is made infinitesimally small (by choosing λ large), the modified method will give correction vectors $\vec{\delta}_t$ at each iteration that are parallel to the correction vector prescribed by the method of steepest descent and convergence will be assured but at the expense of increased

computation time. Essentially, the modified method attempts to find at each iteration the maximum neighborhood $|\vec{\delta}_0|$ within which the truncated Taylor series adequately represents the nonlinear model. Once this has been done, the correction vector $\vec{\delta}_t$ is easily found by solving the resulting system of normal equations (linear), and the iteration process is continued until the stationary point is found.

3. OPERATIONAL DESCRIPTION OF THE CODE

There are two methods that may be employed to determine the equation-of-state coefficients. Since the Martin equation is particularly suited to describing the state of the fluid in the dense gaseous region at supercritical pressures, a pressure-volume fit along an isotherm near the critical temperature is helpful in ensuring the quality of the fit at supercritical temperatures and pressures. As a matter of convenience, the critical isotherm is chosen for this initial step, since application of the Van der Waals conditions at the thermodynamic critical point (first and second derivatives of pressure with respect to volume must vanish) reduces the equation to one of 18 independent parameters.

3.1 Critical Isotherm Data Available

As described in Appendix A, the form of the equation of state for the critical isotherm alone reduces to one of eight parameters, and six of these appear linearly. By applying the constraint conditions at the critical point, three of the linear coefficients are eliminated, and the equation is reduced to one having three linear and two nonlinear parameters. The code STATEQ is used to determine these five coefficients (and, hence, the three dependent coefficients) by supplying only critical isotherm data and by specifying that only five parameters are to be varied. The parameters p_i of Eq. (2.1) are identified with the vector PAR(I), $I = 1 - 21$ in subroutine FCODE of STATEQ. The relationships to the equation-of-state coefficients of Appendix A are as follows:

Dependent parameters [functions of a , b , and $f_i(1)$, $i = 4 - 6$]:

$$\text{PAR}(1) = f_1(1) \quad \text{PAR}(4) = f_2(1) \quad \text{PAR}(7) = f_3(1)$$

Independent parameters:

	PAR(2) = B_1	PAR(3) = C_1
	PAR(5) = B_2	PAR(6) = C_2
	PAR(8) = B_3	PAR(9) = C_3
PAR(10) = $f_4(1)$	PAR(11) = B_4	PAR(12) = C_4
PAR(13) = $f_5(1)$	PAR(14) = B_5	PAR(15) = C_5
PAR(16) = $f_6(1)$	PAR(17) = B_6	PAR(18) = C_6
PAR(19) = K	PAR(20) = a	PAR(21) = b

In all cases, PAR(1), PAR(4), and PAR(7) are not to be varied independently, and this information must be passed on to STATEQ with the input data. Along the critical isotherm ($T_c = 1$), the terms involving the coefficients B_i and C_i ($i = 1 - 6$) and K cancel; and hence, their associated parameters do not enter into the calculations. Information that they are not to be varied should also be included as input, if the critical isotherm alone is to be determined. Initial estimates of the values of all the parameters must be supplied, and this will be taken up in a later paragraph. When the code is operated in this manner, only critical isotherm data (P-V-T) are used. The procedure then determines the coefficients $f_i(1)$ ($i = 1 - 6$), a , and b .

The remaining 13 coefficients are found by operating STATEQ with all available P-V-T data while holding the 8 previously determined coefficients constant. This procedure determines the coefficients B_i , C_i , ($i = 1 - 6$), and K . A greater emphasis can be placed on different regions of the P-V-T domain by weighting these regions more heavily with additional data.

3.2 Critical Isotherm Data Unavailable

If data along the critical isotherm are not available, then all 21 coefficients must be determined simultaneously by STATEQ. All available P-V-T data are supplied as input; and only PAR(1), PAR(4), and PAR(7) are held constant. Frequently, this is the method that must be used, since accurate critical isotherm data are available for only a few compounds.

3.3 Initial Parameter Estimates

STATEQ requires an initial estimate of all 21 parameters, which should be reasonably close to the optimum value in order to minimize machine calculation times. Martin² describes the strategy for estimating the parameters when the critical isotherm is known. This means that results of Method 1 above must be available before the initial values can be determined, but the initial estimates are needed by STATEQ to perform the calculations in Method 1. The problem can be resolved by using as estimates for Method 1 the known equation-of-state parameters of another fluid. The fact that the equation-of-state coefficients are expressed in reduced or dimensionless form makes this possible, since the approximate law of corresponding states asserts that different fluids that are at the same reduced temperature and reduced volume will have nearly the same value of reduced pressure.

The code APPROX, which is based upon the procedure recommended by Martin, was written to provide the estimates of the remaining parameters (exclusive of the eight critical isotherm coefficients). In this code, certain generalized facts about the P-V-T behavior of compounds are used to determine the coefficients. The fit is obtained without the need for P-V-T data; but a knowledge of the second and third virial coefficients, the Boyle temperature, and the slope of the vapor pressure curve at the critical point is required along with other miscellaneous known facts about the compound. In all, twelve known facts are required to set up a system of linear equations which are solved for the remaining unknown equation-of-state coefficients. A value for the nonlinear temperature exponent K must be assumed. The fit obtained is compared with the available P-V-T data, and small adjustments in the facts can be made to improve the accuracy. This technique can be used to refine the coefficients, but the method is tedious and does require a knowledge of the behavior along the critical isotherm. In using this technique to describe the P-V-T behavior of ammonia, Milora³ found that the representation obtained in this manner was considerably less accurate than that determined by the nonlinear least-squares approach (Methods 1 and 2 above). It does, however, provide good estimates for the nonlinear code.

If critical isotherm data are lacking, then APPROX cannot be used to obtain initial parameter estimates for STATEQ; and the estimates must then be obtained from another fluid (preferably a homologous compound). Under these circumstances, Method 2 would be used to refine the estimates.

4. PROCEDURAL OPERATION OF THE CODES STATEQ AND APPROX

4.1 APPROX

When the eight critical isotherm coefficients are known (determined by STATEQ), then APPROX may be used to estimate the remaining 13 coefficients for the compound being considered. The user must supply to the main body of the program (a read or data statement may be substituted) values of the critical temperature T_c in degrees Rankine, the critical pressure P_c in atmospheres, the critical volume v_c in ft^3/lb_m , the critical compressibility factor Z_c (dimensionless), and the specific gas constant R in $\text{atm-ft}^3/(\text{lb}_m\text{-}^\circ\text{R})$. Provision is made for comparing the predicted and experimental values of pressure by transmitting in a read statement the experimental values of pressure, volume, and temperature. This comparison may be omitted by removing the appropriate statements. The sequence for reading the experimental data is identical to that described in subroutine INPUT of STATEQ.

The code variables are identified with the equation-of-state variables of Appendix A as follows:

<u>FORTTRAN variable</u>		<u>Designation</u>
FTC(I)	(I = 1 - 6) supplied by user	$f_i(1)$
A(I)	"	A_i
B(I)	"	B_i
C(I)	"	C_i
AR	} determined by code	a
BR		b
RK		K

<u>FORTTRAN variable</u>	<u>Designation</u>
TC	critical temperature, T_c ($^{\circ}\text{R}$)
PC	critical pressure, P_c (atm)
VC	critical specific volume, v_c (ft^3/lb_m)
ZC	critical compressibility factor, Z_c
R	gas constant [$\text{atm}\cdot\text{ft}^3/(\text{lb}_m\cdot^{\circ}\text{R})$]
TR	reduced temperature, $T_r = T/T_c$
VR	reduced volume, $v_r = v/v_c$
PR	reduced pressure, $P_r = P/P_c$

Additional code variables are defined as follows:

<u>FORTTRAN variable</u>	<u>Designation</u>
PEXP	experimental pressure (psia)
VEXD	experimental specific volume (ft^3/lb_m)
TEXP	experimental temperature ($^{\circ}\text{F}$)

4.1.1 Input for APPROX

For each compound, the thermodynamic constants TC, PC, VC, ZC, and R must be supplied to the main body of the code. In addition, an assumed value of the equation-of-state temperature exponent, RK, must be supplied in this fashion. Only a slight modification to the code would be required to transfer this information via a read statement instead.

APPROX also requires as input the eight known critical isotherm coefficients FTC(I), $I = 1-6$, AR, and BR. This is accomplished by an internal read statement.

If a comparison of the resultant fit is to be made with experimental data, then the isobars [PEXP(I), $I = 1, \text{NEXP}$] and isotherms [TEXP(I), $I = 1, \text{NEXT}$] along with the value of specific volume VEXD(K) corresponding to the j th isotherm and the i th value of pressure must be supplied in a read statement. Data input is accomplished by reading sequentially volume/pressure pairs along consecutive isotherms (see INPUT in description of STATEQ). In its present form, APPROX will accept data in engineering units (psia, $^{\circ}\text{F}$, ft^3/lb_m), although all calculations are performed in reduced or dimensionless variable format. Temperatures are converted to absolute [T ($^{\circ}\text{R}$) = T ($^{\circ}\text{F}$) + 459.69] for the nondimensionalization step.

4.1.2 Output from APPROX

As output, APPROX prints the following information:

a. Input parameters — Critical temperature (TC), critical pressure (PC), critical specific volume (VC), assumed value of the dimensionless temperature exponent (RK), and the dimensionless critical isotherm equation-of-state coefficients [AR, BR, FTC(I), I = 1 – 6].

b. Resultant dimensionless equation-of-state coefficients — A(I), B(I), C(I), for I = 1 – 6.

c. A comparison of calculated and experimental values of pressure using the resulting equation-of-state coefficients — The predicted value of pressure is calculated in subroutine PRESRE for each temperature-volume pair, the temperature in °R and the volume in ft^3/lb_m . The calculated and experimental pressures (in psia) at each thermodynamic state point as well as the percentage error are printed. Temperatures are converted to absolute units (°K) for this step.

If no data are available, then step (c) can be omitted by removing the appropriate sections in the main body of the code.

4.2 STATEQ

STATEQ is the title of the modified version of NLIN that is used to obtain refined estimates of the Martin equation-of-state coefficients. As described in Sects. 3.1 and 3.2, it may be operated in a number of different ways depending upon the type and quality of data available. If the critical isotherm is known accurately, then it is generally advisable to use STATEQ to first generate a critical isotherm fit. Then, by specifying to the code that the 8 known critical isotherm coefficients are to remain unchanged, STATEQ is applied to all additional data to refine the estimates of the remaining 13 coefficients. In the absence of critical isotherm data, the first step must be omitted.

Only those parts of the code relevant to its use are discussed here.

4.2.1 MAIN

The MAIN section of STATEQ serves as a calling program for subroutine MARQ, which performs the least-squares calculation and manages all input

and output steps. In addition, MAIN sets absolute limits for the number of data points (NDPM), the number of function parameters (NPM), and the number of independent variables (NXM). The following values for these parameters are transferred to subroutine MARQ in the argument list:

```

NDPM = 1000 = maximum number of data points,
NPM  =   50 = maximum number of parameters,
NXM  =    6 = maximum number of independent variables.

```

The user need not utilize the full code capability.

4.2.2 Subroutine TSET

TSET assigns values to the input/output units which are identified with the following devices:

```

Card reader           = NI
Line printer          = NO
Card punch            = NP
Scratch disk (not used) = NST

```

Presently, the numerical values 5, 6, 7, and 3 are assigned to NI, NO, NP, and NST, respectively. The user has the option to assign those values which are compatible with the installation being used.

4.2.3 Subroutine MARQ

Subroutine MARQ manages all input and output steps and performs the calculations necessary to obtain the equation-of-state coefficients. In the original version of NLIN, MARQ represents the main or driver section of the code. It has subsequently been rewritten as a subroutine by W. Davis, Jr., of ORNL to allow data to be transmitted from MAIN, but this option is not employed in the application discussed here. If the user wishes to transmit input data in this fashion, the variable IREAD must be assigned an integer value greater than unity in MAIN.

In the method employed here, MARQ calls subroutine INPUT, which provides all necessary P-V-T data including the properties of the compound at the thermodynamic critical point. Switches, algorithm convergence parameters, and other code control parameters are read internally by MARQ.

Subroutine FCODE provides to MARQ the analytical form of the equation-of-state representation. In subroutine PCODE, differentiation of the equation of state with respect to the coefficients is performed by finite differences. Refined values of the coefficients are provided on punched cards by subroutine OUTPUT. Additional results, including a comparison of the fit with the data, are sent to the line printer by MARQ.

The following is an abbreviated list of key MARQ FORTRAN variables as they relate to the equation-of-state variables in Appendix A:

<u>MARQ variable</u>	<u>Designation</u>
B(I), I = 1, 4, 7, 10, 13, 16	$f_i(1)$, $i = 1 - 6$
B(I), I = 2, 5, 8, 11, 14, 17	B_i , $i = 1 - 6$
B(I), I = 3, 6, 9, 12, 15, 18	C_i , $i = 1 - 6$
B(19)	K
B(20)	a
B(21)	b
B(J), J = 22 to 50	Unused portion of parameter vector
F	P; computed value of pressure (dependent variable)
X(I,1), X(I,2), I = 1 to NDPM	T_i, v_i ; values of temperature and specific volume for i th data point (independent variables)
X(I,5), X(I,6), I = 1 to NDPM	$T_{r,i}, v_{r,i}$; reduced value of temperature and specific volume for i th data point
X(I, 3), X(I,4), I = 1 to NDPM	Unused portion of independent variable array
Y(J), J = 1 - 1000	P_j ; vector of experimental pressures
PRNT(1), PRNT(2)	Additional information to be printed along with experimental and calculated values of pressure. Set equal to the temperature and specific volume of the i th data point, respectively (T_i and v_i)
RES	Residual = $[F - Y(I)/Y(I)]$; i.e., 100 times percent difference for i th data point

Other variables and switches that are required as input to the algorithm are discussed in the Sect. 4.2.9. The user is referred to Refs. 1 & 4 for a more detailed description of these variables.

4.2.4 Subroutine INPUT

Subroutine INPUT provides to MARQ all pressure-volume-temperature data as well as the properties of the compound at the thermodynamic critical point. The former are transmitted in punched card format, while the latter must be supplied by way of an internal data statement. In addition, INPUT reduces the data to the dimensionless format required by subroutine FCODE. As presently comprised, INPUT accepts data in units of °F, psia, and ft^3/lb_m and converts temperatures to absolute units (°R) before dividing all properties by their respective critical values which must have units of °R, psia, and ft^3/lb_m . It is a simple matter to modify INPUT to accept data in any system of units. Modification of other subroutines is not required since the calculations are performed in dimensionless format.

INPUT first reads the title, or compound identification cards, which the user supplies (see Sect. 4.2.9). These cards may be left blank, but they must be included in the input deck. The next read statement supplies the total number of isobars (NEXP) and isotherms (NEXT) for which some data are available. The vector of isobars, PEXP(I), is read next. INPUT then reads sequentially the j th isotherm, the number of specific volumes, NDUM, for that isotherm, and the corresponding vector of specific volumes VEXD(I), $I = 1$ to NDUM. Note that VEXD is a dummy array whose elements are renewed at each isotherm. The individual elements of this vector are identified with the specific volumes corresponding to the first NDUM values of the experimental pressure vector PEXP for the isotherm being considered. The value of NDUM is transferred to the j th element of the vector NEXV. This process is repeated until the data for all isotherms have been exhausted.

Table 1 illustrates the procedure described above for an arbitrary compound. During the process of reading the isotherms, the experimental points are transferred to the arrays $X(L,1)$ [absolute temperature], $X(L,2)$ [specific volume], and $Y(L)$ [pressure], according to the numbering sequence shown. The absolute temperature and specific volume arrays are converted to the reduced temperature and reduced volume arrays $X(L,5)$ and $X(L,6)$ for use internally.

Table 1. Sequential ordering of pressure-volume-temperature data for STATEQ and APPROX

	TEXP(1); NEXV(1) = NDUM	TEXP(2); NEXV(2) = NDUM	TEXP(NEXT); NEXV(NEXT) = NDUM
PEXP(1):	VEXD(1) X(1,1) X(1,2) Y(1)	VEXD(1) X[NEXV(1) + 1,1] X[NEXV(1) + 1,2] Y[NEXV(1) + 1]	VEXD(1) X[NEXV(1) + NEXV(2) ... + NEXV(NEXT - 1) + 1,1] X[NEXV(1) + NEXV(2) ... + NEXV(NEXT - 1) + 1,2] Y[NEXV(1) + NEXV(2) ... + NEXV(NEXT - 1)]
PEXP(2):	VEXD(2) X(2,1) X(2,2) Y(2)	VEXD(2) X[NEXV(1) + 2,1] X[NEXV(1) + 2,2] Y[NEXV(1) + 2]	VEXD(2) X[NEXV(1) + NEXV(2) ... + NEXV(NEXT - 1) + 2,1] X[NEXV(1) + NEXV(2) ... + NEXV(NEXT - 1) + 2,2] Y[NEXV(1) + NEXV(2) ... + NEXV(NEXT - 1) + 2]
	:	:	:
PEXP[NEXV(1)]:	VEXD[NEXV(1)] X[NEXV(1), 1] X[NEXV(1), 2] Y[NEXV(1)]	.	.
:	:	:	:
PEXP[NEXV(2)]:		VEXD[NEXV(2)] X[NEXV(1) + NEXV(2), 1] X[NEXV(1) + NEXV(2), 2] Y[NEXV(1) + NEXV(2)]	.
:			.
PEXP[NEXV(NEXT)]:			VEXD[NEXV(NEXT)] X[NEXV(1) + NEXV(2) ... + NEXV(NEXT), 1] X[NEXV(1) + NEXV(2) ... + NEXV(NEXT), 2] Y[NEXV(1) + NEXV(2) ... + NEXV(NEXT)]

In addition to the P-V-T data, the user must supply in a DATA statement the appropriate fluid properties at the thermodynamic critical point:

TC = critical temperature ($^{\circ}\text{R}$),
 VC = critical specific volume (ft^3/lb_m),
 ZC = critical compressibility factor (dimensionless),
 PC = critical pressure (psia).

A READ statement could be substituted for the DATA statement with only slight modification to INPUT.

Pertinent FORTRAN variables that appear in INPUT are:

<u>FORTRAN variable</u>	<u>Designation</u>
TC	T_c , critical temperature
VC	v_c , critical specific volume
ZC	Z_c , critical compressibility factor
PC	P_c , critical pressure
TITLE (18,3)	alphanumeric array for case identification
NEXP	total number of experimental isobars
NEXT	total number of isotherms
PEXP(I), I = 1 - NEXP	P_i , vector of experimental isobars
TEXP(J), J = 1 - NEXT	T_i , vector of experimental isotherms
VEXD(I)	dummy array v_i ; experimental specific volume
NDUM	dummy index; represents the number of experimental points associated with an isotherm
NEXV(I), I = 1 - NEXT	array whose elements signify number of data points for the j th isotherm
Y(L)	P_i , vector of experimental pressures associated with individual data points
X(L,1)	T_i , vector of experimental absolute temperatures corresponding to Y(L)
X(L,2)	v_i , vector of experimental specific volumes corresponding to Y(L)
X(L,5)	T_{ri} , vector of reduced absolute temperatures; one-to-one correspondence with X(L,1)

<u>FORTTRAN variable</u>	<u>Designation</u>
X(L,6)	v_{r1} , vector of reduced specific volumes; one-to-one correspondence with X(L,2)
N	index for counting total number of data points, transferred to MARQ

The dummy arrays TEXP, VEXD, PEXP, and NEXV all have dimension 50. This limits the maximum number of isotherms and isobars to 50, but this number can be increased as long as the total number of data points does not exceed 1000.

4.2.5 Subroutine FCODE

FCODE evaluates for MARQ the analytical expression for the pressure, given the reduced temperature and reduced specific volume and current values of the equation-of-state coefficients. The latter are designated within FCODE by the vector [PAR(I), I = 1 - 21]. There is a one-to-one correspondence between the elements of this vector and the vector B of MARQ. The reduced temperature and reduced volume are identified with the matrix elements X(I,5) and X(I,6), respectively, as in subroutine INPUT. The analytical value of pressure is denoted by the FORTRAN variable P, which corresponds to the variable F of subroutine MARQ.

The experimental pressure is also transmitted to FCODE in the calling sequence for the purpose of calculating the residual, RES. Experimental values of pressure are identified with elements of the vector PEX(I), which is designated as Y(I) in both INPUT and MARQ.

The vector elements PRNT(1) and PRNT(2) are set equal to the experimental values of temperature X(I,1) and specific volume X(I,2). These quantities and the corresponding values of PEX, P, and RES are returned to MARQ to be printed in the comparison of experimental and calculated pressures. As in INPUT, a data statement must supply the values of temperature, specific volume, compressibility factor, and pressure at the thermodynamic critical point.

The key FORTRAN variables and their identification with variables in MARQ and INPUT are listed below:

<u>FCODE variable</u>	<u>INPUT or MARQ variable</u>	<u>Designation</u>
PAR(I)	B(I)	Equation-of-state coefficient
TR	X(I,5)	Reduced temperature
VR	X(I,6)	Reduced specific volume
AR	B(20)	Dummy variable
BR	B(21)	Dummy variable
PEX	Y(I)	Experimental pressure
PRNT	PRNT	Vector of auxiliary information set equal to experimental absolute temperature and specific volume
P	F	Calculated pressure
RES	RES	Residual
TC, VC, ZC, PC	TC, VC, ZC, PC	Previously defined critical point properties

4.2.6 Subroutine PCODE

Subroutine PCODE provides analytical expressions for the partial derivatives of pressure with respect to the equation-of-state parameters.

If preferred, PCODE may be left blank, in which case differentiation is performed by the method of finite differences. This procedure is employed here, and the user need only supply the correct switch in the control section and a numerical value for the finite difference DEL. Too small a value for DEL may be the source of potential round-off errors that produce a division by zero error in the matrix inversion section of MARQ. The internal default value for DEL (10^{-5}) has been found to be adequate.

4.2.7 Subroutine SUBZ

SUBZ is employed here only to provide a value for the variable NPRNT, which specifies the number of auxiliary words that are to be printed as output along with the experimental and analytical values of pressure and the residual. NPRNT is given a value of 2, and the corresponding vector components PRNT(1) and PRNT(2) are set equal to the experimental absolute temperature and specific volume in FCODE.

4.2.8 Subroutine OUTPUT

OUTPUT directs to the card punch the improved values of the equation-of-state coefficients. As in MARQ, the coefficients are identified with the vector elements $B(I)$, $I = 1 - 21$.

4.2.9 Initialization and control of STATEQ

Operation of STATEQ is effected by supplying, as input data, values for control switches, certain essential program parameters, and initial values for the equation-of-state coefficients. This information must precede any P-V-T data which is read by subroutine INPUT. All control information is transferred to subroutine MARQ via the card reader.

The following description of the initialization procedure is essentially that which appears in the original write-up of the NLIN code but with the necessary modifications that make operation pertinent to this specific application.

<u>Card No.</u>	<u>Item</u>	<u>Format</u>	<u>Columns</u>	<u>Comments and instructions</u>
1	N	I3	1-3	Number of data points. Since the actual number is counted by INPUT, it is only necessary to use a number here that is greater than 1. Use 2 in column 3.
1	K	I3	4-6	Total number of parameters. Use 21.
1	IP	I3	7-9	Number of omitted parameters. Three cases can be identified: (1) Critical isotherm behavior not specified - all coefficients to be determined: Use 3 for item IP. (2) Critical isotherm specified - remaining 13 coefficients to be determined: Use 8 for item IP. (3) Critical isotherm alone to be determined: Use 16 for item IP.
1	M	I3	10-12	Number of independent variables. Use 2 in column 12.
1	IFP	I3	13-15	For plotting option. Use zero in column 15 (no plots).
1	NCONS	I3	16-18	Number of constraints. Use zero for no constraints.
1	ISPRD	I3	19-21	Used only if IFP > 0. Use 1.

<u>Card No.</u>	<u>Item</u>	<u>Format</u>	<u>Columns</u>	<u>Comments and instructions</u>
2	IWS1	I3	1-3	Doesn't apply.
2	IWS2	I3	4-6	= 0 for analytical derivatives. = 1 for estimated derivatives. Use 1.
2	IWS3	I3	7-9	= 0 for abbreviated printout. = # for detailed printout for number of iterations. Use 2.
2	IWS4	I3	10-12	= 0 for no force off. = # for force off after number of iterations. Use 25, 15, 35, etc.
2	IWS5	I3	13-15	= 0 for sense switches not interrogated. = 1 for sense switches interrogated. Use 0.
2	IWS6	I3	16-18	= 0 nonlinear confidence limits desired. = 1 omit nonlinear confidence limits. Use 0.
3				Omit if IFP = 0 (no plotting).
4	IB(1)	I3	1-3	Subscripts of the omitted parameters. The following values correspond to three cases cited for item IP above: (1) Critical isotherm not specified; use 1, 4, and 7. (2) Critical isotherm specified; use 1, 4, 7, 10, 13, 16, 20, and 21. (3) Critical isotherm to be fit; use 1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 14, 15, 17, 18, and 19.
4	IB(2)	I3	4-6	
4	IB(3)	I3	...	
	:	:	:	
	:	:	:	
	IB(IP)	I3	...	
5	FF	F10.0	1-10	Variance ratio statistic.
5	T	F10.0	11-20	Student's t.
5	E	F10.0	21-30	Convergence criterion.
5	TAU	F10.0	31-40	Convergence criterion.
5	XL	F10.0	41-50	Program parameter.
5	GAMCR	F10.0	51-60	Critical angle.
5	DEL	F10.0	61-70	Used in finite-difference derivatives.
5	ZETA	F10.0	71-80	Singularity criterion for matrix inversion.

Note: All or any of the items appearing in card 5 may be left blank.
In that case, the program assigns the following default values:

FF = 4.0, T = 2.0, E = 0.00005, TAU = 0.001, XL = 0.002,
GAMCR = $\pi/4$, DEL = 0.00001, ZETA = 1.E - 31.

<u>Card No.</u>	<u>Item</u>	<u>Format</u>	<u>Columns</u>	<u>Comments and instructions</u>
6	B(1)	D12.0	1-12	} Initial guess for parameters. Six per card.
	B(2)	D12.0	13-24	
	:	:	:	
	etc.	D12.0		
7				Leave this card blank.
8				} Cards 8 through 10 are the title cards. They may be left blank.
9				
10				
11				Experimental P-V-T data begins here (see INPUT).

Notes:

1. If the function is insensitive to one or more of the parameters, then round-off errors may occur in the finite-difference derivative evaluation. It would be necessary to then increase the value of DEL. It is also required that E be increased since it must be distinctly larger than DEL.
2. Use cards 8 and 9 to identify the fluid being fit.
3. Use card 10 to identify what case the initial guess came from.
4. The parameter IWS4 limits the number of iterations that the program makes in searching for the position of the stationary point. It is necessary to limit this number, since convergence may not occur in the time allotted for machine calculations, and the accumulated results of the calculation would be lost if the allotted time expires before convergence occurs. The calculation is continued by submitting as input to a new run the results of the previous run. This process is repeated until convergence occurs within the number of specified iterations.

5. EXAMPLES OF THE USE OF STATEQ: THE EQUATION OF STATE FOR ISOBUTANE

The following two examples illustrate the use of the code STATEQ for the two cases mentioned in Sects. 3.1 and 3.2. The compound chosen for study is isobutane, and the examples illustrate the use of the code to

- (1) obtain all 21 parameters when the critical isotherm is unknown and
- (2) obtain an expression for the critical isotherm alone.

To date, no critical isotherm data have been published for isobutane, and so the data for the latter case were obtained by extrapolating to the critical isotherm the available data along suitable isochores.⁵ The region of extrapolation extends only over 5°F; thus, the results should be valid, at least for the purpose of illustration. Following are the critical point properties as they appear in the data statements of subroutines INPUT and FCODE:

Critical Point Properties of Isobutane

$$\begin{aligned}T_c &= 734.65^\circ\text{R} \\v_c &= 0.07244 \text{ ft}^3/\text{lb}_m \\P_c &= 529.1 \text{ psia} \\Z_c &= 0.28255\end{aligned}$$

5.1 Case 1 — Critical Isotherm Data Unavailable, Full Equation of State Sought

The first case treated will be one in which all 21 parameters are to be determined by the nonlinear least-squares code. To adequately represent the behavior of the fluid, data from all regions of the P-V-T domain (excluding the subcooled liquid) have been included; and hence, the amount of input data is large. Card images of the input data are given below for a typical run in which the known equation-of-state coefficients for ammonia were used as the initial estimates for the isobutane parameters. This demonstrates the versatility of the code, since ammonia differs greatly from isobutane in its reduced P-V-T behavior.

Referring to Sect. 4.2.9, the input data convey the following information to the code:

- Card 1: N = 2, K = 21, IP = 3, M = 2, IFP = 0, NCONS = 0, ISPRD = 1.
IP is given value 3 since the Van der Waals conditions at the critical point render 3 of the 21 parameters dependent variables.
- Card 2: IWS1 not used, IWS2 = 1, IWS3 = 2, IWS4 = 15, IWS5 = 0, IWS6 = 0.
- Card 3: Omitted.
- Card 4: 1, 4, and 7 in columns 3, 6, 9, respectively.
- Card 5: Blank, indicating default values for program parameters FF, T, E, TAU, XL, GAMCR, DEL, ZETA.
- Card 6: B(1) = -1.56202D 0, B(2) = 7.43036D-1, B(3) = -2.32186D 1,
B(4) = 1.06562D 0, B(5) = -7.69621D-1, B(6) = -2.67278D 1,
- Cont'd. B(7) = -2.27223D-1, B(8) = 1.52805D 0, B(9) = 1.08407D 2,
B(10) = -3.51859D-2, B(11) = -6.34237D-1, B(12) = -5.74382D 1,
- Cont'd. B(13) = 1.78214D 3, B(14) = 5.07668D 3, B(15) = 7.12931D 5,
B(16) = 6.84438D 4, B(17) = 2.13130D 6, B(18) = -1.92117D 7,
- Cont'd. B(19) = 4.2D 0, B(20) = 1.43333D 1, B(21) = 1.83333D-2.
- Card 7: Blank.
- Card 8: NONLINEAR LEAST-SQUARES FIT TO ISOBUTANE.
- Card 9: DATA IS FROM CANJAR AND MANNING.
- Card 10: INITIAL GUESS IS FROM AMMONIA RUN 914.
- Card 11 and on: These cards contain the P-V-T data that are read in subroutine INPUT. Referring to Sect. 4.2.4, NEXP = 40 and NEXT = 39 represent the number of isobars and isotherms, respectively. The following 5 cards contain the values of 40 isobars [PEXP(I)]; i.e., 1., 14.696, 50. ... 3500 psia. The card immediately following contains the value of the first isotherm [TEXP(1) = -60°F] and the number of experimental points along that isotherm (NDUM = 1). The card that follows supplies the only value of specific volume for that isotherm [VEXD(1) = 73.53 ft³/lb_m]. This value of specific volume is identified with the first element of the experimental pressure vector; i.e., PEXP(1) = 1 psia. This procedure is repeated for all 39 isotherms up to 900°F, where 40 experimental points are given covering the range from 1 psia, 251 ft³/lb_m to 3500 psia, 0.07708 ft³/lb_m.

STATEQ INPUT CARD IMAGES - CASE 1

```

2 21 3 2 0 0 1
1 2 15 C C
1 7 7

```

```

-1.562020 CC 7.430360-01-2.321860 01 1.065620 00-7.696210-01-2.672780 01
-2.272230-01 1.528050 00 1.084070 02-3.513590-02-6.342370-01-5.743820 01
1.782140 03 5.076680 03 7.129310 05 6.844380 04 2.131300 06-1.921170 07
4.200000 00 1.433330 01 1.853330-02

```

NON-LINEAR LEAST SQUARES FIT TO ISOBUTANE DATA.

DATA IS FROM CAMJAN AND MANNING.

INITIAL GUESS IS FROM AMMONIA RUN 914

	40	39						
1.	14.656	50.	100.	150.	200.	250.	300.	350.
400.	420.	440.	460.	480.	500.	520.	540.	560.
580.	600.	620.	640.	660.	680.	700.	750.	800.
850.	900.	950.	1000.	1100.	1200.	1400.	1600.	1800.
2000.	2500.	3000.	3500.					
-60.	1							
73.53								
-40.	1							
77.42								
-20.	1							
80.92								
0.	2							
84.62	5.522							
20.	3							
88.36	5.757	1.495						
40.	3							
92.15	6.067	1.601						
60.	3							
95.74	6.337	1.701						
80.	4							
99.43	6.604	1.790	.7742					
100.	4							
103.1	6.869	1.889	.8367					
120.	4							
106.8	7.133	1.976	.8941					
140.	5							
110.5	7.396	2.060	.9480	.5041				
160.	6							
114.2	7.667	2.152	.9993	.6071	.4004			
180.	7							
117.8	7.919	2.237	1.048	.6468	.4390	.3033		
200.	8							
121.6	8.179	2.320	1.096	.684	.4731	.3404		
.2402								
220.	9							
125.3	8.438	2.402	1.143	.7194	.5044	.3685		
.2771	.2078							
230.	10							
127.2	8.507	2.443	1.166	.7360	.5191	.3858		
.2928	.2208	.150						
240.	10							
129.1	8.696	2.484	1.188	.7534	.5335	.399		
.3059	.2345	.1701						
250.	12							
130.9	8.825	2.524	1.210	.77	.5477	.412		
.3189	.2488	.1901	.1668	.1397				
260.	14							
132.8	8.953	2.564	1.232	.7864	.5615	.4246		
.3312	.2617	.2057	.1848	.1542	.1419	.1149		
270.	16							
134.7	9.081	2.605	1.254	.8025	.5750	.4368		
.3429	.2737	.2188	.1991	.1804	.162	.143		

.1213	.05072					
280.	40					
136.5	9.209	2.645	1.270	.8165	.5183	.4486
.3542	.2849	.2307	.2115	.1938	.1768	.1602
.1438	.1267	.1068	.07535	.05712	.05249	.05014
.04844	.04704	.04622	.04550	.04427	.04326	.04245
.04178	.04121	.0407	.03914	.03850	.03788	.0369
.03655	.03600	.03494	.03410	.03341		
290.	40					
138.4	9.330	2.685	1.258	.8344	.6014	.4603
.365	.2955	.2418	.2231	.2060	.1899	.1742
.1593	.1453	.1308	.110	.09559	.08173	.06788
.05968	.05447	.05209	.05062	.04789	.0461	.0446
.04379	.04299	.04231	.04074	.04001	.03888	.03799
.03725	.03666	.03543	.03451	.03377		
300.	40					
140.2	9.467	2.725	1.32	.85	.6141	.4716
.3755	.3057	.2521	.2335	.2169	.2012	.1864
.1724	.1561	.1462	.1335	.1210	.1083	.09556
.08264	.07155	.06494	.0600	.0539	.05031	.04789
.04643	.04522	.04420	.04282	.04171	.04000	.03891
.03804	.03731	.03594	.03494	.03415		
320.	40					
143.9	9.724	2.804	1.362	.8805	.6389	.4931
.3951	.3245	.2706	.2523	.2356	.2202	.2059
.1926	.18	.1682	.157	.1464	.1362	.1264
.1165	.107	.09857	.09088	.07541	.06524	.05883
.05471	.05180	.04979	.04706	.04515	.04261	.04091
.03969	.03875	.03705	.03585	.03494		
340.	40					
147.6	9.979	2.882	1.464	.9103	.6629	.5138
.4138	.3419	.2874	.269	.2523	.2369	.2220
.2095	.1972	.1857	.175	.1649	.1553	.1462
.1376	.1263	.1217	.1144	.09818	.08470	.07454
.06729	.06202	.05816	.05312	.04980	.04576	.0433
.04161	.04038	.03827	.03684	.03578		
360.	40					
151.3	10.23	2.960	1.445	.9345	.6862	.5337
.4317	.3584	.303	.2844	.2675	.252	.2377
.2248	.2123	.2008	.1902	.1820	.1709	.1621
.1533	.146	.1386	.1317	.1258	.1102	.09061
.0815	.07433	.06874	.06091	.05579	.0496	.04591
.04379	.04227	.03962	.03791	.03608		
380.	40					
154.9	10.49	3.038	1.486	.9663	.709	.5532
.4489	.3741	.3178	.299	.2818	.2661	.2516
.2383	.226	.2145	.2038	.1948	.1845	.1758
.1677	.1598	.1525	.1457	.1301	.1165	.1048
.09501	.08681	.08008	.07034	.06368	.05341	.04441
.04659	.04442	.04111	.03908	.03764		
400.	40					
158.6	10.74	3.115	1.527	.9968	.7317	.5721
.4656	.3894	.332	.3128	.2954	.2798	.2647
.2512	.2367	.2272	.2164	.2064	.197	.1881
.180	.1722	.1671	.1580	.1424	.1289	.1172
.107	.09831	.09086	.0791	.07062	.05949	.05309
.04953	.04687	.04277	.04033	.03867		
440.	40					
166.1	11.25	3.269	1.607	1.053	.7756	.6091
.498	.4186	.3585	.339	.3209	.3044	.2892
.2753	.2624	.2504	.2393	.229	.2194	.2104
.2019	.194	.1865	.1795	.1636	.1490	.1370
.1272	.118	.1099	.09647	.08598	.0712	.06207
.05653	.05238	.04652	.04310	.04093		
480.	40					
173.5	11.76	3.422	1.687	1.108	.819	.6453
.5294	.4466	.3845	.3683	.345	.3278	.3121
.2970	.2842	.2718	.2603	.2436	.2396	.2303

.2215	.4133	.2050	.1404	.102	.1077	.1552
.1443	.1347	.1201	.1115	.09480	.0823d	.07113
.06467	.0506	.05062	.04037	.040348		
520.	40					
180.9	12.27	3.576	1.766	1.103	.0616	.0806
.5595	.4738	.409	.3075	.3079	.35	.3337
.3186	.3047	.2910	.2799	.2688	.2584	.2487
.2395	.2312	.2234	.2150	.1905	.1838	.1704
.1596	.1495	.1400	.1255	.1129	.0934	.0805
.07263	.06537	.05535	.04991	.04024		
560.	40					
106.3	12.70	3.720	1.045	1.217	.9033	.715
.5894	.4658	.4326	.4102	.3849	.3713	.3543
.3386	.3242	.3108	.2984	.2809	.2701	.266
.2505	.2470	.2345	.2317	.214	.1986	.1853
.1736	.1632	.1534	.1380	.1247	.104	.08973
.0804	.07224	.06031	.0537	.0493		
600.	40					
195.6	13.28	3.88	1.923	1.271	.9445	.7488
.6184	.5254	.4550	.4324	.4112	.392	.3743
.3561	.343	.3292	.3163	.3044	.2932	.2827
.2729	.2630	.2552	.2471	.2237	.2128	.1989
.1867	.1758	.1661	.1495	.1356	.1130	.0904
.0874	.0751	.06534	.05765	.05248		
650.	40					
204.9	13.52	4.07	2.014	1.337	.9953	.7905
.654	.5566	.4830	.4592	.4372	.417	.3986
.3615	.3459	.3314	.318	.3254	.3137	.3027
.2925	.2826	.2734	.2624	.2402	.2299	.2159
.2025	.1902	.1799	.1630	.1476	.1252	.1072
.09708	.0877	.07145	.0625	.05041		
700.	40					
214.1	14.55	4.250	2.116	1.403	1.045	.8315
.689	.5872	.511	.4855	.4624	.4414	.4221
.4044	.3861	.3728	.3588	.3458	.3335	.3221
.3115	.304	.2917	.2831	.265	.2455	.2301
.2172	.2045	.1935	.1751	.1604	.1350	.1182
.1053	.09509	.07806	.0677	.06074		
750.	40					
223.3	15.18	4.440	2.212	1.408	1.095	.8721
.7234	.6173	.5370	.5112	.4872	.4653	.4451
.4266	.4096	.3937	.3791	.3655	.3527	.3400
.3290	.3170	.3054	.3001	.2791	.2608	.2448
.2306	.2174	.2065	.1870	.1709	.1451	.1273
.1135	.1026	.08411	.07264	.06495		
800.	40					
232.0	15.62	4.634	2.308	1.533	1.145	.9123
.7574	.6469	.5642	.5366	.5114	.4886	.4670
.4484	.4307	.4142	.3984	.3847	.3714	.359
.3474	.3300	.3263	.3167	.2948	.2757	.259
.2441	.2300	.2169	.1985	.1814	.1554	.136
.1213	.1058	.08945	.07743	.06905		
850.	40					
241.8	16.45	4.821	2.405	1.547	1.194	.9521
.7911	.6762	.5902	.5614	.5354	.5117	.4898
.4693	.4513	.4342	.4182	.4035	.3897	.3768
.3647	.3434	.3420	.3328	.31	.2909	.2727
.2572	.2434	.231	.2047	.192	.1646	.1443
.1288	.1107	.0950	.08222	.07504		
900.	40					
251.0	17.08	5.004	2.498	1.601	1.243	.9917
.8245	.7052	.6158	.586	.5589	.5343	.5116
.4908	.4710	.4534	.4373	.422	.4077	.3943
.3818	.37	.3584	.3480	.3249	.3043	.2861
.27	.2556	.2427	.2205	.2022	.1736	.1524
.1361	.1234	.1011	.08686	.07708		

The printed output for this example appears in Appendix D. The preliminary information includes case identification, the number of data points, and key input variables discussed above such as the number of parameters (K), the number of omitted parameters (IP), etc. The initial assumed values for all 21 parameters appear in rows below the heading (0) PARAMETERS. Following this is a comparison of pressures calculated from these initial parameters and the experimental values. The first column lists the observed or experimental pressure in psia and is followed by the predicted or calculated value in the second column. The residual appears in column 3, and the temperature ($^{\circ}\text{R}$) and specific volume (ft^3/lb_m) are tabulated in columns 4 and 5, respectively. Not surprisingly, the ammonia equation of state fails to model accurately the isobutane behavior, with many points being in error by 10% or more.

The portion of printout that immediately follows the detailed comparison of the model is a partial accounting of the code statistics which is useful for evaluating the progress of the iteration procedure. The PTP CORRELATION MATRIX represents the value of the matrix of normal equations for the approximate linearized model. Note that zeros occur for all off-diagonal elements when either index is 1, 4, or 7. This is an indication that these three parameters are not being varied by the code. Following the PTP matrix are values for PHI, SE, and LAMBDA. PHI represents the sum of squares of the residuals given by Eq. (2.2); SE is the standard error of estimate; and LAMBDA is the value of the Lagrange multiplier, λ , discussed in Sect. 2. During the course of a run, both PHI and SE should converge to their respective minima.

Under the heading INCREMENTS are tabulated the incremental changes in the parameters taken during the course of an iteration. Current values of PHI and LAMBDA are presented along with GAMMA (the angle between the approximate Taylor series and maximum descent methods) and LENGTH (the magnitude of the vector of the increments).

Under the heading (1) PARAMETERS, the 21 parameters arrived at after the first full iteration are presented. A detailed comparison of the fit using these parameters follows immediately. The PTP correlation matrix is printed next, and this is followed by the current values of PHI, SE, the values for the INCREMENTS, etc. In the example presented, the first

iteration results in a marked reduction for both the sum of the squares of residuals (PHI) and the standard error of estimate (SE).

An abbreviated printout is given for all but the last of the number of specified iterations. Only PHI, SE, LENGTH, GAMMA, and LAMBDA are listed for these intermediate iterations. In the example shown, both PHI and SE are decreasing but not rapidly (less than 0.2% per iteration). Convergence did not occur within the specified number of iterations, and the calculation was terminated after 15 iterations. The final detailed comparison shows that the fit has been greatly improved. Errors as large as 5% are still present, particularly near the saturation conditions and just above the critical region, but the fit at higher temperatures is very good. Further refinement of the fit is possible through continued operation of the code.

Of some importance is the parameter correlation matrix. The magnitude of the elements of this matrix is an indication of how well each parameter models the behavior of the fluid separately. A zero value for any matrix element indicates that the parameters identified with the indices of that element are uncorrelated. Conversely, a value of unity signifies complete correlation. A synopsis of the results of the parameter correlation matrix is presented for this example in Table 2. With reference to Appendix A, the following observations can be made about the nature of the model:

1. No correlation exists between $f_1(1)$, $f_2(1)$, $f_3(1)$, and other coefficients since the former are not independent parameters.
2. There is a low-to-moderate (at most) correlation between $\underline{b}$ and all other parameters.
3. Parameters $f_4(1)$, $f_5(1)$, $f_6(1)$, and $\underline{a}$ are strongly coupled, and this is probably due to the fact that these parameters determine the critical isotherm behavior. They are not at all correlated with B_{1-4} and C_{1-4} and moderately to highly correlated with fifth and sixth term coefficients due to the direct coupling demonstrated in Eq. (A-1).
4. There is a very high degree of correlation between the temperature exponent and all C_i 's, which is due to the coupling of these parameters in Eq. (A-4).

Table 2. Parameter correlation matrix
 Key: M = moderate (0.3-0.7), H = high (>0.7),
 0 = no correlation, 1 = complete correlation,
 L = low (<0.3)

	$f_1(1)$	B_1	C_1	$f_2(1)$	B_2	C_2	$f_3(1)$	B_3	C_3	$f_4(1)$	B_4	C_4	$f_5(1)$	B_5	C_5	$f_6(1)$	B_6	C_6	K	a	b
$f_1(1)$	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B_1		1	M	0	H	H	0	M	H	1	M	H	1	M	M	1	1	M	H	1	1
C_1			1	0	L	M	0	L	H	L	L	M	1	L	M	L	L	M	H	1	M
$f_2(1)$				1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B_2					1	M	0	H	M	1	H	M	L	M	M	1	L	L	M	1	1
C_2						1	0	M	H	L	M	H	1	M	H	1	L	M	H	L	L
$f_3(1)$							1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B_3								1	M	1	H	M	L	M	M	L	L	L	1	L	1
C_3									1	L	M	H	L	M	H	L	L	H	H	1	1
$f_4(1)$										1	L	L	H	M	M	H	M	M	L	H	L
B_4											1	M	L	M	L	L	L	L	L	L	1
C_4												1	L	M	H	L	L	M	H	L	L
$f_5(1)$													1	M	M	H	M	M	L	H	L
B_5														1	H	M	L	M	L	M	L
C_5															1	M	L	H	H	M	L
$f_6(1)$																1	M	M	L	H	1
B_6																	1	H	L	M	L
C_6																		1	H	M	M
K																			1	L	M
a																				1	1
b																					1

5. Parameter B_6 has mostly a low correlation with all coefficients except for C_6 where a high correlation exists. The reason for this is as yet unknown.

5.2 Case 2 — Critical Isotherm Fit

The fit to the critical isotherm is obtained by allowing only $f_4(1)$, $f_5(1)$, $f_6(1)$, $\underline{a}$, and $\underline{b}$ to be treated as independent variables. The other critical isotherm coefficients $f_1(1)$, $f_2(1)$, and $f_3(1)$ are treated as dependent variables by virtue of the critical point constraints. The remaining coefficients are considered constant, and when data are supplied solely for a reduced temperature of unity, these coefficients vanish in the expression for pressure. Hence, any initial value may be assumed for the coefficients B_1 , C_1 , and K.

The input data for a critical isotherm fit is not complicated; it consists of the usual control information and pressure-volume data for only a single isotherm. The card images for a typical run appear below. A brief description of the input deck follows: (Underscored numbers indicate parameters that differ from previous example.)

- Card 1: N = 2, K = 21, IP = 16, M = 2, IFP = 0, NCONS = 0, ISPRD = 1.
IP is given value 16 since only the critical isotherm behavior is being sought.
- Card 2: IWS1 not used, IWS2 = 1, IWS3 = 2, IWS4 = 95, IWS5 = 0, IWS6 = 0.
The code is allowed to run for 95 iterations (instead of 15 previously) because the fit to the critical isotherm requires substantially less computation time during a single iteration.
- Card 3: Omitted.
- Card 4: 1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 14, 15, 17, 18, 19 in columns 3, 6, 9, 12, ..., etc. Only five parameters are treated as independent variables.
- Card 5: Blank.
- Card 6: B(1) = -1.33110D 0, B(2) = 9.34776D-1, B(3) = -2.17413D 1,
B(4) = 7.65252D-1, B(5) = -9.51859D-1, B(6) = -3.35394D 1,
- Cont'd B(7) = -1.23797D-1, B(8) = 1.46257D 0, B(9) = 1.10871D 2,
B(10) = -2.83036D 2, B(11) = -6.17794D-1, B(12) = -5.43971D 1,
- Cont'd B(13) = 1.61253D 3, B(14) = 1.25498D 4, B(15) = 1.00959D 6,
B(16) = 6.86034D 5, B(17) = 1.56416D 6, B(18) = 2.30770D 8,
- Cont'd B(19) = 5.23773D 0, B(20) = 1.39357D 1, B(21) = 8.81712D-2.
- Card 7: Blank.
- Card 8: CRITICAL ISOTHERM FIT FOR ISOBUTANE.
- Card 9: DATA IS FROM CANJAR AND MANNING.
- Card 10: INITIAL ESTIMATES ARE FROM JOB 810.
- Card 11 and on: These cards contain the 29 values of pressure and specific volume for the critical isotherm alone; i.e., NEXP = NDUM = 29, NEXT = 1. The manner in which the data are read is described in the previous example.

STATEQ INPUT CARD IMAGES - CASE 2

```

2 21 16 2 0 0 1
  1 2 95 0 0
1 2 3 4 5 6 7 8 9 11 12 14 15 17 18 19

-1.33110D 00 0.34776D-01-2.17413D 01 7.65252D-01-9.51859D-01-3.35194D 01
-1.23797D-01 1.46257D 00 1.10871D 02-2.83036D-02-6.17794D-01-5.43971D 01
1.61253D 03 1.25498D 04 1.00959D 06 6.86034D 05 1.56416D 06 2.30770D 08
5.23773D 00 1.39357D 01 8.81712D-02

```

CRITICAL ISO-THERM FIT FOR ISORUTANE
 DATA IS FROM CANJAP AND MANNING
 INITIAL ESTIMATES ARE FROM JOB 910.

```

29 1
1.0 14.696 50. 100. 150. 200. 250. 300. 350.
400. 440. 460. 480. 520. 529.1 558. 590.44 605.02
038.8 886.6 779.44 827.72 920.2 1190. 1292.9 1565. 1745.
1888.6 2374.
274.96 29
135.6 9.145 2.625 1.265 .8105 .5816 .4427
.3484 .2794 .2250 .1873 .1698 .1525 .11
.07244 .05249 .04844 .04704 .04558 .04427 .04245
.04121 .0407 .0385 .03788 .0369 .03655 .03606
.03494

```

The output from this run (Appendix E) is similar to the previous example, with the exception that only 29 data points are present and only 8 parameters are changing (5 independently). The calculation terminated after 46 iterations when one of the algorithm convergence criteria was satisfied (Epsilon test).

The parameter correlation matrix presented in Table 3 reveals a very high degree of correlation between the parameters $f_4(1)$, $f_5(1)$, $f_6(1)$, and a . The correlation of b is highest with $f_5(1)$ and $f_6(1)$, and very little correlation exists with $f_4(1)$. This behavior is not unlike that of the previous example.

Table 3. Parameter correlation matrix of critical isotherm fit

	$f_1(1)$	$f_2(1)$	$f_3(1)$	$f_4(1)$	$f_5(1)$	$f_6(1)$	a	b
$f_1(1)$	1	0	0	0	0	0	0	0
$f_2(1)$		1	0	0	0	0	0	0
$f_3(1)$			1	0	0	0	0	0
$f_4(1)$				1	0.90	0.94	0.98	0.11
$f_5(1)$					1	0.99	0.96	0.49
$f_6(1)$						1	0.98	0.48
a							1	0.21
b								1

6. USE OF THE CODE APPROX

As mentioned earlier, the code APPROX, which is much less complicated than STATEQ, may be used to obtain the entire equation-of-state representation. A disadvantage is that the critical isotherm must be specified which requires the prior use of STATEQ or a similar code to optimize the eight critical isotherm coefficients. In addition, the procedure for using STATEQ is tedious, since it requires the user to examine the results of the fit and manipulate some or all of 12 parameters to improve the representation. It is possible, however, to improve the fit in certain regions of the P-V-T domain by using this technique, and this may be a desirable feature.

The input procedure for APPROX is described briefly in Sect. 4.1.1. The format for reading P-V-T data is identical to that used by subroutine INPUT of STATEQ. A listing of the input variables and card format is given in Table 4. Card images of the data are not presented since they are identical to those listed in Sect. 5.1. The critical isotherm was determined by assuming representative values for $\underline{a}$ (AR) and $\underline{b}$ (BR) and then solving the simple linear least-squares problems for $f_1(l)$ [FTC(1)]. The fit obtained from STATEQ in Sect. 5.2 would provide a superior critical isotherm representation.

A typical printout from APPROX appears in Appendix F. The input variables are printed first; that is, T_c ($^{\circ}\text{R}$), P_c (atm), v_c (ft^3/lb_m), a , b , K , and the six $f_1(l)$ parameters. The resultant coefficients A_1 , B_1 , and C_1 follow (the A_1 's are redundant). The calculated and experimental pressures (in psia) are then compared for each temperature-volume pair. The representation obtained in this example is poor in comparison to that obtained by STATEQ, with some errors as high as 21% in the high-density gaseous region. The fit would probably be improved by following the procedure suggested by Martin,² but STATEQ provides a more expeditious way to accomplish this.

Table 4. Card input data for APPROX

Card number	Columns	Format	FORTTRAN variable
1	1-20	D20.7	AR
1	21-40	D20.7	BR
2	1-20	D20.7	FTC(1)
2	21-40	D20.7	FTC(2)
2	41-60	D20.7	FTC(3)
2 (cont'd)	1-20	D20.7	FTC(4)
:	:	:	:
2 (cont'd)	41-60	D20.7	FTC(6)
3	1-5	I5	NEXP
3	6-10	I5	NEXT
4	1-8	F8.3	PEXP(1)
4	9-16	F8.3	PEXP(2)
:	:	:	:
4	65-72	F8.3	PEXP(9)
4 (cont'd)	1-8	F8.3	PEXP(10)
:	:	:	:
4 (cont'd)	65-72	F8.3	PEXP (18)
4 (cont'd)	Repeat pattern until all isobars are read		
5	1-8	F8.3	TEXP(J)
5	9-10	I2	NDUM
6	1-10	F10.5	VEXD(1)
:	:	:	:
6	61-70	F10.5	VEXD(7)
6 (cont'd)	1-10	F10.5	VEXD(8)
7 Repetition of cards 5-6 until all isotherms are completed			
:	:	:	:

REFERENCES

1. D. W. Marquardt, "An Algorithm for Least-Squares Estimation of Nonlinear Parameters," *J. Soc. Ind. Appl. Math.* 11(2), 431 (1963).
2. J. J. Martin, "Equations of State," *Ind. Eng. Chem.* 59, 34-52 (1967).
3. S. L. Milora, Application of the Martin Equation of State to the Thermodynamic Properties of Ammonia, ORNL-TM-4413 (December 1973).
4. D. W. Marquardt, "Least-Squares Estimation of Nonlinear Parameters," IBM Share Program No. 1428.
5. L. N. Canjar and F. S. Manning, Thermodynamic Properties and Reduced Correlations for Gases, Gulf Publishing Company, Houston, Tex., 1967.

Appendix A

THE MARTIN EQUATION OF STATE IN REDUCED FORMAT

The full 21-parameter Martin-Hou equation of state as described in Ref. 2 can be written in reduced, or dimensionless, form as follows:

$$P = (P_c/Z_c) \left[\frac{T_r}{(v_r - b)} + \frac{f_1(T_r)}{(v_r - b)^2} + \frac{f_2(T_r)}{(v_r - b)^3} + \frac{f_3(T_r)}{(v_r - b)^4} + \frac{f_4(T_r)}{(v_r - b)^5} + f_5(T_r) e^{-av_r} + f_6(T_r) e^{-2av_r} \right] . \quad (A-1)$$

The parameters b and a and the f functions are chosen so as to fit the P-V-T data in the least-squares sense. The form of the f functions is prescribed as follows:

$$f_i(T_r) \cong A_i + B_i T_r + C_i e^{-KT_r}, \quad i = 1 - 6 . \quad (A-2)$$

In the above form, the equation has a total of 21 parameters, 18 of which are linear (A_i, B_i, C_i) and 3 of which appear nonlinearly (a, b, K). Essentially, the number of free or independent parameters can be reduced to 18 if the critical point is fixed and the Van der Waals conditions are applied there; that is,

$$\left. \begin{aligned} P &= P_c \\ \left(\frac{\partial P}{\partial v} \right)_T &= \left(\frac{\partial^2 P}{\partial v^2} \right)_T = 0 \end{aligned} \right\} \text{ at } T_r, v_r = 1 . \quad (A-3)$$

Since the critical point plays an important role in parameter selection, it is useful to eliminate A_i in Eq. (A-2) and introduce six new linear constants $f_i(1)$, the temperature functions $f_i(T_r)$ evaluated at $T_r = 1$. The preferred form of the temperature functions then becomes

$$f_i(T_r) = f_i(1) + B_i(T_r - 1) + C_i(e^{-KT_r} - e^{-K}) . \quad (A-4)$$

In this representation, the critical isotherm takes the form

$$P(v_r, T_r = 1) = \frac{P_c}{Z_c} \left[\frac{T_r}{(v_r - b)} + \frac{f_1(1)}{(v_r - b)^2} + \dots + f_6(1) e^{-2av_r} \right], \quad (A-5)$$

and the three conditions at the critical point reduce to

$$\begin{aligned} \frac{f_1(1)}{(1-b)^2} + \frac{f_2(1)}{(1-b)^3} + \frac{f_3(1)}{(1-b)^4} + \frac{f_4(1)}{(1-b)^5} + f_5(1) e^{-a} + f_6(1) e^{-2a} \\ = Z_c - \frac{1}{(1-b)}, \end{aligned} \quad (A-6)$$

$$\begin{aligned} \frac{2f_1(1)}{(1-b)} + \frac{3f_2(1)}{(1-b)^2} + \frac{4f_3(1)}{(1-b)^3} + \frac{5f_4(1)}{(1-b)^4} + ae^{-a} (1-b)^2 f_5(1) \\ + 2a e^{-2a} (1-b)^2 f_6(1) = -1, \end{aligned} \quad (A-7)$$

$$\begin{aligned} \frac{6f_1(1)}{(1-b)} + \frac{12f_2(1)}{(1-b)^2} + \frac{20f_3(1)}{(1-b)^3} + \frac{30f_4(1)}{(1-b)^4} + a^2 e^{-a} (1-b)^3 f_5(1) \\ + 4a^2 e^{-2a} (1-b)^3 f_6(1) = -2. \end{aligned} \quad (A-8)$$

Equations (A-6), (A-7), and (A-8) can be solved easily for any three linear parameters in terms of the remaining linear and nonlinear terms. If the parameters $f_1(1)$, $f_2(1)$, and $f_3(1)$ are chosen as the three dependent parameters, their dependence on the remaining five independent parameters will be as follows:

$$f_1(1) = 6(1-b)^2 R_1 - 4(1-b) R_2 + \frac{(1-b)}{2} R_3, \quad (A-9)$$

$$f_2(1) = -8(1-b)^3 R_1 + 7(1-b)^2 R_2 - (1-b)^2 R_3, \quad (A-10)$$

$$f_3(1) = 3(1-b)^4 R_1 - 3(1-b)^3 R_2 + \frac{(1-b)^3}{2} R_3, \quad (A-11)$$

where the quantities R_1 , R_2 , and R_3 are functions only of $f_4(1)$, $f_5(1)$, $f_6(1)$, a , and b , and are given by

$$R_1 = Z_c - \frac{1}{(1-b)} - \frac{f_4(1)}{(1-b)^5} - f_5(1) e^{-a} - f_6(1) e^{-2a}, \quad (A-12)$$

$$R_2 = - \frac{5f_4(1)}{(1-b)^4} - \left[f_5(1) a e^{-a} + 2a e^{-2a} f_6(1) \right] (1-b)^2 - 1, \quad (A-13)$$

$$R_3 = -2 - \frac{30f_4(1)}{(1-b)^4} - \left[a^2 e^{-a} f_5(1) + 4a^2 e^{-2a} f_6(1) \right] (1-b)^3. \quad (A-14)$$

This last result reduces the number of independent parameters in Eq. (A-1) to 18.

There are two strategies for estimating the remaining unknown parameters. If the critical isotherm is known accurately, then Eq. (A-5), along with the results of Eqs. (A-9) through (A-11), can be used to obtain a least-squares estimate of the critical isotherm functions $f_i(1)$ and the parameters a and b . This can be done, for example, by writing a linear least-squares algorithm for the $f_i(1)$ and manually adjusting the parameters a and b until a satisfactory fit to the critical isotherm data is obtained. Alternatively, the STATEQ program can be used for the special case in which only critical isotherm data are considered. The details of this latter method were discussed earlier in this report.

Appendix B

FORTRAN LISTING OF THE CODE STATEQ

```

C      CALLING PROGRAM FOR THE NONLINEAR-LEAST-SQUARES PROGRAM OF      10
C      D. W. MARQUADT      20
C      NDPH      = MAXIMUM NUMBER OF DATA POINTS      30
C      NPM      = MAXIMUM NUMBER OF PARAMETERS      40
C      NXM      = MAXIMUM NUMBER OF INDEPENDENT VARIABLES      50
C      IMPLICIT REAL*8 (A-H,O-Z)      60
C      REAL*4 TITLE      70
C      INTEGER PMT,PA,Q      80
C      DIMENSION A(50,50),B(50),BA(50),BB(50),BS(50),C(50),CONS(25)      90
C      DIMENSION DB(50),PMT(18),G(50),IB(50),P(50),PA(50),PRMT(5),Q(50)      100
C      DIMENSION SA(50),SPRMT(5),TITLE(18,3),W(50)      110
C      DIMENSION X(1000,6),Y(1000)      120
C      COMMON/LBCOM1/IPR(10),PMT(50)      130
C      COMMON/TAPES/NI,NO,NP,NTTOC      140
C      COMMON/STAPE/NST      150
C      CALL TSET      160
C      NDPH=1000      170
C      NPM = 50      180
C      NXM=6      190
C      -----      200
C      THIS VERSION OF THE MARQUADT PROGRAM CONTAINS MODIFICATIONS, BY      210
C      W.DAVIS, TO MAKE IT USEABLE WITH INPUT FROM A CALLING PROGRAM      220
C      AS WELL AS WITH THE USUAL DATA-INPUT PROCEDURE.      230
C      THIS DUALITY IS ACCOMPLISHED BY HAVING AS ARGUMENTS OF MARQ ALL      240
C      THE INPUT DATA THAT CAN BE READ BY MARQ ** PLUS ** A FINAL      250
C      ARGUMENT ** IREAD ** THAT IS DEFINED IN THE CALLING PROGRAM.      260
C      IREAD .EQ. 1 MEANS THAT THE SUBROUTINE MARQ(**) EXPECTS      270
C      TO READ INPUT DATA IN THE NORMAL MANNER.      280
C      IREAD .NE. 1 MEANS THAT ALL DATA NORMALLY READ INTO      290
C      MARQ(**) MUST BE PASSED FROM THE CALLING      300
C      PROGRAM. NO DATA WILL BE READ BY MARQ.      310
C      -----      320
C      IREAD = 1      330
C      CALL MARQ(A,B,BA,BB,BS,C,CONS,DB,G,P,PRMT,SA,SPRMT,W,X,Y,      340
1      YHN,SPRD,PF,T,E,TAU,XL,GAMCB,DEL,ZETA,      350
2      TITLE,PMT,IB,PA,Q,W,X,IP,B,IPP,NCONS,ISPRD,      360
3      IWS1,IWS2,IWS3,IWS4,IWS5,IWS6,IREAD,NDPH,NPM,NXM)      361
C      STOP 13579      362
C      END      363
C      SUBROUTINE TSET      370
C      COMMON/TAPES/NI,NO,NP,NTTOC      380
C      COMMON/STAPE/NST      TSET 10
C      NI=5      TSET 20
C      NO = 6      TSET 30
C      NP = 7      TSET 40
C      NST = 3      TSET 50
C      RETURN      TSET 60
C      END      TSET 70
C      SUBROUTINE INPUT(B,PRMT,X,Y,PMT,TITLE,N,NDPH)      TSET 80
C      IMPLICIT REAL*8 (A-H,O-Z)      TSET 90
C      INTEGER PMT      INPUT 10
C      REAL*4 TITLE      INPUT 20
C      DIMENSION B(50),PMT(18),PRMT(5),TITLE(18,3)      INPUT 30
C      DIMENSION X(NDPH,6),Y(1000)      INPUT 40
C      DIMENSION TEXP(50),VEXD(50),PEXP(50),NEXV(50)      INPUT 50
C      COMMON /LBCOM1/IPR(10),PMT(50)      INPUT 60
C      COMMON/TAPES/NI,NO,NP,NTTOC      INPUT 70
C      DATA TC,VC,ZC,PC/734.65,.07244,.28255,529.10/      INPUT 80
C      TC,VC,ZC,PC MUST BE SUPPLIED IN UNITS CONSISTENT WITH THE DATA OR      INPUT 90
C      VICE VERSA.      INPUT 100
C      READ (NI,1003) (TITLE(I,1),I=1,18)      INPUT 110
C      READ (NI,1003) (TITLE(I,2),I=1,18)      INPUT 120
C      READ (NI,1003) (TITLE(I,3),I=1,18)      INPUT 130
C      READ (NI,1001) NEXP,NEXT,(PEXP(I),I=1,NEXP)      INPUT 140

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C
C      NEXP IS NUMBER OF EXPERIMENTAL PRESSURES
C      NEXT IS NUMBER OF EXPERIMENTAL TEMPERATURES
C      PEXP(I) REPRESENT THE TOTAL NUMBER OF PRESSURES.
C
1001  FORMAT(2I5/,9P8.3))
      L=1
      DO 2 J=1,NEXT
      READ(NI,1002) TEXP(J),NDUM,(VEXD(I),I=1,NDUM)
1002  FORMAT(7F9.3,I2/(7F10.5))
      NEXV(J)=NDUM
      DO 1 K=1,NDUM
      X(L,1)=TEXP(J)+459.6900
      X(L,2)=VEXD(K)
      Y(L)=PEXP(K)
C
C      X(L,5) AND X(L,6) ARE DIMENSIONLESS INDEPENDENT VARIABLES
C      REQUIRED BY FCODE.
C      Y(L,1) AND X(L,2) ARE DATA.
C      Y(L) ARE THE EXPERIMENTAL PRESSURES.
C      VEXD(I) ARE THE VOLUMES ASSOCIATED WITH THE NDUM PRESSURES
C      OF ISOTHERM TEXP(J).
C
      X(L,5)=X(L,1)/TC
      X(L,6)=X(L,2)/VC
      L=L+1
      2  CONTINUE
      N=L-1
1003  FORMAT(18A4)
      RETURN
      END
      SUBROUTINE SUBZ(B,PRNT,X,Y,TITLE,INNER,N,NDPM,NPRNT)
      IMPLICIT REAL*8 (A-H,O-Z)
      INTEGER PMT
      REAL*4 TITLE
      DIMENSION B(50),PRNT(5),TITLE(18,3)
      DIMENSION X(NDPM,6),Y(1000)
      NPRNT = 2
      RETURN
      END
      SUBROUTINE FCODE(PAR,P,PRNT,RES,X,PEX,I,IB,IP,NDPM)
      IMPLICIT REAL*8 (A-H,O-Z)
      INTEGER PMT
      REAL*4 TITLE
      DIMENSION PAR(50),IB(50),PRNT(5),X(NDPM,6),PEX(1000),P(6)
      COMMON /LBCOR1/IPR(10),PMT(50)
      DATA TC,VC,ZC,PC/734.65,.07244,.28255,529.10/
C
C      THREE PARAMETERS ARE IMPLICIT FUNCTIONS OF THE OTHERS DUE TO
C      THE CONDITIONS AT THE CRITICAL POINT
C      PAR(J),J=1,4,7,10,13,16 = FTC(I),I=1-6
C      PAR(J),J=2,5,8,11,14,17 = B(I),I=1-6
C      PAR(J),J=3,6,9,12,15,18 = C(I),I=1-6
C      PAR(19)=KR
C      PAR(20)=AR
C      PAR(21)=BR
C
C      INITIAL VALUES OF ALL PARAMETERS MUST BE SUPPLIED TO THE MARQ
C      SUBROUTINE. A CARD MUST BE SUPPLIED INDICATING THAT PARAMETERS
C      1,4, AND 7 ARE NOT TO BE VARIED.
C
      TR=X(I,5)
      VR=X(I,6)
      PRNT(1)=X(I,1)
      PRNT(2)=X(I,2)
      AR=PAR(20)
      BR=PAR(21)
      TERM=1./(VR-BR)
      TERM=1./(1.-BR)

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INPU 190
INPU 200
INPU 210
INPU 220
INPU 230
INPU 240
INPU 250
INPU 260
INPU 270
INPU 280
INPU 290
INPU 300
INPU 310
INPU 320
INPU 330
INPU 340
INPU 350
INPU 360
INPU 370
INPU 380
INPU 390
INPU 400
INPU 410
INPU 420
INPU 430
INPU 440
INPU 450
INPU 460
INPU 470
INPU 480
INPU 490
SUBZ 10
SUBZ 20
SUBZ 30
SUBZ 40
SUBZ 50
SUBZ 60
SUBZ 70
SUBZ 80
SUBZ 90
FCODE 10
FCODE 20
FCODE 30
FCODE 40
FCODE 50
FCODE 60
FCODE 70
FCODE 80
FCODE 90
FCOD 100
FCOD 110
FCOD 120
FCOD 130
FCOD 140
FCOD 150
FCOD 160
FCOD 170
FCOD 180
FCOD 190
FCOD 200
FCOD 210
FCOD 220
FCOD 230
FCOD 240
FCOD 250
FCOD 260
FCOD 270
FCOD 280
FCOD 290

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QC=1./TPRMC
IF (I.GT.1) GO TO 1
FOUR=TEPMC+TERMC*TERMC*TERMC
EA=DEXP(-AR)
EB=DEXP(-2.*AR)
R1=ZC-TERMC*(1.+PAR(10)*FOUR)-EA*PAR(13)-EB*PAR(16)
R2=-1.-5.*PAR(10)*FOUR-AR*(EA*PAR(13)+2.*EB*PAR(16))*QC**2
R3=-2.-30.*FOUR*PAR(10)-AR**2*(EA*PAR(13)+4.*EB*PAR(16))*QC**3
PAR(1)=QC*(6.*R1*QC-4.*R2+.5*R3)
PAR(4)=QC**2*(-8.*R1*QC+7.*R2-R3)
PAR(7)=QC**3*(3.*R1*QC-3.*R2+.5*R3)
1 CONTINUE
K=1
DO 2 N=1,6
F(N)=PAR(K)*PAR(K+1)*(TR-1.)*PAR(K+2)*(DEXP(-TR*PAR(19))-DEXP(-PAR
1(19)))
K=K+3
2 CONTINUE
P=(PC/ZC)*TERM*(TR+TERM*(F(1)+TERM*(F(2)+TERM*(F(3)+TERM*(F(4))))
1+(PC/ZC)*DEXP(-AR*VR)*(F(5)+F(6)*DEXP(-AR*VR))
RES=(PEX(I)-P)/PEX(I)
RETURN
END
SUBROUTINE PCODE(B,D,F,PRNT,X,I,IB,IP,NDPM)
IMPLICIT REAL*8 (A-H,O-Z)
INTEGER PMT
REAL*4 TITLE
DIMENSION B(50),D(50),IB(50),PRNT(5),X(NDPM,6)
COMMON /LBCOM1/IPR(10),PMT(50)
RETURN
END
SUBROUTINE OUTPUT(A,B,PRNT,SA,SE,X,Y,TITLE,ITCT,K,N,NDPM,NPM)
IMPLICIT REAL*8 (A-H,O-Z)
INTEGER PMT
REAL*4 TITLE
DIMENSION A(NPM,50),B(50),PRNT(5),SA(50),TITLE(18,3)
DIMENSION X(NDPM,6),Y(1000)
COMMON /LBCOM1/IPR(10),PMT(50)
COMMON /TAPES/NI,NO,NP,MTTC
IF (K.GT.6) GO TO 1
N=1
GO TO 3
1 NC=K/6
J=6*NC
I=0
2 WRITE (NP,1001) B(I+1),B(I+2),B(I+3),B(I+4),B(I+5),B(I+6)
I=I+6
IF (I.LT.J) GO TO 2
N=N+1
3 WRITE (NP,1001) (B(I),I=N,K)
1001 FORMAT(1P6E12.5)
RETURN
END
SUBROUTINE MARQ(A,B,BA,BB,BS,C,CONS,DB,G,P,PRNT,SA,SPRNT,W,X,Y,
1 YMN,SPRD,FP,T,E,TAU,XL,GAMCR,DEL,ZETA,
2 TITLE,PMT,IP,PA,Q,H,K,IP,H,IPP,NCONS,ISPRD,
3 IWS1,IWS2,IWS3,IWS4,IWS5,IWS6,IREAD,NDPM,NPM,NIN)
NONLINEAR LEAST SQUARES
BY D. W. MARQUARDT
PROGRAMMED BY T. BAUMEISTER III,
J. ANN SHELDON AND RUBY M. STANLEY
IBKT=1 MEANS USE UPPER A MATRIX
IBKT=2 MEANS USE TAPE 3
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION A(NPM,50),B(50),BA(50),BB(50),BS(50),C(50),CONS(25)
DIMENSION DB(50),PMT(18),G(50),IB(50),P(50),PA(50),PRNT(5),Q(50)
DIMENSION SA(50),SPRNT(5),TITLE(18,3),W(50)

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FCOD 300
FCOD 310
FCOD 320
FCOD 330
FCOD 340
FCOD 350
FCOD 360
FCOD 370
FCOD 380
FCOD 390
FCOD 400
FCOD 410
FCOD 420
FCOD 430
FCOD 440
FCOD 441
FCOD 450
FCOD 460
FCOD 470
FCOD 471
FCOD 480
FCOD 490
FCOD 500
PCODE 10
PCODE 20
PCODE 30
PCODE 40
PCODE 50
PCODE 60
PCODE 70
PCODE 80
OUTPU 10
OUTPU 20
OUTPU 30
OUTPU 40
OUTPU 50
OUTPU 60
OUTPU 70
OUTPU 80
OUTPU 90
OUTP 100
OUTP 110
OUTP 120
OUTP 130
OUTP 140
OUTP 150
OUTP 160
OUTP 170
OUTP 180
OUTP 190
OUTP 200
OUTP 210
OUTP 220
MARQ 10
MARQ 11
MARQ 12
MARQ 13
MARQ 20
MARQ 30
MARQ 40
MARQ 50
MARQ 60
MARQ 70
MARQ 80
MARQ 90
MARQ 100
MARQ 110
MARQ 120
MARQ 130

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DIMENSION X(NDPH,6),Y(1000)
COMMON/LBCOM1/IPR(10),PNT(50)
COMMON/TAPES/NI,NO,MP,NTOC
COMMON/STAPE/WST
REAL*4 TITLE
INTEGER PNT,PA,Q
C
C -----
C NDPH      = MAXIMUM NUMBER OF DATA POINTS
C NPE      = MAXIMUM NUMBER OF PARAMETERS
C NIN      = MAXIMUM NUMBER OF INDEPENDENT VARIABLES
C IWHER = -1 MEANS DO ANY SPECIAL INITIALIZING FOR CASE
C IWHER = 0 MEANS START NEW CASE OR END RUN
C IWHER = 1 MEANS GET P S AND F
C IWHER GREATER THAN 1 MEANS GET P ONLY
C
C NPRINT=0
1 IWHER = 0
2 GO TO 11
3 IWHER = IWHER
  IF (IWHER) 4,4,7
  IF (IWHER) 5, 10,5
4
5 CONTINUE
C CODING FOR CASE INITIALIZING GOES HERE
C .....
C CALL SUBZ(B,PNT,X,Y,TITLE,IWHER,N,NDPH,NPRINT)
C .....
C IF (IBOUT) 6, 2,6
6 GO TO 1
7 CONTINUE
C CODING TO MAKE F GOES HERE
C F IS Y HAT (I)
C NPRINT IS THE NO OF OTHER WORDS TO BE PRINTED
C THE WORDS TO BE PRINTED ARE IN PNT(1)...PNT(5)
C .....
C CALL FCODE(B,F,PNT,RES,X,Y,I,IB,IP,NDPH)
C .....
C IF (IWHER-1) 2, 8,2
8 IF (IFSS2) 2,9,2
9 CONTINUE
C CODING TO MAKE DF/DB GOES HERE
C MAKE K OF THEM. CALL THEN P(J)
C THEY ARE MADE FROM X(I,L) AND B(J)
C .....
C CALL PCODE(B,P,F,PNT,X,I,IB,IP,NDPH)
C .....
C GO TO 2
10 CALL EXIT
C THIS IS THE END OF THE MAIN ROUTINE
C -----
11 IWHER = IWHER
C - 0 +
  IF (IWHER) 44,13,12
C 1 2 3 4
12 GO TO (65,208,70,76), IWHER
C READ FIRST CARD OF NEXT CASE
13 ITCT=0
  IBOUT=0
  IF (IREAD.EQ.1) READ (NI,1001) N,K,IP,M,IFP,NCONS,ISPRD
  IF (N.EQ.0) RETURN
C HERE I ADD A CONTROL INDEX, ISPRD, TO ALLOW LINEAR OR LOG PLOTTING
C ISPRD = 1 FOR LINEAR PLOTTING
C ISPRD = 2 FOR LOG PLOTTING (LOG(F) AND LOG(Y(I)))
C ISPRD IS USED ONLY IF (IFP.GT.0)
  NTILDA=N+NCONS
  INT=NTILDA
  IF (N) 15,15,14
14 IF (IREAD.EQ.1) READ (NI,1001) IWS1,IWS2,IWS3,IWS4,IWS5,IWS6
  IFSS1=2
  WRITE (NO,1033)

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MARQ 140
 MARQ 150
 MARQ 160
 MARQ 170
 MARQ 180
 MARQ 190
 MARQ 200
 MARQ 210
 MARQ 220
 MARQ 230
 MARQ 240
 MARQ 250
 MARQ 260
 MARQ 270
 MARQ 280
 MARQ 290
 MARQ 300
 MARQ 310
 MARQ 320
 MARQ 330
 MARQ 340
 MARQ 350
 MARQ 360
 MARQ 370
 MARQ 380
 MARQ 390
 MARQ 400
 MARQ 410
 MARQ 420
 MARQ 430
 MARQ 440
 MARQ 450
 MARQ 460
 MARQ 470
 MARQ 480
 MARQ 490
 MARQ 500
 MARQ 510
 MARQ 520
 MARQ 530
 MARQ 540
 MARQ 550
 MARQ 560
 MARQ 570
 MARQ 580
 MARQ 590
 MARQ 600
 MARQ 610
 MARQ 620
 MARQ 630
 MARQ 640
 MARQ 650
 MARQ 660
 MARQ 670
 MARQ 680
 MARQ 690
 MARQ 700
 MARQ 710
 MARQ 720
 MARQ 730
 MARQ 740
 MARQ 750
 MARQ 760
 MARQ 770
 MARQ 780
 MARQ 790
 MARQ 800
 MARQ 810
 MARQ 820

	GO TO 18	MARQ 830
C	END OF LAST PROBLEM	MARQ 840
15	GO TO (17, 16),IBKT	MARQ 850
16	REWIND NST	MARQ 860
17	IWHER=0	MARQ 870
	GO TO 3	MARQ 880
18	IF (IFP) 20, 20, 19	MARQ 890
19	CONTINUE	MARQ 900
	CALL ATHRUZ(IBC,1H)	MARQ 910
	CALL ATHRUZ(IOC,1HO)	MARQ 920
	CALL ATHRUZ(IPC,1HP)	MARQ 930
	CALL ATHRUZ(IYC,1HY)	MARQ 940
	CALL ATHRUZ(IXC,1HX)	MARQ 950
	IF (IREAD.EQ.1) READ (NI,1031) YMW,SPRD	MARQ 960
20	IF (IP) 24,24,21	MARQ 970
21	IF (IREAD.EQ.1) READ (NI,1001) (IB(I),I=1,IP)	MARQ 980
	DO 23 I=1,IP	MARQ 990
	IF (IB(I)) 22,22,23	MAR 1000
22	WRITE (NO,1028)	MAR 1010
	IBOUT=1	MAR 1020
23	CONTINUE	MAR 1030
24	IF (IREAD.EQ.1) READ (NI,1032) FF,T,E,TAU,XL,GAMCR,DEL,ZETA	MAR 1040
C	DUB IN INPUT CONSTANTS IF NOT SUPPLIED	MAR 1050
C	(XL IS CHECKED IN FIRST ITERATION)	MAR 1060
	IF (FF) 25,25,26	MAR 1070
25	FF=4.	MAR 1080
26	IF (E) 27,27,28	MAR 1090
27	E=.00005	MAR 1100
28	IF (TAU) 29,29,30	MAR 1110
29	TAU=.001	MAR 1120
30	IF (T) 31,31,32	MAR 1130
31	T=2.	MAR 1140
32	IF (K-25) 33,33,34	MAR 1150
33	IBKT=1	MAR 1160
	GO TO 35	MAR 1170
34	IBKT=2	MAR 1180
	REWIND NST	MAR 1190
35	IF (GAMCR) 36,36,37	MAR 1200
36	GAMCR = 45.	MAR 1210
37	IF (DEL) 38,38,39	MAR 1220
38	DEL=.00001	MAR 1230
39	IF (ZETA) 40,40,41	MAR 1240
40	ZETA=.1E-30	MAR 1250
41	XKDB = 1.	MAR 1260
42	CONTINUE	MAR 1270
C	READ IN INITIAL B GUESSES 6 TO THE CARD	MAR 1280
	IF (IREAD.EQ.1) READ (NI,1002) (B(I),I=1,K)	MAR 1290
	IF (IREAD.EQ.1) READ (NI,1003) (PMT(I),I=1,18)	MAR 1300
43	CALL INPUT(B,PRNT,X,Y,PMT,TITLE,N,NDPH)	MAR 1310
	NTILDA=N+NCONS	MAR 1320
	IWHER=-1	MAR 1330
	GO TO 3	MAR 1340
44	IBKA=1	MAR 1350
C		MAR 1360
C		MAR 1370
C	START THE CALCULATION OF THE PTP MATRIX	MAR 1380
	WRITE (NO,1033)	MAR 1390
	WRITE (NO,1004) (TITLE(I,1),I=1,18)	MAR 1400
	WRITE (NO,1004) (TITLE(I,2),I=1,18)	MAR 1410
	WRITE (NO,1004) (TITLE(I,3),I=1,18)	MAR 1420
45	WRITE (NO,1009) N,K,IP,H,IFP,GAMCR,DEL,FF,T,E,TAU,XL,ZETA	MAR 1430
46	GO TO 49	MAR 1440
47	CONTINUE	MAR 1450
48	IWS3=IWS3-1	MAR 1460
	IWS3=MAX0(IWS3,0)	MAR 1470
49	DO 50 I=1,K	MAR 1480
	G (I) =0.	MAR 1490
	DO 50 J=1,K	MAR 1500
50	A (I,J)=0.	MAR 1510
	GO TO (51,56,56),IRKA	MAR 1520

51	IF (IWS5.EQ.0) GO TO 52	MAR 1530
	GO TO (54,53),IPSS3	MAR 1540
52	IPSS3=IWS3	MAR 1550
	IPSS2=IWS2	MAR 1560
	GO TO 57	MAR 1570
53	IPSS3=0	MAR 1580
54	GO TO (57,55), IPSS2	MAR 1590
55	IPSS2=0	MAR 1600
	GO TO 57	MAR 1610
56	CONTINUE	MAR 1620
57	WRITE (NO,1010) ITCT,(B(J),J=1,K)	MAR 1630
	IF (IPSS3) 58,61,58	MAR 1640
58	IF (IFP) 60,60,59	MAR 1650
59	WS = YNN+SPRD	MAR 1660
	WRITE (NO,1008) YNN,WS	MAR 1670
	GO TO 61	MAR 1680
60	WRITE (NO,1012)	MAR 1690
61	I=1	MAR 1700
	PHI=0.	MAR 1710
	PHIN=0.	MAR 1720
	ICONS=1	MAR 1730
	IF (IPSS2) 62,64,62	MAR 1740
62	GO TO 68	MAR 1750
63	IF (IPSS2-1) 64,69,64	MAR 1760
C	THIS IS THE ANALYTICAL P S ROUTINE	MAR 1770
64	IWHRR=1	MAR 1780
C	GET P S AND P	MAR 1790
	GO TO 3	MAR 1800
65	IF (IP) 81,81,66	MAR 1810
66	DO 67 II=1,IP	MAR 1820
	IWS=IB(II)	MAR 1830
67	P(IWS)=0.	MAR 1840
	GO TO 81	MAR 1850
C		MAR 1860
C	THIS IS THE ESTIMATED P S ROUTINE	MAR 1870
68	CONTINUE	MAR 1880
69	IWHRR=3	MAR 1890
	GO TO 3	MAR 1900
70	RWS=RES	MAR 1910
	PSAVE=P	MAR 1920
	DO 71 II=1,NPRNT	MAR 1930
71	SPRNT(II)=PRNT(II)	MAR 1940
	J=1	MAR 1950
72	IF (IP) 75,75,73	MAR 1960
73	DO 74 II=1,IP	MAR 1970
	IF (J-IB(II)) 74,77,74	MAR 1980
74	CONTINUE	MAR 1990
75	DBW=B(J)*DEL	MAR 2000
	TWS=B(J)	MAR 2010
	B(J)=B(J)+DBW	MAR 2020
	IWHRR=4	MAR 2030
	GO TO 3	MAR 2040
76	B(J)=TWS	MAR 2050
	F(J)=- (RES-RWS)/DBW	MAR 2060
	GO TO 78	MAR 2070
77	P(J)=0.	MAR 2080
78	J=J+1	MAR 2090
	IF (J-K) 72,72,79	MAR 2100
79	RES=RWS	MAR 2110
	F=PSAVE	MAR 2120
	DO 80 II=1,NPRNT	MAR 2130
80	PRNT(II)=SPRNT(II)	MAR 2140
C	END OF ESTIMATED P S ROUTINE	MAR 2150
C		MAR 2160
C	NOW, USE THE P S TO MAKE PARTIALS MATRIX	MAR 2170
81	DO 82 JJ=1,K	MAR 2180
	G(JJ)=G(JJ)+RES*P(JJ)	MAR 2190

	DO 82 II=JJ,K	HAR 2200
	A(II,JJ)=A(II,JJ)+P(II)*P(JJ)	HAR 2210
82	A(JJ,II)=A(II,JJ)	HAR 2220
	IF (IFP) 105,105,93	HAR 2230
83	IF (IPSS3) 84,110,84	HAR 2240
C	PLOTTING Y(I),F	HAR 2250
84	GO TO (85,86), ISPRD	HAR 2260
85	IO = (Y(I)-YMH)*100./SPRD	HAR 2270
	IPP = (F-YMH)*100./SPRD	HAR 2280
	GO TO 87	HAR 2290
86	IO = (DLOG10(Y(I))-YMH)*100./SPRD	HAR 2300
	IPP = (DLOG10(F)-YMH)*100./SPRD	HAR 2310
87	IF (IO-IPP) 88,89,90	HAR 2320
C	Y(I) OUT FIRST	HAR 2330
88	IP1=IOCH	HAR 2340
	IP2=IPCH	HAR 2350
	I1=IO	HAR 2360
	I2=IPP	HAR 2370
	GO TO 91	HAR 2380
C	ONLY ONE CHARACTER	HAR 2390
89	IP1=IXCH	HAR 2400
	IP2=IXCH	HAR 2410
	I1=IO	HAR 2420
	I2=IPP	HAR 2430
	GO TO 91	HAR 2440
C	F OUT FIRST	HAR 2450
90	IP1=IPCH	HAR 2460
	IP2=IOCH	HAR 2470
	I1=IPP	HAR 2480
	I2=IO	HAR 2490
C	ZERO PLOTS IN THE LEFT HAND COLUMN, SO I1 IS ITS	HAR 2500
C	OWN BLANK COUNTER	HAR 2510
C	OVERFLOWS PLOT X IN COLUMN 102	HAR 2520
C	UNDERFLOWS ALSO PLOT X IN COLUMN ZERO	HAR 2530
91	IF (I2-101) 94,94,92	HAR 2540
92	I2=101	HAR 2550
	IP2=IXCH	HAR 2560
	IF (I1-101) 94,93,93	HAR 2570
93	I1=101	HAR 2580
	IP1=IXCH	HAR 2590
	IP2=IBCH	HAR 2600
	GO TO 97	HAR 2610
94	IF (I1) 95,95,97	HAR 2620
95	I1=0	HAR 2630
	IP1=IXCH	HAR 2640
	IF (I2) 96,96,97	HAR 2650
96	I2=1	HAR 2660
	IP2=IBCH	HAR 2670
97	I1M1=I1	HAR 2680
	I1M2=I2-I1-1	HAR 2690
	IF (I1M1) 98,98,101	HAR 2700
98	IF (I1M2) 99,99,100	HAR 2710
99	WRITE (NO,1030) IP1,IP2	HAR 2720
	GO TO 104	HAR 2730
100	WRITE (NO,1030) IP1,(IBCH,II=1,I1M2),IP2	HAR 2740
	GO TO 104	HAR 2750
101	IF (I1M2) 102,102,103	HAR 2760
102	WRITE (NO,1030) (IBCH,II=1,I1M1),IP1,IP2	HAR 2770
	GO TO 104	HAR 2780
103	WRITE (NO,1030) (IBCH,II=1,I1M1),IP1,(IBCH,II=1,I1M2),IP2	HAR 2790
104	GO TO 110	HAR 2800
105	WS=RES	HAR 2810
	IF (IPSS3) 106,110,106	HAR 2820
106	IF (I-N) 107,107,110	HAR 2830
107	IF (NPRNT) 108,108,109	HAR 2840
108	WRITE (NO,1027) Y(I),F,WS	HAR 2850
	GO TO 110	HAR 2860
109	WRITE (NO,1027) Y(I),F,WS,(PRNT(JJ),JJ=1,NPRNT)	HAR 2870
110	WS=RES	HAR 2880

	PHI=PHI+WS*WS		HAR 2890
	IF (I-N) 111,111,112		HAR 2900
111	PHIN=PHIN+WS*WS		HAR 2910
	GO TO 113		HAR 2920
112	CONS;ICONS)=RES		HAR 2930
	ICONS=ICONS+1		HAR 2940
113	I=I+1		HAR 2950
	IF (I-NILDA) 63,63,114		HAR 2960
114	IF (IP) 118,118,115		HAR 2970
115	DO 117 JJ=1,IP		HAR 2980
	IWS=IB(JJ)		HAR 2990
	DO 116 II=1,K		HAR 3000
	A(IWS,II)=0.		HAR 3010
116	A(II,IWS)=0.		HAR 3020
117	A(IWS,IWS)=1.		HAR 3030
118	GO TO (119,214,216),IBKA		HAR 3040
C	SAVE SQUARE ROOTS OF DIAGONAL ELEMENTS		HAR 3050
119	DO 122 I=1,K		HAR 3060
	IF(A(I,I)) 120,121,122		HAR 3070
120	WRITE (NO,1041) I,I,A(I,I)		HAR 3080
	WRITE (NO,1042) (A(JQ,JQ),JQ=1,K)		HAR 3090
	IF (IREAD .NE. 1) RETURN		HAR 3100
	GO TO 1		HAR 3110
121	WRITE (NO,1042) (A(JQ,JQ),JQ=1,K)		HAR 3120
122	SA(I)=DSQRT(A(I,I))		HAR 3130
	DO 128 I=1,K		HAR 3140
	DO 125 J=1,K		HAR 3150
	WS = SA(I)*SA(J)		HAR 3160
	IF (WS) 123,123,124		HAR 3170
123	A(I,J) =0.		HAR 3180
	GO TO 125		HAR 3190
124	A(I,J)=A(I,J)/WS		HAR 3200
125	CONTINUE		HAR 3210
	IF (SA(I)) 126,126,127		HAR 3220
126	G(I)=0.		HAR 3230
	GO TO 128		HAR 3240
127	G(I)=G(I)/SA(I)		HAR 3250
128	CONTINUE		HAR 3260
	DO 129 I=1,K		HAR 3270
129	A(I,I)=1.		HAR 3280
130	PHIZ=PHI		HAR 3290
C	WE NOW HAVE PHI ZERO		HAR 3300
	GO TO (132,131),IBKT		HAR 3310
131	WRITE (3)A		HAR 3320
	REWIND NST		HAR 3330
	GO TO 134		HAR 3340
132	DO 133 II=1,K		HAR 3350
	III=II+25		HAR 3360
	DO 133 JJ=1,K		HAR 3370
133	A(III,JJ)=A(II,JJ)		HAR 3380
C			HAR 3390
134	CONTINUE		HAR 3400
	IF (ITCT) 139,135,139		HAR 3410
C	FIRST ITERATION		HAR 3420
135	IF (XL) 136,136,137		HAR 3430
136	XL=0.01		HAR 3440
137	DO 138 J=1,K		HAR 3450
138	BS(J)=B(J)		HAR 3460
C	BS(J) CORRESPONDS TO PHIZ		HAR 3470
139	IBK1=1		HAR 3480
	WS=N-K+IP		HAR 3490
	ITCT=ITCT+1		HAR 3500
	SE=DSQRT(PHIN/WS)		HAR 3510
	IF (IFSS3) 140,140,143		HAR 3520
140	IF (IFSS2) 141,142,141		HAR 3530
141	WRITE (NO,1013) PHIZ,SE,XLL,GAMMA,XL		HAR 3540
	GO TO 149		HAR 3550
142	WRITE (NO,1014) PHIZ,SE,XLL,GAMMA,XL		HAR 3560
	GO TO 149		HAR 3570

143	IF (NCONS) 144,145,144	NAR 3580
144	WRITE (NO,1039) (JJ,CONS(JJ),JJ=1,NCONS)	NAR 3590
145	WRITE (NO,1040)	NAR 3600
	DO 146 I=1,K	NAR 3610
	WRITE (NO,1038) I,(A(I,J),J=1,K)	NAR 3620
146	CONTINUE	NAR 3630
	IF (IFSS2) 147,148,147	NAR 3640
147	WRITE (NO,1005) PHIZ,SE,XL	NAR 3650
	GO TO 149	NAR 3660
148	WRITE (NO,1011) PHIZ,SE,XL	NAR 3670
149	GO TO 183	NAR 3680
150	PHIL=PHI	NAR 3690
C	WE NOW HAVE PHI LAMBDA	NAR 3700
	DO 151 J=1,K	NAR 3710
	IF (ABSP (DB(J)/(ABSP(B(J))+TAU)) - E) 151,153,153	NAR 3720
151	CONTINUE	NAR 3730
152	WRITE (NO,1025)	NAR 3740
	GO TO 212	NAR 3750
153	IF (IWS4) 154,157,154	NAR 3760
154	IF (IWS4-1) 155, 156,155	NAR 3770
155	IWS4=IWS4-1	NAR 3780
	GO TO 157	NAR 3790
156	WRITE (NO,1026)	NAR 3800
	GO TO 212	NAR 3810
157	KKDB = 1.	NAR 3820
	IF (PHIL-PHIZ) 158,158,168	NAR 3830
158	XLS=XL	NAR 3840
	DO 159 J=1,K	NAR 3850
	BA(J)=B(J)	NAR 3860
159	B(J)=BS(J)	NAR 3870
	IF (XL-0.00000001) 160,160,162	NAR 3880
160	DO 161 J=1,K	NAR 3890
	B(J)=BA(J)	NAR 3900
161	BS(J)=B(J)	NAR 3910
	GO TO 47	NAR 3920
162	XL=XL/10.	NAR 3930
	IBK1=2	NAR 3940
	GO TO 183	NAR 3950
163	PHL4=PHI	NAR 3960
C	WE NOW HAVE PHI (LAMBDA/10)	NAR 3970
	IF (PHL4-PHIZ) 164,164,166	NAR 3980
164	DO 165 J=1,K	NAR 3990
165	BS(J)=B(J)	NAR 4000
	GO TO 47	NAR 4010
166	XL=XLS	NAR 4020
	DO 167 J=1,K	NAR 4030
	BS(J)=BA(J)	NAR 4040
167	B(J)=BA(J)	NAR 4050
	GO TO 47	NAR 4060
168	IBK1=4	NAR 4070
	XLS=XL	NAR 4080
	XL=XL/10.	NAR 4090
	DO 169 J=1,K	NAR 4100
169	B(J)=BS(J)	NAR 4110
	GO TO 183	NAR 4120
170	IF (PHI-PHIZ) 177,177,171	NAR 4130
171	XL=XLS	NAR 4140
	IBK1=3	NAR 4150
172	XL=XL*10.	NAR 4160
173	DO 174 J=1,K	NAR 4170
174	B(J)=BS(J)	NAR 4180
	GO TO 183	NAR 4190
175	PHIT4=PHI	NAR 4200
C	WE NOW HAVE PHI (10*LAMBDA)	NAR 4210
176	IF (PHIT4-PHIZ) 177,177,179	NAR 4220
177	DO 178 J=1,K	NAR 4230
178	BS(J)=B(J)	NAR 4240
	GO TO 47	NAR 4250
179	IF (GAMMA-GAMCR) 180,172,172	NAR 4260
180	KKDB = KKDB/2.	NAR 4270

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DO 181 J=1,K
IF (ABSF{DB{J}}/{ABSF{B{J}}+TAU))-E) 181,173,173
181 CONTINUE
DO 182 J=1,K
182 B{J}=BS{J}
WRITE (NO,1035)
GO TO 212
C
C .....
C SET UP FOR MATRIX INVERSION
183 GO TO (185,184),IBK1
184 READ (NST) A
REWIND NST
GO TO 187
185 DO 186 II=1,K
III=II+25
DO 186 JJ=1,K
186 A{II,JJ}=A{III,JJ}
187 DO 188 I=1,K
188 A{I,I}=A{I,I}+XL
C GET INVERSE OF A AND SOLVE FOR DB {J}S
IBK1=1
C .....
C THIS IS THE MATRIX INVERSION ROUTINE
C K IS THE SIZE OF THE MATRIX
189 CALL AGJR{A,BB,C,DET,ZETA,PA,Q,K,MSING,NPM)
GO TO (191,190),MSING
190 IF (IREAD - 1) 286, 1,286
191 GO TO (192,226), IBK1
C END OF MATRIX INVERSION, SOLVE FOR DB{J}
192 DO 194 I=1,K
DB{I}=0.
DO 193 J=1,K
193 DB{I}=A{I,J}*G{J}+DB{I}
194 DB{I}=IKDB*DB{I}
XLL=0.
DTG = 0.
GTG = 0.
DO 195 J=1,K
XLL=XLL+DB{J}*DB{J}
DTG = DTG + DB{J}*G{J}
GTG = GTG + G{J}**2
DB{J}=DB{J}/SA{J}
195 B{J}=B{J}+DB{J}
KIP=K-IP
IF (KIP-1) 196,201,196
196 CGAM=DTG/DSQRT(XLL*GTG)
JGAM = 1
IF (CGAM) 197, 197, 198
197 CGAM = ABSF{CGAM}
JGAM = 2
198 IF (CGAM.GT.1.0) CGAM = 1.0
GAMMA = 57.2957795*(1.5707288+CGAM*(-0.2121144+CGAM*(0.074261
1-CGAM*.0187293)))*DSQRT(1.-CGAM)
GO TO (202,199), JGAM
199 GAMMA = 180.-GAMMA
IF (XL-1.0) 202,200,200
200 WRITE (NO,1024) XL,GAMMA
GO TO 212
201 GAMMA=0.
202 XLL=DSQRT(XLL)
IBK2=1
GO TO 206
203 IF (IFSS3) 204, 205, 204
204 WRITE (NO,1006) {DB{J},J=1,K)
WRITE (NO,1007) PHI,XL,GAMMA,XLL
205 GO TO (150,163,175,170),IBK1
C
C .....

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C		CALCULATE PHI	HAR 4960
206	I=1		HAR 4970
	PHI=0.		HAR 4980
	PHIN=0.		HAR 4990
	IWHER=2		HAR 5000
C	IF (IWS5)	2141, 121, 2141	HAR 5010
C2141	CALL SSWTCH(5,NONSK)		HAR 5020
C	IF (NONSK-1)	2151, 101, 2151	HAR 5030
207	GO TO 3		HAR 5040
208	PHI=PHI+(RES**2)		HAR 5050
	IF (I-N)	209, 209, 210	HAR 5060
209	PHIN=PHIN+RES*RES		HAR 5070
210	I=I+1		HAR 5080
	IF (I-NTILDA)	207, 207, 211	HAR 5090
211	GO TO (203, 271, 214, 259, 262, 266), IBK2		HAR 5100
C			HAR 5110
C			HAR 5120
C			HAR 5130
C		THIS IS THE CONFIDENCE LIMIT CALCULATION	HAR 5140
212	DO 213 J=1,K		HAR 5150
213	B(J)=BS(J)		HAR 5160
	WRITE (NO,1034) N,K,IP,N,PP,T,E,TAU		HAR 5170
	IBKA=2		HAR 5180
	NTILDA=N		HAR 5190
C		THIS WILL PRINT THE Y,YHAT,DELTA Y	HAR 5200
	ITCT=ITCT-1		HAR 5210
	IPSS3=1		HAR 5220
	GO TO 49		HAR 5230
214	IF (IFP)	216, 216, 215	HAR 5240
215	IBKA=3		HAR 5250
	IFP=0		HAR 5260
	GO TO 49		HAR 5270
216	IF (NCONS)	217, 218, 217	HAR 5280
217	WRITE (NO,1039) (JJ,CONS(JJ),JJ=1,NCONS)		HAR 5290
218	WS=N-K+IP		HAR 5300
	SE=DSQRT(PHI/WS)		HAR 5310
	PHI2=PHI		HAR 5320
	IF (IPSS2)	219, 220, 219	HAR 5330
219	WRITE (NO,1005) PHIZ,SE,XL		HAR 5340
	GO TO 221		HAR 5350
220	WRITE (NO,1011) PHIZ,SE,XL		HAR 5360
C		NOW WE HAVE MATRIX A	HAR 5370
221	GO TO (223,222),IBKT		HAR 5380
222	WRITE (NST) A		HAR 5390
	REWIND NST		HAR 5400
	GO TO 225		HAR 5410
223	DO 224 II=1,K		HAR 5420
	III=II+25		HAR 5430
	DO 224 JJ=1,K		HAR 5440
224	A(III,JJ)=A(II,JJ)		HAR 5450
225	IBKM=2		HAR 5460
	GO TO 189		HAR 5470
C			HAR 5480
C		NOW WE HAVE C = A INVERSE	HAR 5490
226	DO 228 J=1,K		HAR 5500
	IF (A(J,J))	227, 228, 228	HAR 5510
227	WRITE (NO,1043) J,J,A(J,J),J,J		HAR 5520
	A(J,J)=1.0 D 0		HAR 5530
228	SA(J)=DSQRT(A(J,J))		HAR 5540
229	KST=-4		HAR 5550
	WRITE (NO,1018)		HAR 5560
230	KST=KST+5		HAR 5570
	KEND=KST+4		HAR 5580
	IF (KEND-K)	232, 231, 231	HAR 5590
231	KEND=K		HAR 5600
232	DO 233 I=1,K		HAR 5610
233	WRITE (NO,1020) I,(A(I,J),J=KST,KEND)		HAR 5620
	IF (KEND-K)	230, 234, 234	HAR 5630
234	IF (IBOUT)	235, 236, 235	HAR 5640
235	WRITE (NO,1037)		HAR 5650

	IF (IREAD .NE. 1) RETURN	HAR 5660
	GO TO 1	HAR 5670
236	DO 239 I=1,K	HAR 5680
	DO 239 J=1,K	HAR 5690
	WS=SA(I)*SA(J)	HAR 5700
	IF (WS) 237, 237, 238	HAR 5710
237	A(I,J)=0.	HAR 5720
	GO TO 239	HAR 5730
238	A(I,J)=A(I,J)/WS	HAR 5740
239	CONTINUE	HAR 5750
	DO 240 J=1,K	HAR 5760
240	A(J,J)=1.	HAR 5770
	WRITE (NO,1019)	HAR 5780
	KST=-9	HAR 5790
241	KST=KST+10	HAR 5800
	KEND=KST+9	HAR 5810
	IF (KEND-K) 243,242,242	HAR 5820
242	KEND=K	HAR 5830
243	DO 244 I=1,K	HAR 5840
244	WRITE (NO,1036) I,(A(I,J),J=KST,KEND)	HAR 5850
	IF (KEND-K) 241,245,245	HAR 5860
	GET T*SE*SQRT(C(I,I))	HAR 5870
C		
245	DO 246 J=1,K	HAR 5880
246	SA(J) = SE*SA(J)	HAR 5890
247	WRITE (NO,1021)	HAR 5900
	WS=K-IP	HAR 5910
	DO 252 J=1,K	HAR 5920
	IF (IP) 250, 250, 248	HAR 5930
248	DO 249 I=1,IP	HAR 5940
	IF (J-B(I)) 249, 251, 249	HAR 5950
249	CONTINUE	HAR 5960
250	HJTD=DSQRT(WS*FF)*SA(J)	HAR 5970
	STE=SA(J)	HAR 5980
	OPL=BS(J)-SA(J)*T	HAR 5990
	OPU=BS(J)+SA(J)*T	HAR 6000
	SPL=BS(J)-HJTD	HAR 6010
	SPU=BS(J)+HJTD	HAR 6020
	WRITE (NO,1029) J,STE,OPL,OPU,SPL,SPU	HAR 6030
	GO TO 252	HAR 6040
251	WRITE (NO,1015) J	HAR 6050
252	CONTINUE	HAR 6060
C		
	NONLINEAR CONFIDENCE LIMIT	HAR 6070
	IF (IWS6-1) 253,255,253	HAR 6080
253	WS=K-IP	HAR 6090
	WS1=N-K+IP	HAR 6100
	PKN=WS/WS1	HAR 6110
	PC=PHIZ*(1.+FF*PKN)	HAR 6120
	WRITE (NO,1022) PC	HAR 6130
	WRITE (NO,1023)	HAR 6140
	IFSS3=1	HAR 6150
	DO 284 J=1,K	HAR 6160
	IBKP=1	HAR 6170
	DO 254 JJ=1,K	HAR 6180
254	B(JJ)=BS(JJ)	HAR 6190
	IF (IP) 257, 257, 255	HAR 6200
255	DO 256 JJ=1,IP	HAR 6210
	IF (J-IB(JJ)) 256, 277, 256	HAR 6220
256	CONTINUE	HAR 6230
257	DD=-1.	HAR 6240
	IBKN=1	HAR 6250
258	D=DD	HAR 6260
	B(J)=BS(J)+D*SA(J)	HAR 6270
	IBK2=4	HAR 6280
	GO TO 206	HAR 6290
259	PHI1=PHI	HAR 6300
	IF (PHI1-PC) 260, 264, 264	HAR 6310
260	D=D+DD	HAR 6320
	IF ((D/DD)-5.) 261, 279, 279	HAR 6330
261	B(J)=BS(J)+D*SA(J)	HAR 6340

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IBK2=5
GO TO 206
262 PHID=PHI
IF (PHID-PC) 260, 263, 263
263 IF (PHID-PC) 264, 267, 267
264 D=D/2.
IF ((D/DD) -.001) 279, 279, 265
265 B(J)=BS(J)+D*SA(J)
IBK2=6
GO TO 206
266 PHID=PHI
IF (PHID-PC) 267, 267, 264
267 KK1=PHIZ/D+PHI1/(1.-D)+PHID/(D*(D-1.))
KK2=-(PHIZ*(1.+D)/D+D/(1.-D)+PHI1+PHID/(D*(D-1.)))
KK3=PHIZ-PC
BC = (DSQRT (KK2*KK2-4.*KK1*KK3)-KK2)/(2.*KK1)
GO TO (268, 269), IBKN
268 B(J)=BS(J)-SA(J)*BC
GO TO 270
269 B(J)=BS(J)+SA(J)*BC
270 IBK2=2
GO TO 206
271 GO TO (272, 273), IBKN
272 IBKN=2
DD=1.
BL=B(J)
PL=PHI
GO TO 258
273 BU=B(J)
PU=PHI
GO TO (274, 275, 276, 278), IBKP
274 WRITE (NO, 1020) J, BL, PL, BU, PU
GO TO 284
275 WRITE (NO, 1017) J, BU, PU
GO TO 284
276 WRITE (NO, 1020) J, BL, PL
GO TO 284
277 WRITE (NO, 1015) J
GO TO 284
278 WRITE (NO, 1016) J
GO TO 284
279 GO TO (280, 281), IBKN
C      DELETE LOWER PRINT
280 IBKP=2
GO TO 271
281 GO TO (282, 283), IBKP
C      DELETE UPPER PRINT
282 IBKP=3
GO TO 271
C      LOWER IS ALREADY DELETED, SO DELETE BOTH
283 IBKP=4
GO TO 271
284 B(J)=BS(J)
C      -----
285 CALL OUTPUT(A, B, PENT, SA, SE, X, Y, TITLE, ITCT, K, N, NDPH, NPH)
C      -----
IF (IREAD .NE. 1) RETURN
GO TO 1
286 RETURN
C      .....
1001 FORMAT (25I3)
1002 FORMAT (6D12.0)
1003 FORMAT (18A4)
1004 FORMAT (1X, 18A4)
1005 FORMAT (/13X, 4H PHI 14X, 4H S E 9X, 7H LAMBDA 6X,
1 25H ESTIMATED PARTIALS USED / 5X, 2E18.8, E13.3)
1006 FORMAT (/12H INCREMENTS 5E18.8/(12X, 5E18.8) )
1007 FORMAT (13X, 4H PHI 10X, 7H LAMBDA 6X, 7H GAMMA 6X, 7H LENGTH /
1 5X, E18.8, 3E13.3)
1008 FORMAT (1X, 1E9.2, 86X, 1E9.2 /1X, 1E+ 99X, 1E+ )

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MAR 6350
MAR 6360
MAR 6370
MAR 6380
MAR 6390
MAR 6400
MAR 6410
MAR 6420
MAR 6430
MAR 6440
MAR 6450
MAR 6460
MAR 6470
MAR 6480
MAR 6490
MAR 6500
MAR 6510
MAR 6520
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MAR 6900
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MAR 6920
MAR 6930
MAR 6940
MAR 6950
MAR 6960
MAR 6970
MAR 6980
MAR 6990
MAR 6991
MAR 7000
MAR 7010
MAR 7011
MAR 7020

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1009 FORMAT( 5HON = I3,5X,5H K = I3,5X,5HIP = I3,5X,5H M = I3,5X,      MAR 7030
1 7H IFF = I3,5X,13HGAMMA CRIT = E10.3,5X,6HDEL = E10.3/6H PF =      MAR 7031
2E10.3,5X,5H T = E10.3,5X,5H E = E10.3,5X,7H TAU = E10.3,5X,6H XL = MAR 7032
3 E10.3 , 4X, 7HZETA = E10.3 /)
1010 FORMAT (/2H (I3,13H) PARAMETERS 5E18.8/(18X,5E18.8))      MAR 7040
1011 FORMAT (/13X,4H PHI 14X,4H S E 9X,7H LAMBDA 6X,      MAR 7050
1 25H ANALYTIC PARTIALS USED /5X, 2E18.8, F13.3)      MAR 7051
1012 FORMAT(1H /5X,9X,4H OBS 13X,5H PRED 13X,5H RES )      MAR 7060
1013 FORMAT (/13X,4H PHI 14X,4H S E 11X,7H LENGTH 6X, 7H GAMMA 6X,      MAR 7070
1 7H LAMBDA 6X, 25HESTIMATED PARTIALS USED /5X, 2E18.8, 3E13.3)      MAR 7071
1014 FORMAT (/13X,4H PHI 14X,4H S E 11X,7H LENGTH 6X, 7H GAMMA 6X,      MAR 7080
1 7H LAMBDA 6X, 24HANALYTIC PARTIALS USED /5X, 2E18.8, 3E13.3)      MAR 7081
1015 FORMAT(2X,I3,20H PARAMETER NOT USED )      MAR 7090
1016 FORMAT(2X,I3,12H NONE POUND )      MAR 7100
1017 FORMAT(2X,I3,36X,2E18.8 )      MAR 7110
1018 FORMAT(1H /13H PTP INVERSE )      MAR 7120
1019 FORMAT(1H /30H PARAMETER CORRELATION MATRIX )      MAR 7130
1020 FORMAT( 2X,I3,5E18.8)      MAR 7140
1021 FORMAT( 1H /1H / 13X,4H STD 17X, 16H ONE - PARAMETER 21X,      MAR 7150
1 14H SUPPORT PLANE / 3X, 2H B 7X,6H ERROR 12X, 6H LOWER 12X,
2 6H UPPER 12X, 6H LOWER 12X, 6H UPPER )      MAR 7152
1022 FORMAT( 1H /1H /30H NONLINEAR CONFIDENCE LIMITS / /      MAR 7160
1 16H PHI CRITICAL = E15.8 )      MAR 7161
1023 FORMAT(1H / 6H PARA 6X,8H LOWER B 8X,10H LOWER PHI 10X,8H UPPER B MAR 7170
1 8X,10H UPPER PHI )      MAR 7171
1024 FORMAT (1H1,60X,17HGAMMA LAMBDA TEST 6X,2E13.3)      MAR 7180
1025 FORMAT (1H1,90X,12HEPSILON TEST )      MAR 7190
1026 FORMAT (1H1,90X,10HFORCE OFF )      MAR 7200
1027 FORMAT (5X,6E18.8/59X,2E18.8)      MAR 7210
1028 FORMAT ( 40H BAD DATA, SUBSCRIPTS FOR UNUSED BS = 0 / / / )      MAR 7220
1029 FORMAT(2X,I3,5E18.8 )      MAR 7230
1030 FORMAT(1H , 110A1 )      MAR 7240
1031 FORMAT (7F10.0)      MAR 7250
1032 FORMAT (8F10.0)      MAR 7260
1033 FORMAT(1H1)      MAR 7270
1034 FORMAT (5HON = ,I3,5X,5H K = ,I3,5X,5H P = ,I3,5X,5H M = ,I3,5X,      MAR 7280
1/6H PF = ,E10.3,5X,5H T = ,E10.3,
25X,5H E = ,E10.3,5X,7H TAU = ,E10.3/)      MAR 7281
1035 FORMAT (1H1,80X,18HGAMMA EPSILON TEST )      MAR 7282
1036 FORMAT (3X,I5,2X,10F10.4)      MAR 7290
1037 FORMAT (27H0 NEGATIVE DIAGONAL ELEMENT )      MAR 7300
1038 FORMAT (3X,I5,2X,10F10.4/(10X,10F10.4))      MAR 7310
1039 FORMAT (1H /25H CONSTRAINT RESIDUALS .../(3X,I5,33X,E18.8))      MAR 7320
1040 FORMAT (1H /23H PTP CORRELATION MATRIX )      MAR 7330
1041 FORMAT (1H /11H ELEMENT A(,I2,1H,,I2,3H) =,1PE14.4)      MAR 7340
1042 FORMAT(10E12.3)      MAR 7350
1043 FORMAT(15H WARNING*** A(,I2,1H,,I2,4H) = ,1PD16.8/55H TO PERMIBAR 7370
1 THE CALCULATION TO CONTINUE WE NOW SET A(,I2,1H,,I2,9H) =1.0D 0/MAR 7371
2120H **** SUBROUTINE OUTPUT SHOULD BE PROGRAMMED TO HANDLE THISMAR 7372
3 SITUATION, POSSIBLY BY CHECKING FOR SA(J)=0.0 /120H MAR 7373
4 WE DO NOT SET A(J,J) = 0.0 SINCE THIS IS ALREADY THE CASE WHENMAR 7374
5H PARAMETERS ARE HELD CONSTANT. /1H0)      MAR 7375
END      MAR 7380
SUBROUTINE ATHRUZ(I,J)      MAR 7380
C ACCORDING TO D M FROM DU POWT      ATHRU 10
I=J      ATHRU 20
RETURN      ATHRU 30
END      ATHRU 40
SUBROUTINE AGJR(A,B,C,DET,EPS,P,Q,W,MSING,NPH)      ATHRU 50
C GAUSS-JORDAN-RUTISHAUSER MATRIX INVERSION WITH DOUBLE PIVOTING.      AGJR 10
REAL*8 A,B,C,PIVOT,Z      AGJR 20
DIMENSION A(NPH,50),B(50),C(50),P(50),Q(50)      AGJR 30
COMMON/TAPES/NI,NO,NP,NTTOD      AGJR 40
INTEGER P,Q      AGJR 50
DET=1.0D 0      AGJR 60
MSING=1      AGJR 70
DO 16 K=1,N      AGJR 80
C DETERMINATION OF THE PIVOT ELEMENT      AGJR 90
PIVOT=0.      AGJR 100
DO 2 I=K,N      AGJR 110

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	DO 2 J=K,N	AGJR 130
	IF (DABS(A(I,J))-DABS(PIVOT)) 2,2,1	AGJR 140
1	PIVOT=A(I,J)	AGJR 150
	ICOL=I	AGJR 160
	IROW=J	AGJR 170
	P(K)=I	AGJR 180
	Q(K)=J	AGJR 190
2	CONTINUE	AGJR 200
	IF (ICOL-IROW) 3,4,3	AGJR 210
3	DET=-DET	AGJR 220
4	IF (DABS(PIVOT)-EPS) 24,24,5	AGJR 230
C	EXCHANGE OF THE PIVOTAL ROW WITH THE KTH ROW	AGJR 240
5	IF (P(K)-K) 6,8,6	AGJR 250
6	DO 7 J=1,N	AGJR 260
	L=P(K)	AGJR 270
	Z=A(L,J)	AGJR 280
	A(L,J)=A(K,J)	AGJR 290
7	A(K,J)=Z	AGJR 300
C	EXCHANGE OF THE PIVOTAL COLUMN WITH THE KTH COLUMN	AGJR 310
8	IF (Q(K)-K) 9,11,9	AGJR 320
9	DO 10 I=1,N	AGJR 330
	L=Q(K)	AGJR 340
	Z=A(I,L)	AGJR 350
	A(I,L)=A(I,K)	AGJR 360
10	A(I,K)=Z	AGJR 370
11	CONTINUE	AGJR 380
	DET=DET*PIVOT	AGJR 390
C	JOORDAN STEP	AGJR 400
	DO 15 J=1,N	AGJR 410
	IF (J-K) 13,12,13	AGJR 420
12	B(J)=1./PIVOT	AGJR 430
	C(J)=1.	AGJR 440
	GO TO 14	AGJR 450
13	B(J)=-A(K,J)/PIVOT	AGJR 460
	C(J)=A(J,K)	AGJR 470
14	A(K,J)=0.	AGJR 480
15	A(J,K)=0.	AGJR 490
	DO 16 J=1,N	AGJR 500
	DO 16 I=1,N	AGJR 510
16	A(I,J)=A(I,J)+C(I)*B(J)	AGJR 520
C	REORDERING THE MATRIX	AGJR 530
	DO 22 M=1,N	AGJR 540
	K=N-M+1	AGJR 550
	IF (P(K)-K) 17,19,17	AGJR 560
17	DO 18 I=1,N	AGJR 570
	L=P(K)	AGJR 580
	Z=A(I,L)	AGJR 590
	A(I,L)=A(I,K)	AGJR 600
18	A(I,K)=Z	AGJR 610
19	IF (Q(K)-K) 20,22,20	AGJR 620
20	DO 21 J=1,N	AGJR 630
	L=Q(K)	AGJR 640
	Z=A(L,J)	AGJR 650
	A(L,J)=A(K,J)	AGJR 660
21	A(K,J)=Z	AGJR 670
22	CONTINUE	AGJR 680
23	RETURN	AGJR 690
24	WRITE (NO,1001) P(K),Q(K),PIVOT	AGJR 700
1001	FORMAT(16H0SINGULAR MATRIX3H I=I3,3H J=J3,7H PIVOT=E16.8/)	AGJR 710
	MSING=2	AGJR 720
	GO TO 23	AGJR 730
	END	AGJR 740

Appendix C

FORTRAN LISTING OF THE CODE APPROX

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      IMPLICIT REAL*8 (A-H,C-Z)
      DIMENSION FTC(6),A(6),E(6),C(6),DUM1(3,3),RHS1(3),DUM2(3,3),RHS2(
13),DUM3(4,4),RHS3(4),DUM4(4,4),RHS4(4),PEXP(50),VEXD(50),TEXP(50),
2NE XV(50), VEXF(1000)
C
C THIS PROGRAM OBTAINS INITIAL ESTIMATES OF THE 13 MARTIN EQUATION
C OF STATE PARAMETERS WHEN THE 8 CRITICAL ISOTHERM COEFFICIENTS ARE
C KNOWN. FOR A GIVEN VALUE OF THE NONLINEAR TEMPERATURE EXPONENT, R
C A SYSTEM OF 12 LINEAR EQUATIONS IN 12 UNKNOWN IS SOLVED.
C THE SYSTEM OF EQUATIONS IS OBTAINED BY MAKING USE OF
C 12 KNOWN 'FACTS' ABOUT THE P-V-T BEHAVIOR OF THE COMPOUND.
C THESE INCLUDE A KNOWLEDGE OF THE BOYLE TEMPERATURE, THE
C SLOPE OF THE VAPOR PRESSURE CURVE AT THE CRITICAL POINT, THE
C OBSERVED LINEARITY OF CERTAIN ISOCHORES ETC.
C ALL 12 FACTS MAY BE ADJUSTED TO OBTAIN A BETTER REPRESENTATION
C OF THE DATA.
C
C IT IS ADVISABLE TO START WITH A VALUE OF RK NEAR 4.0 AND TO
C MAKE SMALL CHANGES IN THIS PARAMETER UNTIL A GOOD FIT TO
C THE DATA IS OBTAINED.
C FOR MORE DETAILED INFORMATION SEE REFERENCES 1 AND 2.
C
      TC=734.65
      PC=36.003
      VC=.07244
      R=.0125642
      ZC=.28255
C
C TC IS CRITICAL TEMPERATURE IN DEG.R.
C PC IS CRITICAL PRESSURE IN ATM.
C VC IS CRITICAL SPECIFIC VOLUME IN CU.FT./LBM.
C ZC IS THE CRITICAL COMPRESSIBILITY FACTOR, ZC=PC*VC/(R*TC).
C R IS THE GAS CONSTANT FOR THE COMPOUND BEING CONSIDERED.
C PC, VC, TC, ZC, AND R MUST BE SUPPLIED BY THE USER.
C
      TRC=1.
      VRC=1.
      NUM1=3
      NUM2=3
      NUM3=4
      NUM4=4
C
C READ IN THE 8 KNOWN CRITICAL ISOTHERM COEFFICIENTS.
C
      READ(5,1001)AR,BR,(FTC(I),I=1,6)
1001 FORMAT(2D20.7/(3D20.7))
C
C IF A COMPARISON OF THE THE PREDICTED AND EXPERIMENTAL PRESSURES IS
C DESIRED, THEN READ THE EXPERIMENTAL P-V-T DATA HERE; OTHERWISE,
C REMOVE THIS SECTION(THROUGH STATEMENT 2).
C
      READ(5,1002)NEXP,NEXT,(PEXP(I),I=1,NEXP)
C
C NEXP IS NUMBER OF EXPERIMENTAL PRESSURES
C NEXT IS NUMBER OF EXPERIMENTAL TEMPERATURES
C
1002 FORMAT(2I5/(9F8.3))
      L=1
      DO 2 J=1,NEXT
      READ(5,1003)TEXP(J),NDUM,(VEXD(I),I=1,NDUM)
1003 FORMAT(F8.3,I2/(7F10.5))
      NEXV(J)=NDUM
      DO 1 K=1,NDUM
      VEXP(K)=VEXD(K)
1
      L=L+1
2
      CONTINUE
C
C BSTAR IS DEFINED AS THE GENERALIZED SECOND VIRIAL COEFFICIENT:
C SECOND VIRIAL COEFFICIENT = BSTAR*VC/ZC.
C CSTAR IS DEFINED AS THE GENERALIZED THIRD VIRIAL COEFFICIENT:
C THIRD VIRIAL COEFFICIENT = CSTAR*(VC/ZC)**2.
C BSTAR AND CSTAR ARE RELATED TO THE FIRST TWO REDUCED TEMPERATURE
C FUNCTIONS F(1) AND F(2) BY THE RELATIONSHIPS:
C F(1) = TR*(BSTAR/ZC-BF).
C F(2) = TR*(CSTAR/ZC**2-2*ER*BSTAR/ZC+ER**2).
C
C FACT 1: GENERALIZED SECOND VIRIAL COEFFICIENT IS ZERO AT THE BOYLE
C TEMPERATURE.
C TRB= REDUCED BOYLE TEMPERATURE(TEMPERATURE OF FACT 1 AND FACT 3).
C TRB=2.3
C BSTRB=0.
C
C FACT 2: VALUE OF GENERALIZED SECOND VIRIAL COEFFICIENT AT TR=TRS.
C TRS= REDUCED TEMPERATURE OF FACT 2 AND FACT 4.
C TRS=.8
C BSTRS=TRS*(ZC-1.)
C
C FACT 3: VALUE OF GENERALIZED THIRD VIRIAL COEFFICIENT AT THE BOYLE
C TEMPERATURE.
C CSTRB=.014

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      B(1)=RHS1(2)
      C(1)=RHS1(3)
      CALL SIMQ(DUM2,RHS2,NUN2,KS2)
      A(2)=RHS2(1)
      B(2)=RHS2(2)
      C(2)=RHS2(3)
C
C      USE FACTS 6,7,11 AND 12.
C
      DO 13 I=1,4
      SU TO (8,9,10,11),I
      DPRSQ=DPRSQ1
      VR=VR1
      GU TO 12
      DPRSQ=DPRSQ2
      VR=VR2
      SU TO 12
      DPRSQ=DPRSQ3
      TR=TR3
      VR=VR3
      SU TO 12
      DPRSQ=DPRSQ4
      TR=TR4
      VR=VR4
      TERM=1./(VR-BF)
      JUM3(1,1)=TERM**4
      JUM3(1,2)=TERM**5
      JUM3(1,3)=DEXF(-AR*VR)
      JUM3(1,4)=DEXF(-2.*AR*VR)
      RHS3(1)=(ZC/RK**2)*DPRSC*DEXP(RK*TR)-C(1)*TERM**2-C(2)*TERM**3
      CONTINUE
      CALL SIMQ(DUM3,RHS3,NUN3,KS3)
      C(3)=RHS3(1)
      C(4)=RHS3(2)
      C(5)=RHS3(3)
      C(6)=RHS3(4)
C
C      USE FACTS 5,8,9 AND 10.
C
      DO 19 I=1,4
      SU TO (14,15,16,17),I
      DPR=DPR1
      VR=VRD1
      TR=TRD1
      GU TO 18
      DPR=DPR2
      VR=VRD2
      TR=TRD2
      SU TO 18
      DPR=DPR3
      VR=VRD3
      TR=TRD3
      SU TO 18
      DPR=DPR4
      VR=VRD4
      TR=TRD4
      TERM=1./(VR-BF)
      JUM4(1,1)=TERM**4
      JUM4(1,2)=TERM**5
      JUM4(1,3)=DEXF(-AR*VR)
      JUM4(1,4)=DEXF(-2.*AR*VR)
      RHS4(1)=DPR*ZC-TERM-B(1)*TERM**2-B(2)*TERM**3+RK*DEXP(-RK*TR)*(C(1)
1) *TERM**2+C(2)*TERM**3+C(3)*TERM**4+C(4)*TERM**5+C(5)*DEXP(-AR*VR)
2+C(6)*DEXP(-2.*AR*VR)
      CONTINUE
      CALL SIMQ(DUM4,RHS4,NUN4,KS4)
      B(3)=RHS4(1)
      B(4)=RHS4(2)
      B(5)=RHS4(3)
      B(6)=RHS4(4)
      DO 20 J=3,6
C
C      ALL 12 LINEAR COEFFICIENTS HAVE NOW BEEN OBTAINED.
C
      20 A(J)=FTC(J)-B(J)-C(J)*DEXP(-RK)
      WRITE(6,1004)TC,PC,VC
      1004 FORMAT(1H1,'CRITICAL TEMPERATURE',3X,'CRITICAL PRESSURE',5X,
1,'CRITICAL VOLUME',3D20.6//)
      WRITE(6,1005)AR,BF,RK
      1005 FORMAT(1H1,17X,'AR',18X,'BF',18X,'RK',3D20.6//)
      WRITE(6,1006)(FTC(I),I=1,6)
      1006 FORMAT(1H1,9X,'FTC(1)',10X,'FTC(2)',10X,'FTC(3)',10X,'FTC(4)',
110X,'FTC(5)',10X,'FTC(6)',6D16.6//)
      WRITE(6,1007)(A(I),I=1,6)
      1007 FORMAT(1H1,11X,'A(1)',12X,'A(2)',12X,'A(3)',12X,'A(4)',12X,
1'A(5)',12X,'A(6)',6D16.6//)
      WRITE(6,1008)(B(I),I=1,6)
      1008 FORMAT(1H1,11X,'B(1)',12X,'B(2)',12X,'B(3)',12X,'B(4)',12X,
1'B(5)',12X,'B(6)',6D16.6//)
      WRITE(6,1009)(C(I),I=1,6)
      1009 FORMAT(1H1,11X,'C(1)',12X,'C(2)',12X,'C(3)',12X,'C(4)',12X,
1'C(5)',12X,'C(6)',6D16.6//)
      WRITE(6,1010)

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1010 FORMAT(1H,5X,'TEMP.',14X,'VOLUME',5X,'PRESSURE(EXPT.)',5X,
1 'PRESSURE(CALC.)',7X,'PERCENT DIFF.//')
C
C THIS SECTION IS FOR COMPARING EXPERIMENTAL AND PRECICTED
C PRESSURES. IF A COMPARISON IS NOT WANTED, THEN REMOVE CARDS
C THROUGH STATEMENT 22.
C
L=1
DO 22 J=1,NEXT
TEXPE=TEXP(J)+459.69
NOUM=NEXV(J)
DO 21 K=1,NOUM
VEXPE=VEXP(L)
L=L+1
CALL PRESRE(PCAL,VEXPE,TEXPE,PC,VC,TC,ZC,AR,BR,RK,A,B,C)
C
C PCAL IS CALCULATED PRESSURE IN ATM.
C PRESRE REQUIRES VOLUME AND TEMPERATURE IN ENGLISH UNITS
C
PCAL=PCAL*14.696
PERCNT=100.*(PCAL-FEXP(K))/FEXP(K)
WRITE(6,1011)TEXPE,VEXPE,PCAL,PERCNT
21 FORMAT(1H,10F10.3,4E20.6)
22 CONTINUE
23 CONTINUE
C
C REFERENCES:
C
C J.J.MARTIN, "EQUATIONS OF STATE," INC. ENG. CHEM. VOL 59 (1967)
C
C S.L.MILORA, "APPLICATION OF THE MARTIN EQUATION TO THE THERMO-
C DYNAMIC PROPERTIES OF AMMONIA," CAK RIDGE NATIONAL LABORATORY,
C ORNL-TM-4413 (DECEMBER 1973)
C
END
SUBROUTINE PRESRE(P,V,T,PC,VC,TC,ZC,AR,BR,RK,A,B,C)
IMPLICIT REAL*8 (A-H,C-Z)
DIMENSION A(6),E(6),C(6),F(6)
VM=V/VC
TR=T/TC
TERM=1./(VR-BR)
DO 1 I=1,6
F(I)=A(I)+B(I)*TR+C(I)*DEXP(-RK*TR)
P=(PC/ZC)*(TR*TERM+F(1)*TERM**2+F(2)*TERM**3+F(3)*TERM**4+F(4)*TE
1 RM**5+F(5)*DEXP(-AR*VR)+F(6)*DEXP(-2.*AR*VR))
RETURN
END
SUBROUTINE SING(A,E,N,KS)
C
C PURPOSE
C OBTAIN SOLUTION OF A SET OF SIMULTANEOUS LINEAR EQUATIONS.
C AX=B
C
C USAGE
C CALL SING(A,E,N,KS)
C
C DESCRIPTION OF PARAMETERS
C A - MATRIX OF COEFFICIENTS STORED COLUMNWISE. THESE ARE
C DESTROYED IN THE COMPUTATION. THE SIZE OF MATRIX A IS
C N BY N.
C B - VECTOR OF ORIGINAL CONSTANTS (LENGTH N). THESE ARE
C REPLACED BY FINAL SOLUTION VALUES, VECTOR X.
C N - NUMBER OF EQUATIONS AND VARIABLES. N MUST BE > 0. ONE.
C KS - OUTPUT DIGIT
C 0 FOR A NORMAL SOLUTION
C 1 FOR A SINGULAR SET OF EQUATIONS
C
IMPLICIT REAL*8 (A-H,C-Z)
DIMENSION A(1),E(1)
C
C FORWARD SOLUTION
C
TOL=0.0
KS=0
JJ=-N
DO 9 J=1,N
JY=J+1
JJ=JJ+N+1
BIGA=0
IT=JJ-J
DO 2 I=J,N
C
C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
C
IJ=IT+1
IF(DABS(BIGA)-DABS(A(IJ))) 1,2,2
1 BIGA=A(IJ)
IMAX=I
2 CONTINUE
C
C TEST FOR PIVOT LESS THAN TOLERANCE (SINGULAR MATRIX)

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2970
2980
2990
3000
3010
3020
PRESR 10
PRESR 20
PRESR 30
PRESR 40
PRESR 50
PRESR 60
PRESR 70
PRESR 80
PRESR 90
PRESR 91
PRES 100
PRES 110
SIMQ 10
SIMQ 20
SIMQ 30
SIMQ 40
SIMQ 50
SIMQ 60
SIMQ 70
SIMQ 80
SIMQ 90
SIMQ 100
SIMQ 110
SIMQ 120
SIMQ 130
SIMQ 140
SIMQ 150
SIMQ 160
SIMQ 170
SIMQ 180
SIMQ 190
SIMQ 200
SIMQ 210
SIMQ 220
SIMQ 230
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SIMQ 260
SIMQ 270
SIMQ 280
SIMQ 290
SIMQ 300
SIMQ 310
SIMQ 320
SIMQ 330
SIMQ 340
SIMQ 350
SIMQ 360
SIMQ 370
SIMQ 380
SIMQ 390
SIMQ 400
SIMQ 410
SIMQ 420
SIMQ 430
SIMQ 440
SIMQ 450

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3	IF (DABS(BIGA)-TOL) 3,3,4	SIMQ 460
	KS=1	SIMQ 470
	RETURN	SIMQ 480
C		SIMQ 490
C	INTERCHANGE ROWS IF NECESSARY	SIMQ 500
C		SIMQ 510
4	I1=J+N*(J-2)	SIMQ 520
	IT=IMAX-J	SIMQ 530
	DO 5 K=J,N	SIMQ 540
	I1=I1+N	SIMQ 550
	I2=I1+IT	SIMQ 560
	SAVE=A(I1)	SIMQ 570
	A(I1)=A(I2)	SIMQ 580
	A(I2)=SAVE	SIMQ 590
C		SIMQ 600
C	DIVIDE EQUATION BY LEADING COEFFICIENT	SIMQ 610
C		SIMQ 620
5	A(I1)=A(I1)/BIGA	SIMQ 630
	SAVE=B(IMAX)	SIMQ 640
	B(IMAX)=B(J)	SIMQ 650
	B(J)=SAVE/BIGA	SIMQ 660
C		SIMQ 670
C	ELIMINATE NEXT VARIABLE	SIMQ 680
C		SIMQ 690
6	IF (J-N) 6,9,6	SIMQ 700
	IQS=N*(J-1)	SIMQ 710
	DO 8 IX=JY,N	SIMQ 720
	IXJ=IQS+IX	SIMQ 730
	IT=J-IX	SIMQ 740
	DO 7 JX=JY,N	SIMQ 750
	IXJX=N*(JX-1)+IX	SIMQ 760
	JJX=IXJX+IT	SIMQ 770
7	A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))	SIMQ 780
8	B(IX)=B(IX)-(B(J)*A(IXJ))	SIMQ 790
C		SIMQ 800
C	BACK SOLUTION	SIMQ 810
C		SIMQ 820
9	NY=N-1	SIMQ 830
	IT=N*N	SIMQ 840
	DO 10 J=1,NY	SIMQ 850
	IA=IT-J	SIMQ 860
	IB=N-J	SIMQ 870
	IC=N	SIMQ 880
	DO 10 K=1,J	SIMQ 890
	B(IB)=B(IB)-A(IA)*B(IC)	SIMQ 900
	IA=IA-N	SIMQ 910
10	IC=IC-1	SIMQ 920
	RETURN	SIMQ 930
	END	SIMQ 940

Appendix D

OUTPUT FROM STATEQ — CASE 1

0.1500000000 03	0.148027007 03	0.131533550-01	0.699690000 03	0.753400000 00
0.2000000000 03	0.196330700 03	0.183464810-01	0.699690000 03	0.533500000 00
0.2500000000 03	0.243832650 03	0.246693860-01	0.699690000 03	0.399000000 00
0.3000000000 03	0.290427380 03	0.319087440-01	0.699690000 03	0.305900000 00
0.3500000000 03	0.335752620 03	0.407067910-01	0.699690000 03	0.234500000 00
0.4000000000 03	0.379396350 03	0.515091150-01	0.699690000 03	0.170100000 00
0.4500000000 01	0.420028700 01	-0.287036080-03	0.709690000 03	0.130900000 03
0.5000000000 02	0.467484900 02	0.143921030-02	0.709690000 03	0.882500000 01
0.5500000000 02	0.498116100 02	0.376779730-02	0.709690000 03	0.252400000 01
0.6000000000 03	0.492738280 02	0.726171970-02	0.709690000 03	0.121000000 01
0.6500000000 03	0.448284000 03	0.114395650-01	0.709690000 03	0.770000000 00
0.7000000000 03	0.196833170 03	0.158341620-01	0.709690000 03	0.547700000 00
0.7500000000 03	0.244836190 03	0.206552490-01	0.709690000 03	0.412000000 00
0.8000000000 03	0.292156190 03	0.261460450-01	0.709690000 03	0.318900000 00
0.8500000000 03	0.338701630 03	0.322810580-01	0.709690000 03	0.248800000 00
0.9000000000 03	0.384419080 03	0.389523100-01	0.709690000 03	0.190100000 00
0.9500000000 03	0.402626700 03	0.413649930-01	0.709690000 03	0.166800000 00
1.0000000000 01	0.421031850 03	0.431094320-01	0.709690000 03	0.139700000 00
1.0500000000 01	0.499909180 00	0.908167690-04	0.719690000 03	0.132800000 03
1.1000000000 02	0.146777490 02	0.124190430-02	0.719690000 03	0.895300000 01
1.1500000000 02	0.498360090 02	0.327981850-02	0.719690000 03	0.256400000 01
1.2000000000 03	0.993694320 02	0.630567600-02	0.719690000 03	0.123200000 01
1.2500000000 03	0.148498150 03	0.100123590-01	0.719690000 03	0.786400000 00
1.3000000000 03	0.197275550 03	0.136222670-01	0.719690000 03	0.561500000 00
1.3500000000 03	0.245644040 03	0.174238550-01	0.719690000 03	0.424600000 00
1.4000000000 03	0.293533400 03	0.215553230-01	0.719690000 03	0.331200000 00
1.4500000000 03	0.340987360 03	0.257503890-01	0.719690000 03	0.261700000 00
1.5000000000 03	0.387905700 03	0.302357430-01	0.719690000 03	0.205700000 00
1.5500000000 03	0.406964460 03	0.310369920-01	0.719690000 03	0.184800000 00
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0.1620000000 04	0.1620820406 04	-0.406326150-03	0.1359690000 04	0.2427000000 00
0.1640000000 04	0.1640840383 04	0.651503110-03	0.1359690000 04	0.2205000000 00
0.1660000000 04	0.1660860369 04	0.240656420-02	0.1359690000 04	0.2022000000 00
0.1680000000 04	0.1680880350 04	0.598830140-02	0.1359690000 04	0.1736000000 00
0.1700000000 04	0.1700900330 04	0.100874230-01	0.1359690000 04	0.1524000000 00
0.1720000000 04	0.1720920310 04	0.144275300-01	0.1359690000 04	0.1361000000 00
0.1740000000 04	0.1740940290 04	0.203380750-01	0.1359690000 04	0.1234000000 00
0.1760000000 04	0.1760960270 04	0.352698960-01	0.1359690000 04	0.1011000000 00
0.1780000000 04	0.1780980250 04	0.495837780-01	0.1359690000 04	0.8686000000-01
0.1800000000 04	0.1801000230 04	0.615066600-01	0.1359690000 04	0.7708000000-01

PTP CORRELATION MATRIX

1	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0000	-0.9426	0.0	0.9099	-0.8232	0.0	0.7951	-0.7174	0.3528
3	0.0	0.7006	0.2685	0.4865	-0.4586	0.1544	0.2903	-0.2750	-0.2110	0.1075
4	0.0	0.5661	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	-0.8081	0.7780	-0.3828	-0.6162	0.5967	-0.2262	-0.3914	-0.8763	0.8504
6	0.0	-0.6596	0.0	0.0	1.0000	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

PHI	0.128410630 01	SE	0.385294160-01	LAMBDA	0.1000-01	ESTIMATED PARTIALS USED	
INCREMENTS	0.0	0.148248680 00	0.974233450 00	0.0	0.235458120 00	0.201998280-01	
	-0.468828480 00	0.0	-0.993287930-02	0.0	0.235458120 00	-0.571098740-04	
	-0.878640200-02	0.351972790 00	-0.193059970 03	-0.356196060 03	0.400192160 05	0.400192160 05	
	0.334169750 06	0.951074290 05	0.223821120 08	0.441825920 00	0.209471390 00	0.209471390 00	
	0.710926440-02						
PHI	0.366474790 00	LAMBDA	0.1000-01	GAMMA	0.6530 02	LENGTH	0.1800 01
INCREMENTS	0.0	0.217172950 00	0.169193340 01	0.0	0.968607730 00	-0.107500270 00	
	-0.309820630 01	0.0	-0.478384930-01	0.0	0.968607730 00	0.229672890-02	
	0.252170130-02	0.160669600 01	-0.366842600 03	0.233912850 04	0.168594720 06	0.168594720 06	
	0.539247340 06	-0.622721220 06	0.109695550 09	0.631180700 00	-0.562103630-01	-0.562103630-01	
	0.391777690-01						
PHI	0.104714760 00	LAMBDA	0.1000-02	GAMMA	0.7990 02	LENGTH	0.4480 01
1 1) PARAMETERS	-0.131616920 01	0.960208950 07	-0.215266670 02	0.732337030 00	-0.877121270 00	-0.877121270 00	
	-0.298260060 02	-0.101146540 00	0.148021150 01	0.109375610 03	-0.328891710-01	-0.328891710-01	
	-0.831715300 00	-0.558315040 02	0.141529740 04	0.741580850 04	0.981525720 06	0.981525720 06	
	0.607691140 06	0.150857880 07	0.904838490 08	0.483118070 01	0.142770900 02	0.142770900 02	
	0.575110690-01						

0.1000000000 01	0.999939830 00	0.601650300-04	0.719690000 03	0.132800000 03
0.1469600000 02	0.146643930 02	0.789785480-03	0.719690000 03	0.895300000 01
0.5000000000 02	0.499138010 02	0.172397400-02	0.719690000 03	0.256400000 01
0.1000000000 03	0.996855530 02	0.314445480-02	0.719690000 03	0.123200000 01
0.1500000000 03	0.149219450 03	0.520365500-02	0.719690000 03	0.786400000 00
0.2000000000 03	0.198574890 03	0.712553060-02	0.719690000 03	0.561500000 00
0.2500000000 03	0.247695920 03	0.921631210-02	0.719690000 03	0.424600000 00
0.3000000000 03	0.296501530 03	0.116533700-01	0.719690000 03	0.331200000 00
0.3500000000 03	0.345011260 03	0.142535550-01	0.719690000 03	0.261700000 00
0.4000000000 03	0.393000360 03	0.174991070-01	0.719690000 03	0.205700000 00
0.4500000000 03	0.442421870 03	0.180431610-01	0.719690000 03	0.184800000 00
0.5000000000 03	0.491504450 03	0.193080760-01	0.719690000 03	0.164200000 00
0.5500000000 03	0.540546420 03	0.205512630-01	0.719690000 03	0.141900000 00
0.6000000000 03	0.589690040 03	0.227906840-01	0.719690000 03	0.114900000 00
0.6500000000 03	0.638838070 03	0.432701200-03	0.729690000 03	0.134700000 03
0.7000000000 03	0.687986030 02	0.678234580-03	0.729690000 03	0.908100000 01
0.7500000000 03	0.737134000 02	0.191800120-02	0.729690000 03	0.260500000 01
0.8000000000 03	0.786281970 02	0.289757790-02	0.729690000 03	0.125400000 01
0.8500000000 03	0.835430000 02	0.466746980-02	0.729690000 03	0.802500000 00
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0.9500000000 03	0.933725250 03	0.808382060-02	0.729690000 03	0.436800000 00
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0.1500000000 03	0.156574000 03	0.134389870-01	0.729690000 03	0.218800000 00
0.2000000000 03	0.205722250 03	0.134547990-01	0.729690000 03	0.199100000 00
0.2500000000 03	0.254797940 03	0.138995510-01	0.729690000 03	0.180400000 00
0.3000000000 03	0.303901630 03	0.143163440-01	0.729690000 03	0.162000000 00
0.3500000000 03	0.353054000 03	0.145858350-01	0.729690000 03	0.143000000 00
0.4000000000 03	0.402204410 03	0.149417790-01	0.729690000 03	0.121300000 00
0.4500000000 03	0.451444880 03	0.245387490-01	0.729690000 03	0.907200000-01
0.5000000000 03	0.500698800 03	0.644023210-04	0.739690000 03	0.136500000 03
0.5500000000 03	0.549903560 00	0.585769130-03	0.739690000 03	0.920900000 01
0.6000000000 03	0.599138010 02	0.180484330-02	0.739690000 03	0.264500000 01
0.6500000000 03	0.648309750 02	0.260944750-02	0.739690000 03	0.127600000 01
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0.7500000000 03	0.746683220 03	0.583901250-02	0.739690000 03	0.588300000 00
0.8000000000 03	0.795823210 03	0.707150570-02	0.739690000 03	0.448600000 00
0.8500000000 03	0.845037030 03	0.876537880-02	0.739690000 03	0.354200000 00
0.9000000000 03	0.894250570 03	0.998355770-02	0.739690000 03	0.284900000 00
0.9500000000 03	0.943469200 03	0.107698200-01	0.739690000 03	0.230700000 00
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0.1500000000 03	0.150949340 03	0.102493430-01	0.739690000 03	0.176800000 00
0.2000000000 03	0.200097130 03	0.984971320-02	0.739690000 03	0.160200000 00
0.2500000000 03	0.249508140 03	0.983704590-02	0.739690000 03	0.143800000 00
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0.3500000000 03	0.347048430 03	0.980587010-02	0.739690000 03	0.106800000 00
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0.4500000000 03	0.445382350 03	0.140028940-01	0.739690000 03	0.571200000-01
0.5000000000 03	0.494587590 03	0.972851490-02	0.739690000 03	0.524900000-01
0.5500000000 03	0.543788320 03	0.706640340-02	0.739690000 03	0.501400000-01
0.6000000000 03	0.593016290 03	0.196445250-02	0.739690000 03	0.484400000-01
0.6500000000 03	0.642281720 03	-0.744947460-02	0.739690000 03	0.470400000-01
0.7000000000 03	0.691561650 03	-0.629601220-02	0.739690000 03	0.462200000-01
0.7500000000 03	0.740723600 03	-0.284879910-02	0.739690000 03	0.455800000-01
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0.8500000000 03	0.838927140 03	0.899271460-02	0.739690000 03	0.432600000-01
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0.9500000000 03	0.937139520 03	0.184494230-01	0.739690000 03	0.417800000-01
1.0000000000 03	0.986236160 03	0.227771700-01	0.739690000 03	0.412100000-01
0.1000000000 04	0.974675060 03	0.253249420-01	0.739690000 03	0.407000000-01
0.1500000000 04	0.116343250 04	-0.576658880-01	0.739690000 03	0.391400000-01
0.2000000000 04	0.126824870 04	-0.568739280-01	0.739690000 03	0.385000000-01
0.2500000000 04	0.139028400 04	0.693996740-02	0.739690000 03	0.378800000-01
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0.3500000000 04	0.174363630 04	0.313131430-01	0.739690000 03	0.365500000-01
0.4000000000 04	0.191543170 04	0.422841720-01	0.739690000 03	0.360600000-01
0.4500000000 04	0.242670380 04	0.293184690-01	0.739690000 03	0.349400000-01
0.5000000000 04	0.295578360 04	0.147388090-01	0.739690000 03	0.341000000-01
0.5500000000 04	0.351869530 04	-0.534152320-02	0.739690000 03	0.334100000-01
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0.6500000000 04	0.468994140 02	-0.232328390-03	0.749690000 03	0.933000000 01
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0.7500000000 04	0.587137180 02	0.286281620-02	0.749690000 03	0.129800000 01
0.8000000000 04	0.646380240 03	0.613171380-02	0.749690000 03	0.834400000 00
0.8500000000 04	0.705908160 03	0.545920520-02	0.749690000 03	0.601400000 00
0.9000000000 04	0.765353100 03	0.658759580-02	0.749690000 03	0.460300000 00
0.9500000000 04	0.824769790 03	0.747350470-02	0.749690000 03	0.365000000 00
1.0000000000 04	0.884262210 03	0.849653890-02	0.749690000 03	0.295500000 00
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0.1500000000 05	0.101631310 03	0.877820740-02	0.749690000 03	0.223100000 00
0.2000000000 05	0.150996110 03	0.909975870-02	0.749690000 03	0.206000000 00
0.2500000000 05	0.200153760 03	0.923095930-02	0.749690000 03	0.189900000 00
0.3000000000 05	0.250098110 03	0.812894060-02	0.749690000 03	0.174200000 00
0.3500000000 05	0.300230140 03	0.753971040-02	0.749690000 03	0.159300000 00
0.4000000000 05	0.350161250 03	0.843746650-02	0.749690000 03	0.145300000 00
0.4500000000 05	0.400174150 03	0.793610120-02	0.749690000 03	0.130800000 00
0.5000000000 05	0.450155410 03	0.795509290-02	0.749690000 03	0.116000000 00
0.5500000000 05	0.500158240 03	0.761845110-02	0.749690000 03	0.995900000-01
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0.6500000000 05	0.600119770 03	0.141972120-01	0.749690000 03	0.678800000-01
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0.660000000 03	0.660327760 03	-0.496606480-03	0.749690000 03	0.544700000-01
0.680000000 03	0.682642330 03	-0.388577630-02	0.749690000 03	0.520900000-01
0.700000000 03	0.701339170 03	-0.191310370-02	0.749690000 03	0.506200000-01
0.750000000 03	0.751511310 03	-0.201508210-02	0.749690000 03	0.478900000-01
0.800000000 03	0.801134180 03	-0.141772750-02	0.749690000 03	0.461000000-01
0.850000000 03	0.849968330 03	0.372586190-04	0.749690000 03	0.448000000-01
0.900000000 03	0.898245300 03	0.194966160-02	0.749690000 03	0.437900000-01
0.950000000 03	0.944847860 03	0.542330620-02	0.749690000 03	0.429900000-01
0.100000000 04	0.991718030 03	0.828197130-02	0.749690000 03	0.423100000-01
0.110000000 04	0.113404740 04	-0.309522090-01	0.749690000 03	0.407400000-01
0.120000000 04	0.122193070 04	-0.182755820-01	0.749690000 03	0.400100000-01
0.140000000 04	0.139637130 04	0.259189720-02	0.749690000 03	0.388800000-01
0.160000000 04	0.157777720 04	0.138892250-01	0.749690000 03	0.379900000-01
0.180000000 04	0.176839260 04	0.175596880-01	0.749690000 03	0.372500000-01
0.200000000 04	0.195347940 04	0.232602840-01	0.749690000 03	0.366600000-01
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0.100000000 01	0.999927780 00	0.722186790-04	0.759690000 03	0.140200000 03
0.146960000 02	0.146862960 02	0.660303010-03	0.759690000 03	0.946700000 01
0.500000000 02	0.499123720 02	0.175255000-02	0.759690000 03	0.272500000 01
0.100000000 03	0.996960420 02	0.303958320-02	0.759690000 03	0.132000000 01
0.150000000 03	0.149421320 03	0.385787210-02	0.759690000 03	0.850000000 00
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0.250000000 03	0.248496790 03	0.401282740-02	0.759690000 03	0.471600000 00
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0.420000000 03	0.416646340 03	0.798491020-02	0.759690000 03	0.233800000 00
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0.950000000 03	0.952066320 03	-0.217507250-02	0.759690000 03	0.452200000-01
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0.120000000 04	0.118937990 04	0.885012390-02	0.759690000 03	0.417100000-01
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0.160000000 04	0.157931130 04	0.129304600-01	0.759690000 03	0.389100000-01
0.180000000 04	0.177116920 04	0.160170870-01	0.759690000 03	0.380400000-01
0.200000000 04	0.197245480 04	0.137725760-01	0.759690000 03	0.373100000-01
0.220000000 04	0.248896390 04	0.441443400-02	0.759690000 03	0.359400000-01
0.300000000 04	0.302923470 04	-0.974489670-02	0.759690000 03	0.349400000-01
0.350000000 04	0.359609510 04	-0.274557300-01	0.759690000 03	0.341500000-01
0.100000000 01	0.999917120 00	0.828837310-04	0.779690000 03	0.143900000 03
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0.1200000000 04	0.121194910 04	-0.995756610-02	0.105969000 04	0.135600000 00
0.1400000000 04	0.142113530 04	-0.150966160-01	0.105969000 04	0.113800000 00
0.1600000000 04	0.162834840 04	-0.177177700-01	0.105969000 04	0.984000000-01
0.1800000000 04	0.181824630 04	-0.101368190-01	0.105969000 04	0.879000000-01
0.2000000000 04	0.202762130 04	-0.138106530-01	0.105969000 04	0.791000000-01
0.2500000000 04	0.252577110 04	-0.101084240-01	0.105969000 04	0.653900000-01
0.3000000000 04	0.299049360 04	0.316879360-02	0.105969000 04	0.576300000-01
0.3500000000 04	0.344232900 04	0.164774260-01	0.105969000 04	0.524800000-01
0.1000000000 01	0.999863610 00	0.136390980-03	0.110969000 04	0.204900000 03
0.1469600000 02	0.146904240 02	0.379390100-03	0.110969000 04	0.135200000 02

0.500000000 03	0.503248910 03	-0.649781920-02	0.120969300 04	0.426600000 00
0.520000000 03	0.523407400 03	-0.635268410-02	0.120969300 04	0.409600000 00
0.540000000 03	0.543791160 03	-0.702067100-02	0.120969300 04	0.393700000 00
0.560000000 03	0.563970120 03	-0.708949370-02	0.120969300 04	0.379100000 00
0.580000000 03	0.584174690 03	-0.719774550-02	0.120969300 04	0.365500000 00
0.600000000 03	0.604572450 03	-0.762075790-02	0.120969300 04	0.352700000 00
0.620000000 03	0.624870340 03	-0.785539070-02	0.120969300 04	0.340800000 00
0.640000000 03	0.645274400 03	-0.824124620-02	0.120969300 04	0.329600000 00
0.660000000 03	0.669902890 03	-0.150043770-01	0.120969300 04	0.317000000 00
0.680000000 03	0.685700790 03	-0.838351200-02	0.120969300 04	0.309400000 00
0.700000000 03	0.706091050 03	-0.870150400-02	0.120969300 04	0.300100000 00
0.750000000 03	0.756994800 03	-0.932640130-02	0.120969300 04	0.279100000 00
0.800000000 03	0.807863920 03	-0.982989550-02	0.120969300 04	0.260800000 00
0.850000000 03	0.858426210 03	-0.991318590-02	0.120969300 04	0.244800000 00
0.900000000 03	0.909060490 03	-0.100672110-01	0.120969300 04	0.230600000 00
0.950000000 03	0.959848830 03	-0.103671860-01	0.120969300 04	0.217900000 00
0.100000000 04	0.101070110 04	-0.107011260-01	0.120969300 04	0.206500000 00
0.110000000 04	0.111200920 04	-0.109174790-01	0.120969300 04	0.187000000 00
0.120000000 04	0.121321950 04	-0.110162700-01	0.120969300 04	0.170900000 00
0.140000000 04	0.142378640 04	-0.169902940-01	0.120969300 04	0.145100000 00
0.160000000 04	0.162233420 04	-0.139588630-01	0.120969300 04	0.127300000 00
0.180000000 04	0.182437630 04	-0.135423650-01	0.120969300 04	0.113500000 00
0.200000000 04	0.202929830 04	-0.146491560-01	0.120969300 04	0.102600000 00
0.250000000 04	0.253414860 04	-0.136594220-01	0.120969300 04	0.841100000-01
0.300000000 04	0.303151130 04	-0.105037630-01	0.120969300 04	0.726400000-01
0.350000000 04	0.351647970 04	-0.470849970-02	0.120969300 04	0.649500000-01
0.400000000 01	0.409920280 00	0.797205070-04	0.125969300 04	0.232600000 03
0.460000000 02	0.466884300 02	0.515115290-03	0.125969300 04	0.158200000 02
0.500000000 02	0.500285950 02	-0.571692080-03	0.125969300 04	0.463400000 01
0.520000000 03	0.520122160 03	-0.122156550-02	0.125969300 04	0.230800000 01
0.540000000 03	0.540258770 03	-0.172514050-02	0.125969300 04	0.153300000 01
0.560000000 03	0.560546970 03	-0.273485980-02	0.125969300 04	0.114500000 01
0.580000000 03	0.580929210 03	-0.371683490-02	0.125969300 04	0.912300000 00
0.600000000 03	0.601344090 03	-0.448030070-02	0.125969300 04	0.757400000 00
0.620000000 03	0.621790580 03	-0.511594810-02	0.125969300 04	0.646900000 00
0.640000000 03	0.642216350 03	-0.554087060-02	0.125969300 04	0.564200000 00
0.660000000 03	0.662435700 03	-0.579927640-02	0.125969300 04	0.536600000 00
0.680000000 03	0.682764770 03	-0.628357730-02	0.125969300 04	0.511400000 00
0.700000000 03	0.702928020 03	-0.636525290-02	0.125969300 04	0.488600000 00
0.720000000 03	0.723203310 03	-0.667356450-02	0.125969300 04	0.467600000 00
0.740000000 03	0.743682800 03	-0.673655440-02	0.125969300 04	0.448400000 00
0.760000000 03	0.764301370 03	-0.676430130-02	0.125969300 04	0.430700000 00
0.780000000 03	0.780726190 03	-0.707261920-02	0.125969300 04	0.414200000 00
0.800000000 03	0.803466540 03	-0.734665440-02	0.125969300 04	0.398900000 00
0.820000000 03	0.825251180 03	-0.752511890-02	0.125969300 04	0.384700000 00
0.840000000 03	0.840707300 03	-0.784549790-02	0.125969300 04	0.371400000 00
0.860000000 03	0.862500390 03	-0.807083480-02	0.125969300 04	0.359000000 00
0.880000000 03	0.882452690 03	-0.824520930-02	0.125969300 04	0.347600000 00
0.900000000 03	0.903653830 03	-0.815712260-02	0.125969300 04	0.336600000 00
0.920000000 03	0.925776380 03	-0.849467170-02	0.125969300 04	0.326300000 00
0.940000000 03	0.940595580 03	-0.850831610-02	0.125969300 04	0.316700000 00
0.960000000 03	0.960823080 03	-0.909743920-02	0.125969300 04	0.294800000 00
0.980000000 03	0.980767970 03	-0.959969640-02	0.125969300 04	0.275700000 00
0.100000000 04	0.100800060 03	-0.966200250-02	0.125969300 04	0.259000000 00
0.102000000 04	0.102000250 03	-0.100889610-01	0.125969300 04	0.244100000 00
0.104000000 04	0.104000540 04	-0.105289430-01	0.125969300 04	0.230800000 00
0.106000000 04	0.106000840 04	-0.108054250-01	0.125969300 04	0.218900000 00
0.108000000 04	0.108001140 04	-0.110540290-01	0.125969300 04	0.198500000 00
0.110000000 04	0.110001440 04	-0.112429930-01	0.125969300 04	0.181400000 00
0.112000000 04	0.112001740 04	-0.117393620-01	0.125969300 04	0.155400000 00
0.114000000 04	0.114002040 04	-0.128990460-01	0.125969300 04	0.136000000 00
0.116000000 04	0.116002340 04	-0.133801390-01	0.125969300 04	0.121300000 00
0.118000000 04	0.118002640 04	-0.138477630-01	0.125969300 04	0.109800000 00
0.120000000 04	0.120002940 04	-0.139434860-01	0.125969300 04	0.899500000-01
0.122000000 04	0.122003240 04	-0.125577590-01	0.125969300 04	0.774800000-01
0.124000000 04	0.124003540 04	-0.875361850-02	0.125969300 04	0.690500000-01
0.126000000 04	0.126003840 04	-0.712398520-04	0.130969300 04	0.241800000 03
0.128000000 04	0.128004140 04	0.393611120-03	0.130969300 04	0.164500000 02
0.130000000 04	0.130004440 04	-0.775190450-03	0.130969300 04	0.482100000 01
0.132000000 04	0.132004740 04	-0.148265630-02	0.130969300 04	0.240300000 01
0.134000000 04	0.134005040 04	-0.224755410-02	0.130969300 04	0.159700000 01
0.136000000 04	0.136005340 04	-0.307451630-02	0.130969300 04	0.119400000 01
0.138000000 04	0.138005640 04	-0.407262770-02	0.130969300 04	0.952100000 00
0.140000000 04	0.140005940 04	-0.480855280-02	0.130969300 04	0.791100000 00
0.142000000 04	0.142006240 04	-0.547377520-02	0.130969300 04	0.676200000 00
0.144000000 04	0.144006540 04	-0.592566990-02	0.130969300 04	0.590200000 00
0.146000000 04	0.146006840 04	-0.636480200-02	0.130969300 04	0.561400000 00
0.148000000 04	0.148007140 04	-0.648199690-02	0.130969300 04	0.535400000 00
0.150000000 04	0.150007440 04	-0.653752480-02	0.130969300 04	0.511700000 00
0.152000000 04	0.152007740 04	-0.695057660-02	0.130969300 04	0.489800000 00
0.154000000 04	0.154008040 04	-0.814075320-02	0.130969300 04	0.469300000 00
0.156000000 04	0.156008340 04	-0.731279090-02	0.130969300 04	0.451300000 00
0.158000000 04	0.158008640 04	-0.748632440-02	0.130969300 04	0.434200000 00
0.160000000 04	0.160008940 04	-0.796244520-02	0.130969300 04	0.418200000 00
0.162000000 04	0.162009240 04	-0.797324550-02	0.130969300 04	0.403500000 00
0.164000000 04	0.164009540 04	-0.820288100-02	0.130969300 04	0.389700000 00
0.166000000 04	0.166009840 04	-0.842363840-02	0.130969300 04	0.376500000 00
0.168000000 04	0.168010140 04	-0.867813410-02	0.130969300 04	0.364700000 00
0.170000000 04	0.170010440 04	-0.876319580-02	0.130969300 04	0.353400000 00
0.172000000 04	0.172010740 04	-0.876355650-02	0.130969300 04	0.342800000 00
0.174000000 04	0.174011040 04	-0.879816670-02	0.130969300 04	0.332800000 00
0.176000000 04	0.176011340 04	-0.938769520-02	0.130969300 04	0.310000000 00

0.8000000000	0.805758690	-0.719836090	0.130969000	0.290900000
0.8500000000	0.858500830	-0.100009710	0.130969000	0.272700000
0.9000000000	0.509296320	-0.103292470	0.130969000	0.257200000
0.9500000000	0.959799190	-0.105044120	0.130969000	0.243400000
0.1000000000	0.101072220	-0.107222160	0.130969000	0.231000000
0.1100000000	0.111209300	-0.109936080	0.130969000	0.209700000
0.1200000000	0.121386180	-0.115515200	0.130969000	0.192000000
0.1400000000	0.141654640	-0.118188610	0.130969000	0.164600000
0.1600000000	0.162016810	-0.126050360	0.130969000	0.144300000
0.1800000000	0.182397570	-0.133198500	0.130969000	0.128800000
0.2000000000	0.202687210	-0.134360430	0.130969000	0.116700000
0.2500000000	0.253492660	-0.139706270	0.130969000	0.956000000
0.3000000000	0.304070940	-0.135697960	0.130969000	0.822200000
0.3500000000	0.354010500	-0.114585790	0.130969000	0.730900000
0.1000000000	0.100021010	-0.210056090	0.135969000	0.251000000
0.1469600000	0.146916360	0.296933480	0.135969000	0.170800000
0.5000000000	0.500354900	-0.709790640	0.135969000	0.500900000
0.1000000000	0.100161480	-0.161482100	0.135969000	0.249800000
0.1500000000	0.150384910	-0.256603420	0.135969000	0.166100000
0.2000000000	0.200633350	-0.316672820	0.135969000	0.124300000
0.2500000000	0.251080830	-0.432331400	0.135969000	0.991700000
0.3000000000	0.301541190	-0.513728850	0.135969000	0.824500000
0.3500000000	0.352041480	-0.589280730	0.135969000	0.705200000
0.4000000000	0.402589650	-0.647412660	0.135969000	0.615800000
0.4200000000	0.422835150	-0.675034620	0.135969000	0.586000000
0.4400000000	0.443103960	-0.705446030	0.135969000	0.558900000
0.4600000000	0.463267470	-0.710320280	0.135969000	0.534300000
0.4800000000	0.483578760	-0.745575200	0.135969000	0.511600000
0.5000000000	0.503825270	-0.765054540	0.135969000	0.490800000
0.5200000000	0.524086170	-0.785801810	0.135969000	0.471600000
0.5400000000	0.544270230	-0.790782930	0.135969000	0.453900000
0.5600000000	0.564673030	-0.834469760	0.135969000	0.437300000
0.5800000000	0.584888930	-0.842918880	0.135969000	0.422000000
0.6000000000	0.605145690	-0.857614360	0.135969000	0.407700000
0.6200000000	0.625452340	-0.879409250	0.135969000	0.394300000
0.6400000000	0.645672460	-0.886321760	0.135969000	0.381800000
0.6600000000	0.666007170	-0.910176770	0.135969000	0.370000000
0.6800000000	0.686350410	-0.933884390	0.135969000	0.358900000
0.7000000000	0.706381800	-0.911686020	0.135969000	0.348600000
0.7500000000	0.757283760	-0.971167580	0.135969000	0.324900000
0.8000000000	0.807963850	-0.995480920	0.135969000	0.304300000
0.8500000000	0.858824790	-1.038210600	0.135969000	0.286100000
0.9000000000	0.909564150	-1.062643170	0.135969000	0.270000000
0.9500000000	0.960411380	-1.095934800	0.135969000	0.255600000
0.1000000000	0.101115500	-0.111549900	0.135969000	0.242700000
0.1100000000	0.111266740	-0.115158510	0.135969000	0.220500000
0.1200000000	0.121361440	-0.113453380	0.135969000	0.202200000
0.1400000000	0.141614510	-0.115322080	0.135969000	0.173600000
0.1600000000	0.161920570	-0.120035570	0.135969000	0.152400000
0.1800000000	0.182338310	-0.129906190	0.135969000	0.136100000
0.2000000000	0.202577700	-0.128885020	0.135969000	0.123400000
0.2500000000	0.253409830	-0.136393130	0.135969000	0.101100000
0.3000000000	0.304155430	-0.138514380	0.135969000	0.086800000
0.3500000000	0.354468140	-0.128232570	0.135969000	0.770800000

PTP CORRELATION MATRIX

1	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0000	-0.9340	0.0	0.9109	-0.8172	0.0	0.7970	-0.7145	-0.3587
3	0.7025	-0.6347	0.2856	0.5149	-0.4825	0.1664	0.3116	-0.2933	-0.3707	-0.0641
4	0.4782	-0.9340	1.0000	0.0	-0.9410	0.9369	0.0	-0.8812	0.8570	-0.5036
5	-0.8147	0.7854	-0.4126	-0.6513	0.6310	-0.2477	-0.4221	0.4044	0.4027	0.1311
6	-0.5058	0.0	0.0	0.0	1.0000	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0	0.0	0.0
8	0.0	0.9109	-0.9410	0.0	1.0000	-0.9601	0.0	0.9684	-0.9107	0.5045
9	0.9101	-0.8518	0.4285	0.7443	-0.7056	0.2696	0.4922	-0.4662	-0.3151	-0.1134
10	0.5796	-0.8172	0.9369	0.0	-0.9601	1.0000	0.0	-0.9754	0.9785	-0.6228
11	0.0	-0.4495	0.9366	-0.8284	0.8105	-0.3496	-0.5827	0.5611	0.3782	0.1903
12	-0.5546	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0	0.0
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0000	0.0
15	0.0	0.7970	-0.8812	0.0	0.9684	-0.9754	0.0	1.0000	-0.9741	0.5817
16	0.9832	-0.9451	0.5199	0.8723	-0.8379	0.3507	0.6245	-0.5949	-0.3818	-0.1569
17	0.6011	0.0	-0.7145	0.8570	0.0	-0.9107	0.9785	0.0	-0.9741	1.0000
18	0.0	-0.9837	0.9678	-0.6152	-0.9172	0.9052	-0.4260	-0.6944	0.6720	0.4486
19	-0.5616	0.0	0.3587	-0.5036	0.0	0.5045	-0.6228	0.0	0.5817	-0.6770
20	0.0	-0.6244	-0.7036	0.5715	0.6526	-0.7088	0.7722	0.6046	-0.6312	-0.4306
21	-0.1689	0.0	0.7025	-0.8147	0.0	0.9101	-0.9495	0.0	0.9832	0.6244
22	0.0	1.0000	-0.9317	0.5815	0.9446	-0.9168	0.4180	0.7261	-0.6957	-0.4698
23	0.6054	0.0	-0.6347	0.7854	0.0	-0.8518	0.9366	0.0	-0.9451	0.9878
24	-0.9817	1.0000	-0.6641	-0.9643	0.9593	-0.4893	-0.7801	0.7586	0.5262	0.2763

	PHI	S F	LAMBDA	ESTIMATED PARTIALS USED			
	0.104714130 00	0.110025810-01	0.1000-02				
INCREMENTS	0.0	-0.284984530-01	-0.373724260 00	0.0	-0.683310530-01		
	-0.237506610 01	0.0	-0.153353210-01	0.124997200 01	0.226374260-03		
	0.165914050 01	0.120471700 01	0.424378910 02	0.491262250 04	0.107663450 06		
	0.373455080 05	-0.771003330 06	0.116251910 09	0.371274760 00	-0.273810020 00		
	0.294803080-01						
	PHI	LAMBDA	GAMMA	LENGTH			
	0.182364250 00	0.1000-02	0.8370 02	0.2380 01			
INCREMENTS	0.0	-0.302212270-01	0.200012360 00	0.0	-0.127653570 00		
	-0.622676130 01	0.0	-0.847439650-01	0.138934780 01	-0.303942110-03		
	0.429512870-01	0.240722940 01	0.163116340 03	0.103434500 05	0.381973050 06		
	-0.319465500 05	-0.396792540 07	0.113146130 09	0.518841230 00	-0.745822940 00		
	0.572844660-01						
	PHI	LAMBDA	GAMMA	LENGTH			
	0.502661860 01	0.1000-03	0.8690 02	0.5880 01			
INCREMENTS	0.0	-0.229026210-01	0.527303260 00	0.0	-0.755640730-02		
	-0.211799420 00	0.0	0.178214220-02	0.243220340 00	0.937420390-04		
	0.574662730 02	0.179891530 00	-0.425078140 01	0.163541640 04	0.217236470 04		
	0.303426550 05	-0.110905740 00	0.513825990 08	0.210155280 00	-0.332014080-01		
	0.339844230-02						
	PHI	LAMBDA	GAMMA	LENGTH			
	0.504662350-01	0.1000-01	0.6580 02	0.5410 00			
2) PARAMETERS	-0.131668240 01	0.937306130 00	-0.209993630 02	0.733256210 00	-0.884677680 00		
	-0.300378060 02	-0.161643360 00	0.148199160 01	0.109618830 03	-0.327954290-01		
	-0.625566680 00	-0.556516120 02	0.141104660 04	0.905122490 04	0.983698090 06		
	0.638033800 06	0.139767300 07	0.141866450 09	0.504133600 01	0.142438880 02		
	0.609095110-01						
	PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED	
	0.504660220-01	0.763820800-02	0.5410 00	0.6580 02	0.1000-01		
3) PARAMETERS	-0.131686080 01	0.936114190 00	-0.209668290 02	0.733695350 00	-0.885770490 00		
	-0.300356780 02	-0.101931400 00	0.148161740 01	0.109657680 03	-0.327500400-01		
	-0.625773090 00	-0.556244150 02	0.141271850 04	0.917747940 04	0.884465950 06		
	0.638834170 06	0.136288310 07	0.148285200 09	0.506274330 01	0.142389990 02		
	0.611463210-01						
	PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED	
	0.498352910-01	0.759032630-02	0.5180-01	0.6470 02	0.1000 00		
4) PARAMETERS	-0.131705660 01	0.936270580 00	-0.210043840 02	0.734083000 00	-0.886766200 00		
	-0.300884310 02	-0.102191640 00	0.148110740 01	0.109695490 03	-0.327025370-01		
	-0.625676580 00	-0.555973800 02	0.141431380 04	0.929529390 04	0.885119780 06		
	0.639387540 06	0.137484120 07	0.152599980 09	0.507028680 01	0.142345550 02		
	0.614710610-01						
	PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED	
	0.495398470-01	0.756779350-02	0.5380 00	0.6470 02	0.1000 00		
5) PARAMETERS	-0.131722640 01	0.936560790 00	-0.210571410 02	0.734458080 00	-0.887922140 00		
	-0.301238160						

61	PARAMETERS	-0.121735590 01	0.936839390 00	-0.211143430 02	0.734833870 00	-0.888934300 00
		-0.301618380 02	-0.102705000 00	0.147991150 01	0.109768280 03	-0.326022160 01
		-0.625626440 00	-0.555436940 02	0.141743560 04	0.950144080 04	0.886781360 06
		0.639858240 06	0.141694170 07	0.159556710 09	0.508302630 01	0.142260930 02
		0.621589500 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.491272720-01	0.753621480-02	0.3710 00	0.8470 02	0.1000 00	

71	PARAMETERS	-0.131756700 01	0.937088520 00	-0.211720610 02	0.735213970 00	-0.889993750 00
		-0.302015600 02	-0.102967270 00	0.147930990 01	0.109802370 03	-0.325497000 01
		-0.625617600 00	-0.555178170 02	0.141904520 04	0.959554150 04	0.887714360 06
		0.639938200 06	0.143864730 07	0.162615660 09	0.508926650 01	0.142219330 02
		0.625056880 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.484557160-01	0.752304480-02	0.3670 00	0.8490 02	0.1000 00	

81	PARAMETERS	-0.131773980 01	0.937309540 00	-0.212285100 02	0.735598760 00	-0.891080350 00
		-0.302423670 02	-0.103233780 00	0.147872360 01	0.109835080 03	-0.324959390 01
		-0.625607770 00	-0.554926210 02	0.142069420 04	0.968513870 04	0.888699490 06
		0.639955440 06	0.145925660 07	0.165491680 09	0.509531890 01	0.142177970 02
		0.628519350 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.487957870-01	0.751071580-02	0.3620 00	0.8500 02	0.1000 00	

91	PARAMETERS	-0.131791410 01	0.937506070 00	-0.212828420 02	0.735987690 00	-0.892158700 00
		-0.302838800 02	-0.103503950 00	0.147815660 01	0.109866510 03	-0.324411430 01
		-0.625543940 00	-0.554680680 02	0.142237810 04	0.977077080 04	0.889732550 06
		0.639924550 06	0.147850230 07	0.168213620 09	0.510114740 01	0.142136830 02
		0.631565280 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.486437300-01	0.749903500-02	0.3580 00	0.8500 02	0.1000 00	

101	PARAMETERS	-0.131808960 01	0.937681240 00	-0.213346820 02	0.736379950 00	-0.893226060 00
		-0.303258730 02	-0.103777140 00	0.147761070 01	0.109896790 03	-0.323854890 01
		-0.625574870 00	-0.554441190 02	0.142409090 04	0.985280720 04	0.890810860 06
		0.639855440 06	0.149633460 07	0.170798280 09	0.510674220 01	0.142095900 02
		0.635293530 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.484494900-01	0.748790860-02	0.3550 00	0.8510 02	0.1000 00	

111	PARAMETERS	-0.131826590 01	0.937837340 00	-0.213838980 02	0.736774790 00	-0.894281150 00
		-0.303682070 02	-0.104052750 00	0.147708620 01	0.109926000 03	-0.323291050 01
		-0.625549920 00	-0.554207380 02	0.142582710 04	0.993153120 04	0.891932210 06
		0.639755380 06	0.151278900 07	0.173256930 09	0.511210480 01	0.142055210 02
		0.638802430 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.483618690-01	0.747727880-02	0.3510 00	0.8520 02	0.1000 00	

121	PARAMETERS	-0.131844290 01	0.937976050 00	-0.214304850 02	0.737171540 00	-0.895323560 00
		-0.304107940 02	-0.104330260 00	0.147658280 01	0.109954200 03	-0.322721220 01
		-0.625518970 00	-0.553978930 02	0.142758200 04	0.100071770 05	0.893094510 06
		0.639629910 06	0.152793300 07	0.175598220 09	0.511172410 01	0.142014770 02
		0.642190780 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.482307350-01	0.746710200-02	0.3480 00	0.8520 02	0.1000 00	

131	PARAMETERS	-0.131862030 01	0.938098660 00	-0.214745020 02	0.737569640 00	-0.896353280 00
		-0.304535770 02	-0.104609260 00	0.147609980 01	0.109981470 03	-0.322146330 01
		-0.625482070 00	-0.553755580 02	0.142935150 04	0.100799490 05	0.894295710 06
		0.639483400 06	0.154184410 07	0.177829340 09	0.512216130 01	0.141974600 02
		0.645557610 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.481043190-01	0.745734060-02	0.3450 00	0.8530 02	0.1000 00	

141	PARAMETERS	-0.131875790 01	0.938206240 00	-0.215160410 02	0.737968600 00	-0.897370560 00
		-0.304965190 02	-0.104889360 00	0.147563640 01	0.110007840 03	-0.321567220 01
		-0.625439410 00	-0.553537070 02	0.143113210 04	0.101500280 05	0.895533780 06
		0.639319290 06	0.155460100 07	0.179956630 09	0.512687250 01	0.141934690 02
		0.648902090 01				

PHI	S F	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
0.479833820-01	0.744796070-02	0.3420 00	0.8530 02	0.1000 00	

FORCE OFF

N = 883	K = 21	P = 3	M = 2	
FF = 0.4000 01	T = 0.2000 01	F = 0.5000 04	TAU = 0.1000 02	

141	PARAMETERS	-0.131875790 01	0.938206240 00	-0.215160410 02	0.737968600 00	-0.897370560 00
		-0.304965190 02	-0.104889360 00	0.147563640 01	0.110007840 03	-0.321567220 01
		-0.625439410 00	-0.553537070 02	0.143113210 04	0.101500280 05	0.895533780 06
		0.639319290 06	0.155460100 07	0.179956630 09	0.512687250 01	0.141934690 02
		0.648902090 01				

DBS	PRED	RES			
0.100000000 01	0.598405110 00	0.159489120-02	0.399690300 03	0.735300000 02	
0.100000000 01	0.996519660 00	0.348053750-02	0.419690300 03	0.774200000 02	
0.100000000 01	0.599503930 00	0.496068250-03	0.439690000 03	0.809200000 02	
0.100000000 01	0.999817260 00	0.182736080-03	0.459690300 03	0.846200000 02	
0.146960000 02	0.146058940 02	0.613135020-02	0.459690300 03	0.552200000 01	
0.100000000 01	0.999601340 00	0.398659560-03	0.479690300 03	0.883600000 02	
0.146960000 02	0.146263450 02	0.473973240-02	0.479690000 03	0.579700000 01	
0.500000000 02	0.494349900 02	0.113001990-01	0.479690300 03	0.149500000 01	
0.100000000 01	0.998820800 00	0.117919650-02	0.499690300 03	0.921500000 02	
0.146960000 02	0.146458940 02	0.340951900-02	0.499690300 03	0.606700000 01	
0.500000000 02	0.495758930 02	0.848214090-02	0.499690300 03	0.160100000 01	
0.100000000 01	0.100014920 01	-0.149237770-03	0.519690300 03	0.957400000 02	
0.146960000 02	0.146555100 02	0.275515280-02	0.519690300 03	0.633700000 01	
0.500000000 02	0.496741750 02	0.651650670-02	0.519690300 03	0.170100000 01	
0.100000000 01	0.100035070 01	-0.350724820-03	0.539690300 03	0.994300000 02	
0.146960000 02	0.146644240 02	0.216100540-02	0.539690000 03	0.660400000 01	
0.500000000 02	0.497590520 02	0.481895250-02	0.539690300 03	0.179600000 01	
0.100000000 03	0.982414780 02	0.175852220-01	0.539690000 03	0.774200000 02	
0.100000000 01	0.100071030 01	-0.710308230-03	0.559690000 03	0.103100000 00	
0.146960000 02	0.146712470 02	0.168433540-02	0.559690300 03	0.686900000 01	
0.500000000 02	0.497916270 02	0.416745330-02	0.559690300 03	0.188900000 01	
0.100000000 03	0.987400030 02	0.125999670-01	0.559690300 03	0.836700000 00	
0.100000000 01	0.100074720 01	-0.747166230-03	0.579690300 03	0.106800000 03	
0.146960000 02	0.146755650 02	0.139051330-02	0.579690300 03	0.713300000 01	
0.500000000 02	0.498434930 02	0.313014730-02	0.579690300 03	0.197800000 01	
0.100000000 03	0.990638170 02	0.936183160-02	0.579690300 03	0.894100000 00	
0.100000000 01	0.100076740 01	-0.767366880-03	0.599690300 03	0.110500000 03	
0.146960000 02	0.146781370 02	0.121548720-02	0.599690300 03	0.739600000 01	
0.500000000 02	0.498602460 02	0.279508510-02	0.599690300 03	0.206600000 01	
0.100000000 03	0.992778190 02	0.722181480-02	0.599690300 03	0.948000000 00	
0.150000000 03	0.147676050 03	0.154930070-01	0.599690300 03	0.564100000 00	
0.100000000 01	0.100077460 01	-0.774586340-03	0.619690000 03	0.114200000 03	
0.146960000 02	0.146627340 02	0.226360800-02	0.619690000 03	0.766700000 01	
0.500000000 02	0.498770100 02	0.245980350-02	0.619690300 03	0.215200000 01	
0.100000000 03	0.994227120 02	0.577287570-02	0.619690300 03	0.999300000 00	
0.150000000 03	0.148305850 03	0.112943350-01	0.619690300 03	0.607100000 00	
0.200000000 03	0.195712700 03	0.214364950-01	0.619690300 03	0.400400000 00	
0.100000000 01	0.100162030 01	-0.162034960-02	0.639690000 03	0.117800000 03	
0.146960000 02	0.146806470 02	0.104473860-02	0.639690000 03	0.791900000 01	
0.500000000 02	0.498803630 02	0.239314610-02	0.639690300 03	0.223700000 01	
0.100000000 03	0.995715620 02	0.428437510-02	0.639690300 03	0.104800000 01	
0.150000000 03	0.148696180 03	0.869215630-02	0.639690000 03	0.646800000 00	
0.200000000 03	0.197031770 03	0.148411630-01	0.639690000 03	0.439000000 00	
0.250000000 03	0.243565430 03	0.257382810-01	0.639690000 03	0.303300000 00	
0.100000000 01	0.100076100 01	-0.760968900-03	0.659690000 03	0.121600000 03	
0.146960000 02	0.146814770 02	0.988197960-03	0.659690000 03	0.817900000 01	
0.500000000 02	0.498974960 02	0.205008760-02	0.659690300 03	0.232000000 01	
0.100000000 03	0.996157150 02	0.384285330-02	0.659690300 03	0.109600000 01	
0.150000000 03	0.148967750 03	0.688167700-02	0.659690300 03	0.688400000 00	
0.200000000 03	0.197827880 03	0.108606040-01	0.659690300 03	0.473100000 00	
0.250000000 03	0.245740090 03	0.170396510-01	0.659690300 03	0.347400000 00	
0.300000000 03	0.291728590 03	0.275713770-01	0.659690300 03	0.240200000 00	
0.100000000 01	0.100074420 01	-0.744170180-03	0.679690300 03	0.125300000 03	
0.146960000 02	0.146824310 02	0.923334030-03	0.679690300 03	0.843800000 01	
0.500000000 02	0.499118100 02	0.176379520-02	0.679690300 03	0.240200000 01	
0.100000000 03	0.996177750 03	0.382224630-02	0.679690300 03	0.114300000 01	
0.150000000 03	0.149151870 03	0.565416690-02	0.679690000 03	0.719400000 01	
0.200000000 03	0.198312850 03	0.843575420-02	0.679690000 03	0.504400000 00	
0.250000000 03	0.248251800 03	0.699280530-02	0.679690300 03	0.368500000 00	
0.300000000 03	0.294745230 03	0.175025060-01	0.679690300 03	0.277100000 00	
0.350000000 03	0.335268100 03	0.420911570-01	0.679690300 03	0.207800000 00	
0.100000000 01	0.100034090 01	-0.340902320-03	0.689690300 03	0.127200000 03	
0.146960000 02	0.146832300 02	0.868910300-03	0.689690000 03	0.856700000 01	
0.500000000 02	0.499117430 02	0.176514870-02	0.689690300 03	0.244300000 01	
0.100000000 03	0.996210390 02	0.378960930-02	0.689690300 03	0.116600000 01	
0.150000000 03	0.149213200 03	0.524535870-02	0.689690000 03	0.736600000 00	
0.200000000 03	0.198531470 03	0.734263320-02	0.689690300 03	0.519100000 00	
0.250000000 03	0.247260850 03	0.109566150-01	0.689690000 03	0.385800000 00	
0.300000000 03	0.295268840 03	0.157705440-01	0.689690000 03	0.292800000 00	
0.350000000 03	0.341201200 03	0.251394210-01	0.689690000 03	0.220800000 00	
0.400000000 03	0.381130310 03	0.471742270-01	0.689690300 03	0.150000000 00	
0.100000000 01	0.999948170 00	0.518317990-04	0.699690000 03	0.129100000 03	
0.146960000 02	0.146837090 02	0.836359820-03	0.699690000 03	0.869600000 01	
0.500000000 02	0.499076150 02	0.184769410-02	0.699690300 03	0.248400000 01	
0.100000000 03	0.996797520 02	0.320247610-02	0.699690000 03	0.118800000 01	
0.150000000 03	0.149278150 03	0.481235470-02	0.699690000 03	0.753400000 00	
0.200000000 03	0.198677090 03	0.661453500-02	0.699690300 03	0.533500000 00	
0.250000000 03	0.247710580 03	0.915766990-02	0.699690300 03	0.399000000 00	
0.300000000 03	0.296358010 03	0.121399710-01	0.699690300 03	0.305900000 00	
0.350000000 03	0.344345790 03	0.161548990-01	0.699690300 03	0.234500000 00	
0.400000000 03	0.391190570 03	0.220235740-01	0.699690300 03	0.170100000 00	
0.100000000 01	0.100032860 01	-0.328635580-03	0.709690000 03	0.130900000 03	
0.146960000 02	0.146839000 02	0.823345210-03	0.709690300 03	0.882500000 01	
0.500000000 02	0.499189030 02	0.162193580-02	0.709690300 03	0.252400000 01	
0.100000000 03	0.997182420 02	0.281757930-02	0.709690000 03	0.121000000 01	
0.150000000 03	0.149320050 03	0.453300640-02	0.709690300 03	0.770000000 00	
0.200000000 03	0.198744350 03	0.627824430-02	0.709690300 03	0.547700000 00	
0.250000000 03	0.247838240 03	0.824705240-02	0.709690000 03	0.412000000 00	
0.300000000 03	0.296795460 03	0.106817990-01	0.709690000 03	0.318900000 00	
0.350000000 03	0.345240620 03	0.135982300-01	0.709690000 03	0.248800000 00	
0.400000000 03	0.393124630 03	0.171884280-01	0.709690300 03	0.190100000 00	

0.5400000000 03	0.538771360 03	0.227525070-02	0.899690000 03	0.258460000 00
0.5500000000 03	0.558805710 03	0.213264920-02	0.899690000 03	0.239300000 00
0.5600000000 03	0.578781740 03	0.210045430-02	0.899690000 03	0.229000000 00
0.5700000000 03	0.598738060 03	0.210323660-02	0.899690000 03	0.219400000 00
0.5800000000 03	0.618749250 03	0.201734420-02	0.899690000 03	0.210400000 00
0.5900000000 03	0.638750390 03	0.167036580-02	0.899690000 03	0.201900000 00
0.6000000000 03	0.658752300 03	0.163180880-02	0.899690000 03	0.194400000 00
0.6100000000 03	0.678754210 03	0.129707130-02	0.899690000 03	0.186500000 00
0.6200000000 03	0.698756120 03	0.122414840-02	0.899690000 03	0.179500000 00
0.6300000000 03	0.718758030 03	0.679925540-03	0.899690000 03	0.163600000 00
0.6400000000 03	0.738759940 03	0.281796160-03	0.899690000 03	0.149800000 00
0.6500000000 03	0.758761850 03	0.266350090-03	0.899690000 03	0.137800000 00
0.6600000000 03	0.778763760 03	-0.699302550-04	0.899690000 03	0.127200000 00
0.6700000000 03	0.798765670 03	0.421146800-03	0.899690000 03	0.118000000 00
0.6800000000 03	0.818767580 03	0.102667180-02	0.899690000 03	0.109900000 00
0.6900000000 03	0.838769490 03	0.247069700-02	0.899690000 03	0.964700000-01
0.7000000000 03	0.858771400 03	0.352916590-02	0.899690000 03	0.859800000-01
0.7100000000 03	0.878773310 03	0.163602190-02	0.899690000 03	0.712000000-01
0.7200000000 03	0.898775220 03	-0.227153130-02	0.899690000 03	0.620700000-01
0.7300000000 03	0.918777130 03	0.160754660-02	0.899690000 03	0.565300000-01
0.7400000000 03	0.938779040 03	-0.380732140-02	0.899690000 03	0.523800000-01
0.7500000000 03	0.958780950 03	0.166647020-02	0.899690000 03	0.465200000-01
0.7600000000 03	0.978782860 03	0.742920680-02	0.899690000 03	0.431600000-01
0.7700000000 03	0.998784770 03	0.124600440-01	0.899690000 03	0.409300000-01
0.7800000000 03	1.018786680 03	0.227843480-03	0.939690000 03	0.173500000 00
0.7900000000 03	1.038788590 03	0.259601440-03	0.939690000 03	0.117600000 02
0.8000000000 03	1.058790500 03	0.737537820-03	0.939690000 03	0.362300000 01
0.8100000000 03	1.078792410 03	0.101507900-02	0.939690000 03	0.168700000 01
0.8200000000 03	1.098794320 03	0.105484950-02	0.939690000 03	0.110800000 01
0.8300000000 03	1.118796230 03	0.170922720-02	0.939690000 03	0.819000000 00
0.8400000000 03	1.138798140 03	0.196067830-02	0.939690000 03	0.645300000 00
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16	0.14619305	0.0	0.34109141	0.0	0.46933953	0.0	0.37466261	0.0
17	0.34109141	0.0	0.56787374	0.0	0.32346304	0.0	0.25197299	0.0
18	0.48536711	0.0	0.32346304	0.0	0.33650252	0.0	0.88817167	0.0
19	0.37466261	0.0	0.25197299	0.0	0.88817167	0.0	0.18902533	0.0
20	0.19803961	0.0	0.73797534	0.0	0.10058611	0.0	0.70078653	0.0
21	0.20179265	0.0	0.10637310	0.0	0.32765749	0.0	0.13463516	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	-0.47359159	0.0	-0.19771181	0.0	0.0	0.0	0.0	0.0
3	-0.19771181	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.11281903	0.0	-0.34877368	0.0	0.0	0.0	0.0	0.0
6	-0.34877368	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	-0.36597648	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	0.10840525	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	0.33982324	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	0.15990865	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	-0.53832723	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	0.60134830	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.39600170	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	0.14239383	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	0.20779265	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	0.10637310	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	0.32765749	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	0.13463516	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	0.15466536	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	0.31160340	0.0	0.0	0.0	0.0	0.0	0.0	0.0

PARAMETER CORRELATION MATRIX

1	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0000	-0.5066	0.0	-0.8488	-0.8887	0.0	0.6724	0.8489
3	0.0	-0.5066	1.0000	0.0	0.1185	0.6920	0.0	0.0909	-0.8254
4	0.0	0.0	0.0	1.0000	0.0	0.0	0.0	0.0	0.0
5	0.0	-0.8488	0.1185	0.0	1.0000	0.6813	0.0	-0.9552	-0.9939
6	0.0	-0.8887	0.6920	0.0	0.6813	1.0000	0.0	-0.4906	-0.9840
7	0.0	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0
8	0.0	0.6724	0.8489	0.0	-0.9552	-0.4906	0.0	1.0000	0.3952
9	0.0	0.8489	-0.8054	0.0	-0.9939	-0.9840	0.0	0.3952	1.0000
10	0.0	0.0469	-0.1071	0.0	0.0420	-0.1004	0.0	-0.1113	0.0999
11	0.0	-0.5882	-0.1311	0.0	0.9057	0.4151	0.0	-0.9872	-0.7285
12	0.0	-0.8411	0.8150	0.0	0.6895	0.9774	0.0	-0.3976	-0.9987
13	0.0	0.0443	-0.1455	0.0	0.0305	-0.1221	0.0	-0.0940	0.1299
14	0.0	0.4283	-0.0881	0.0	-0.5496	-0.3862	0.0	0.4130	0.3526
15	0.0	0.6719	-0.6840	0.0	-0.4784	-0.8158	0.0	0.3182	0.8359
16	0.0	0.0446	-0.1291	0.0	0.0746	-0.1142	0.0	-0.1009	0.1185

17	0.0	0.0001	-0.1575	0.0	-0.0003	-0.1848	0.0	-0.0869	0.1764	0.2995
18	0.0	0.0010	-0.0657	0.0	-0.0006	-0.0739	0.0	0.0002	0.7030	0.5198
19	0.0	0.0011	-0.0649	0.0	-0.0006	-0.0800	0.0	0.1256	0.9445	0.1148
20	0.0	0.0062	-0.1015	0.0	0.0026	-0.1042	0.0	-0.0867	0.1042	0.9728
21	0.0	-0.0122	-0.0452	0.0	0.0023	-0.1755	0.0	-0.1537	0.2479	0.0053
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	-0.0392	-0.0411	0.1443	0.4283	0.0719	0.0446	0.0281	0.4919	0.7233	0.0462
4	-0.0111	-0.0150	-0.0455	-0.0081	-0.0040	-0.1291	-0.1303	-0.0650	-0.9449	-0.1015
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	0.0057	0.0040	0.0305	-0.0040	-0.0476	0.0366	-0.0001	-0.2076	-0.3566	0.0765
7	0.0011	0.0077	-0.1221	-0.1867	-0.0158	-0.1142	-0.1848	-0.0673	-0.8800	-0.1042
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	-0.0072	-0.1676	-0.0960	0.0133	0.1162	-0.1009	-0.0869	0.0002	0.1256	-0.0862
10	-0.1245	-0.0467	0.1795	0.1526	0.0559	0.1165	0.1766	0.7030	0.9445	0.1042
11	0.1866	-0.0026	0.0446	0.0784	0.0638	0.9750	0.2995	0.5399	0.1148	0.9728
12	0.0000	0.0035	0.1551	-0.0000	-0.0011	0.1691	0.1580	0.0991	-0.0628	0.1531
13	0.1375	0.0030	-0.1076	-0.1698	-0.0002	-0.0942	-0.1810	-0.0880	-0.9441	-0.0798
14	0.1597	-0.1036	0.0000	0.0511	0.0795	0.9959	0.3221	0.5707	0.1482	0.9971
15	-0.0000	-0.1698	0.0511	0.0000	0.0000	0.0318	-0.0276	0.2996	0.2716	0.6379
16	-0.0011	-0.0027	0.0255	0.0043	0.0000	0.0118	0.2467	0.7949	0.7949	0.5990
17	0.1540	-0.1610	0.0959	0.0118	0.0118	1.0000	0.3317	0.5712	0.1362	0.9977
18	0.0000	-0.1610	0.0221	-0.0276	0.2996	0.1317	1.0000	0.7189	0.1634	0.3176
19	-0.0000	-0.1610	0.0221	0.2996	0.7949	0.5712	0.7189	1.0000	0.7268	0.5463
20	0.1518	-0.0000	0.1442	0.2016	0.7949	0.1362	0.1634	0.7268	1.0000	0.1110
21	0.1509	-0.0000	0.0911	0.0378	0.5997	0.9977	0.3176	0.5463	0.1110	1.0000
1	0.0	-0.0000	0.1591	0.1007	0.2977	0.3663	0.0800	0.3107	0.3726	0.0284
2	-0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	-0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	-0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	-0.1755	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	-0.1537	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	0.2479	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	0.0053	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	0.1042	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	-0.0053	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	0.1531	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.1362	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	0.0977	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	0.0463	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	0.3107	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	0.3726	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	0.0284	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

	UPPER	LOWER	UPPER	LOWER	UPPER	LOWER
1	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
2	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
3	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
4	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
5	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
6	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
7	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
8	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
9	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
10	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
11	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
12	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
13	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
14	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
15	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
16	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
17	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
18	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
19	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
20	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01
21	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01	0.1311391000-01	-0.1311391000-01

NONLINEAR LIMITS

PHI CRITICAL = 0.519773750-01

PARAM	LOWER	UPPER	UPPER PHI
1 PARAMETER NOT USED			
2 0.924800730-00	0.924800730-00	0.924800730-00	0.519773750-01
3 -0.221702650-02	-0.221702650-02	-0.221702650-02	0.519770660-01
4 PARAMETER NOT USED			
5 -0.908480660-00	0.908480660-00	0.908480660-00	0.519769360-01
6 -0.308689300-02	0.308689300-02	0.308689300-02	0.519768480-01
7 PARAMETER NOT USED			
8 0.146873890-01	0.146873890-01	0.146873890-01	0.519771320-01
9 0.109805410-03	0.109805410-03	0.109805410-03	0.519769070-01
10 -0.331014100-01	0.331014100-01	0.331014100-01	0.519773580-01
11 -0.629231240-00	0.629231240-00	0.629231240-00	0.519770340-01
12 -0.554577770-02	0.554577770-02	0.554577770-02	0.519768270-01
13 0.140249090-04	0.140249090-04	0.140249090-04	0.519770300-01

14	0.576970470 04	C.570390209-01	0.105517440 05	0.519772480-01
15	0.585668760 06	0.487023330-01	0.905433370 06	0.519767630-01
16	0.615430010 06	0.575174750-01	0.664681930 06	0.519772270-01
17	0.100471160 07	0.544797480-01	0.221575630 07	0.519771870-01
18	0.161764730 09	0.493769300-01	0.194305270 09	0.519769110-01
19	0.506199370 01	0.493544850-01	0.521514320 01	0.522630830-01
20	0.141814300 02	C.478581190-01	0.142125590 02	0.523396620-01
21	0.635420280-01	0.515482090-01	0.660973080-01	0.519574650-01

Appendix E

OUTPUT FROM STATEQ — CASE 2

BLANK PAGE

	PMI 0.472477643-U1	SE 0.149334420-U1	LAMBDA 0.1000-U1	ESTIMATED PARAMETERS USED	
1) PARAMETERS	0.0 0.0 0.0 0.49764443 U1 0.13033153-U3	0.0 0.0 0.0 0.0	0.0 0.0 0.0 0.0	0.0 0.0 0.0 0.0 0.0	0.0 -0.472477643-U1 0.0 -0.049764443-U3
	PMI 0.477424533-U2	LAMBDA 0.1000-U1	GAMMA 0.3340 U2	LENGTH 0.1120-U1	
2) PARAMETERS	0.0 0.0 0.0 0.49715443 U4 0.13061200-U2	0.0 0.0 0.0 0.0	0.0 0.0 0.0 0.0	0.0 0.0 0.0 0.0 0.0	0.0 -0.304976133-U4 0.0 -0.776314433-U2
	PMI 0.474028803-U2	LAMBDA 0.1000-U2	GAMMA 0.3450 U2	LENGTH 0.1070 U3	
3) PARAMETERS	-0.133150553 U1 -0.335346003 U2 -0.061774003 U3 -0.068703308 U6 0.064325940-U1	-0.434776000 U0 -0.124274420 U0 -0.543971000 U2 0.156416000 U7	-0.217413000 U2 0.146257003 U1 0.161606005 U4 0.230770000 U9	0.766146000 U0 0.110671000 U3 0.125446000 U5 0.523773000 U1	-0.921627000 U0 -0.263167000-U4 0.100424000 U7 0.134940000 U2
	PMI 0.472322473-U2	SE 0.140285860-U1	LENGTH 0.1070 U0	GAMMA 0.3450 U2	LAMBDA 0.1000-U1
4) PARAMETERS	-0.133154440 U1 -0.335346003 U2 -0.061774000 U3 0.068753113 U6 0.085612700-U1	0.134776000 U0 -0.124207280 U0 -0.543971000 U2 0.156416000 U7	-0.217413000 U2 0.146257000 U1 0.161604390 U4 0.230770000 U9	0.766221500 U0 0.110871000 U3 0.125446000 U5 0.523773000 U1	-0.951627000 U0 -0.263167000-U4 0.100424000 U7 0.134940000 U2
	PMI 0.472223010-U2	SE 0.140221020-U1	LENGTH 0.1070 U0	GAMMA 0.3450 U2	LAMBDA 0.1000-U1
5) PARAMETERS	-0.133159140 U1 -0.335346000 U2 -0.061774000 U3 0.068802966 U6 0.086806800-U1	0.134776000 U0 -0.124332750 U0 -0.543971000 U2 0.156416000 U7	-0.217413000 U2 0.146257000 U1 0.161614490 U4 0.230770000 U9	0.766224750 U0 0.110871000 U3 0.125446000 U5 0.523773000 U1	-0.951627000 U0 -0.263167000-U4 0.100424000 U7 0.134940000 U2

	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47212762D-02	0.14025685D-01	0.106D 00	0.79D 02	0.100D-01	
(5) PARAMETERS	-0.13316329D 01 -0.33539400D 02 -0.61779400D 00 0.68852865D 06 0.88814798D-01	0.93477600D 00 -0.12455635D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16233485D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16233485D 04 0.23077000D 09	0.76636508D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47293672D-02	0.14024335D-01	0.106D 00	0.72D 02	0.100D-01	
(6) PARAMETERS	-0.13316735D 01 -0.33539400D 02 -0.61779400D 00 0.68902806D 06 0.88939637D-01	0.93477600D 00 -0.12437810D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16234900D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16234900D 04 0.23077000D 09	0.76643637D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47195021D-02	0.14023050D-01	0.105D 00	0.442D 02	0.100D-01	
(7) PARAMETERS	-0.13317135D 01 -0.33539400D 02 -0.61779400D 00 0.68752788D 06 0.89063211D-01	0.93477600D 00 -0.12439803D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16276244D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16276244D 04 0.23077000D 09	0.76630082D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47186803D-02	0.14021829D-01	0.105D 00	0.67D 02	0.100D-01	
(8) PARAMETERS	-0.13317521D 01 -0.33539400D 02 -0.61779400D 00 0.69002807D 06 0.89185534D-01	0.93477600D 00 -0.12441613D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16297518D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16297518D 04 0.23077000D 09	0.76656507D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47179010D-02	0.14020671D-01	0.104D 00	0.78D 02	0.100D-01	
(9) PARAMETERS	-0.13317901D 01 -0.33539400D 02 -0.61779400D 00 0.69052863D 06 0.89306620D-01	0.93477600D 00 -0.12443244D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16318723D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16318723D 04 0.23077000D 09	0.76662714D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47171635D-02	0.14019575D-01	0.104D 00	0.822D 02	0.100D-01	
(10) PARAMETERS	-0.13318271D 01 -0.33539400D 02 -0.61779400D 00 0.69102956D 06 0.89426483D-01	0.93477600D 00 -0.12444696D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16339861D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16339861D 04 0.23077000D 09	0.76668704D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47164670D-02	0.14018540D-01	0.103D 00	0.841D 02	0.100D-01	
(11) PARAMETERS	-0.13318635D 01 -0.33539400D 02 -0.61779400D 00 0.69153084D 06 0.89445137D-01	0.93477600D 00 -0.12445970D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16360932D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16360932D 04 0.23077000D 09	0.76674479D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47159110D-02	0.14017565D-01	0.103D 00	0.852D 02	0.100D-01	
(12) PARAMETERS	-0.13318987D 01 -0.33539400D 02 -0.61779400D 00 0.69203296D 06 0.89662594D-01	0.93477600D 00 -0.12447069D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16381937D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16381937D 04 0.23077000D 09	0.76680041D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47151947D-02	0.14016649D-01	0.102D 00	0.860D 02	0.100D-01	
(13) PARAMETERS	-0.13319332D 01 -0.33539400D 02 -0.61779400D 00 0.69253441D 06 0.89778867D-01	0.93477600D 00 -0.12447994D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16398610D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16398610D 04 0.23077000D 09	0.76685392D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47146175D-02	0.14015791D-01	0.102D 00	0.865D 02	0.100D-01	
(14) PARAMETERS	-0.13322793D 01 -0.33539400D 02 -0.61779400D 00 0.69701450D 06 0.90954216D-01	0.93477600D 00 -0.12469079D 00 -0.54397100D 02 0.15641600D 07	0.14625700D 01 0.16392035D 04 0.23077000D 09	0.21741300D 02 0.14625700D 01 0.16392035D 04 0.23077000D 09	0.76744688D 00 0.11087100D 03 0.12549800D 05 0.52377300D 01	-0.95185900D 00 -0.28349900D-01 0.10095900D 07 0.13931523D 02
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.47136759D-02	0.14014094D-01	0.101D 00	0.869D 02	0.100D-02	

(15) PARAMETERS	-0.133263420 01 -0.335394000 02 -0.617794000 00 0.701605420 06 0.920084480-01	0.934776000 00 -0.124898240 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169616400 04 0.230770000 09	0.768554220 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.470407710-02	S E 0.140001150-01	LENGTH 0.7260 00	GAMMA 0.8890 02	LAMBDA 0.1000-02	ESTIMATED PARTIALS USED
(16) PARAMETERS	-0.133296730 01 -0.335394000 02 -0.617794000 00 0.705950720 06 0.929804740-01	0.934776000 00 -0.125076460 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169658950 04 0.230770000 09	0.768619660 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469892780-02	S E 0.139924500-01	LENGTH 0.6990 00	GAMMA 0.8810 02	LAMBDA 0.1000-02	ESTIMATED PARTIALS USED
(17) PARAMETERS	-0.133296240 01 -0.335394000 02 -0.617794000 00 0.706188570 06 0.929820190-01	0.934776000 00 -0.125067510 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169653000 04 0.230770000 09	0.768607660 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469843910-02	S E 0.139917220-01	LENGTH 0.8110-03	GAMMA 0.3610 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(18) PARAMETERS	-0.133295670 01 -0.335394000 02 -0.617794000 00 0.706390900 06 0.929806060-01	0.934776000 00 -0.125057780 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169646290 04 0.230770000 09	0.768594290 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469796660-02	S E 0.139910180-01	LENGTH 0.3410-02	GAMMA 0.5610 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(19) PARAMETERS	-0.133295100 01 -0.335394000 02 -0.617794000 00 0.706571290 06 0.929862720-01	0.934776000 00 -0.125048000 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169639550 04 0.230770000 09	0.768560090 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469774390-02	S E 0.139903230-01	LENGTH 0.3230-02	GAMMA 0.5900 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(20) PARAMETERS	-0.133294540 01 -0.335394000 02 -0.617794000 00 0.706736400 06 0.929885110-01	0.934776000 00 -0.125038490 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169633100 04 0.230770000 09	0.768567430 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469705710-02	S E 0.139896640-01	LENGTH 0.3080-02	GAMMA 0.6020 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(21) PARAMETERS	-0.133294000 01 -0.335394000 02 -0.617794000 00 0.706869610 06 0.929907110-01	0.934776000 00 -0.125029360 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169627040 04 0.230770000 09	0.768554730 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469664490-02	S E 0.139890570-01	LENGTH 0.2940-02	GAMMA 0.6090 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(22) PARAMETERS	-0.133293490 01 -0.335394000 02 -0.617794000 00 0.707032780 06 0.929928460-01	0.934776000 00 -0.125020670 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169621430 04 0.230770000 09	0.768542660 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469627900-02	S E 0.139885060-01	LENGTH 0.2810-02	GAMMA 0.6120 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(23) PARAMETERS	-0.133293010 01 -0.335394000 02 -0.617794000 00 0.707167070 06 0.929949060-01	0.934776000 00 -0.125012420 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169616270 04 0.230770000 09	0.768531240 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469594490-02	S E 0.139880080-01	LENGTH 0.2690-02	GAMMA 0.6150 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(24) PARAMETERS	-0.133292560 01 -0.335394000 02 -0.617794000 00 0.707293260 06 0.929968890-01	0.934776000 00 -0.125004600 00 -0.543971000 02 0.156416000 07	-0.217413000 02 0.146257000 01 0.169611550 04 0.230770000 09	0.768520450 00 0.110871000 03 0.125498000 05 0.523773000 01	-0.951859000 00 -0.285624000-01 0.100959000 07 0.139057100 02	
	PHI 0.469564450-02	S E 0.139875610-01	LENGTH 0.2590-02	GAMMA 0.6170 02	LAMBDA 0.1000 01	ESTIMATED PARTIALS USED
(25) PARAMETERS	-0.133292130 01 -0.335394000 02	0.934776000 00 -0.124997170 00	-0.217413000 02 0.146257000 01	0.768510260 00 0.110871000 03	-0.951859000 00 -0.285624000-01	

	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469537460-02	0.139871590-01	0.2490-02	0.6190 02	0.1000 01	
(26) PARAMETERS	-0.133291730 01 -0.33534000 02 -0.617794000 00 0.707523680 06 0.930006370-01	0.934776000 00 -0.124990140 00 -0.543971000 02 0.156416000 07	0.169607240 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469513210-02	0.1398697980-01	0.2490-02	0.6210 02	0.1000 01	
(27) PARAMETERS	-0.133291350 01 -0.33534000 02 -0.617794000 00 0.707523680 06 0.930006370-01	0.934776000 00 -0.124990140 00 -0.543971000 02 0.156416000 07	0.169607240 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469491410-02	0.139864730-01	0.2310-02	0.6230 02	0.1000 01	
(28) PARAMETERS	-0.133291000 01 -0.33534000 02 -0.617794000 00 0.707727990 06 0.930041140-01	0.934776000 00 -0.124977110 00 -0.543971000 02 0.156416000 07	0.169596370 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469471790-02	0.139861800-01	0.2240-02	0.6230 02	0.1000 01	
(29) PARAMETERS	-0.133290600 01 -0.33534000 02 -0.617794000 00 0.707821350 06 0.930057610-01	0.934776000 00 -0.124977110 00 -0.543971000 02 0.156416000 07	0.169596370 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469449110-02	0.139859170-01	0.2170-02	0.6230 02	0.1000 01	
(30) PARAMETERS	-0.133290350 01 -0.33534000 02 -0.617794000 00 0.707909360 06 0.930073520-01	0.934776000 00 -0.124965400 00 -0.543971000 02 0.156416000 07	0.169596370 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469438150-02	0.139856790-01	0.2100-02	0.6230 02	0.1000 01	
(31) PARAMETERS	-0.133290050 01 -0.33534000 02 -0.617794000 00 0.707992320 06 0.930088900-01	0.934776000 00 -0.124959960 00 -0.543971000 02 0.156416000 07	0.169588850 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469423740-02	0.139854650-01	0.2040-02	0.6300 02	0.1000 01	
(32) PARAMETERS	-0.133289770 01 -0.33534000 02 -0.617794000 00 0.708070550 06 0.930103780-01	0.934776000 00 -0.124954790 00 -0.543971000 02 0.156416000 07	0.169588850 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469410700-02	0.139852710-01	0.1990-02	0.6320 02	0.1000 01	
(33) PARAMETERS	-0.133289510 01 -0.33534000 02 -0.617794000 00 0.708144350 06 0.930118200-01	0.934776000 00 -0.124949870 00 -0.543971000 02 0.156416000 07	0.169588850 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469398880-02	0.139850940-01	0.1940-02	0.6330 02	0.1000 01	
(34) PARAMETERS	-0.133289260 01 -0.33534000 02 -0.617794000 00 0.708211980 06 0.930132190-01	0.934776000 00 -0.124945180 00 -0.543971000 02 0.156416000 07	0.169588850 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	
	0.469388150-02	0.139849350-01	0.1900-02	0.6350 02	0.1000 01	
(35) PARAMETERS	-0.133289030 01 -0.33534000 02 -0.617794000 00 0.708279710 06	0.934776000 00 -0.124940700 00 -0.543971000 02 0.156416000 07	0.169588850 04 0.230770000 09	0.125498000 05 0.523773000 01	0.100959000 07 0.139059000 02	

	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469378400-02	0.139847890-01	0.1850-02	0.6300 02	0.1000 01	
(36) PARAMETERS	-0.133288810 01	0.934776000 00	-0.217413000 02	0.768429320 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708341770 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930158950-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469369520-02	0.139846570-01	0.1820-02	0.6300 02	0.1000 01	
(37) PARAMETERS	-0.133288800 01	0.934776000 00	-0.217413000 02	0.768424120 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708400390 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930171780-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469361410-02	0.139845360-01	0.1780-02	0.6300 02	0.1000 01	
(38) PARAMETERS	-0.133288800 01	0.934776000 00	-0.217413000 02	0.768419180 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708557790 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930184270-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469354000-02	0.139844260-01	0.1750-02	0.6300 02	0.1000 01	
(39) PARAMETERS	-0.133288820 01	0.934776000 00	-0.217413000 02	0.768414500 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708508150 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930196990-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469347210-02	0.139843250-01	0.1720-02	0.6300 02	0.1000 01	
(40) PARAMETERS	-0.133288800 01	0.934776000 00	-0.217413000 02	0.768410000 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708557670 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930208310-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469340970-02	0.139842320-01	0.1700-02	0.6300 02	0.1000 01	
(41) PARAMETERS	-0.133287880 01	0.934776000 00	-0.217413000 02	0.768405830 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708634530 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930219900-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469335240-02	0.139841460-01	0.1680-02	0.6300 02	0.1000 01	
(42) PARAMETERS	-0.133287720 01	0.934776000 00	-0.217413000 02	0.768401810 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708648870 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930231210-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469329960-02	0.139840680-01	0.1650-02	0.6300 02	0.1000 01	
(43) PARAMETERS	-0.133287570 01	0.934776000 00	-0.217413000 02	0.768397990 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708690880 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930242320-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469325080-02	0.139839950-01	0.1640-02	0.6300 02	0.1000 01	
(44) PARAMETERS	-0.133287430 01	0.934776000 00	-0.217413000 02	0.768394330 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708730670 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930253170-01					
	PHI	S E	LENGTH	GAMMA	LAMBDA	ESTIMATED PARTIALS USED
	0.469320560-02	0.139839280-01	0.1620-02	0.6300 02	0.1000 01	
(45) PARAMETERS	-0.133287300 01	0.934776000 00	-0.217413000 02	0.768390880 00	-0.951829000 00	
	-0.335394000 02	-0.124936430 00	0.146257000 01	0.110871000 03	-0.285750760-01	
	-0.617794000 00	-0.543971000 02	0.169578500 04	0.125498000 05	0.100959000 07	
	0.708768400 06	0.156416000 07	0.230770000 09	0.523773000 01	0.139059670 02	
	0.930263800-01					

	PHI 0.46931636J-02	S E 0.13983865U-01	LENGTH 0.160D-02	GAMMA 0.643D 02	LAMBDA 0.100D 01	ESTIMATED PARTIALS USED
(46) PARAMETERS	-0.13328718D 01	0.93477600C 00	-0.21741300D 02	0.76838758D 00	-0.95182900U 00	
	-0.33539400D 02	-0.12490257D 00	0.14622700U 01	0.11087100U 03	-0.28283422J-01	
	-0.61779400D 00	-0.54397100D 02	0.18957941D 04	0.12549800U 05	0.10049000U 07	
	0.70880419D 06	0.15641600D 07	0.23077000D 09	0.52377300D 01	0.13908000U 02	
	0.93027423D-01					

	PHI 0.46931246J-02	S E 0.13983807D-01	LENGTH 0.159D-02	GAMMA 0.642D 02	LAMBDA 0.100D 01	ESTIMATED PARTIALS USED
EPSILON TEST						
N = 29	K = 21	P = 16	F = 2	FAU = 0.100D-02		
FF = 0.400D 01	r = 0.200D 01					

(46) PARAMETERS	-0.13328718D 01	0.93477600C 00	-0.21741300D 02	0.76838758D 00	-0.95182900U 00
	-0.33539400D 02	-0.12490257D 00	0.14622700U 01	0.11087100U 03	-0.28283422J-01
	-0.61779400D 00	-0.54397100D 02	0.18957941D 04	0.12549800U 05	0.10049000U 07
	0.70880419D 06	0.15641600D 07	0.23077000D 09	0.52377300D 01	0.13908000U 02
	0.93027423D-01				

DBS	PRE	RES
0.10000000D 01	0.49970831D 00	0.29168874D-03
0.146960C0 02	0.14588085D 02	0.53854794D-03
0.50000000D 02	0.49924073D 02	0.14185413D-02
0.10000000D 03	0.49807026D 02	0.19297426D-02
0.15000000D 03	0.14953330D 03	0.31113412D-02
0.20000000D 03	0.19915563D 03	0.42218377D-02
0.25000000D 03	0.24865675D 03	0.53729950D-02
0.30000000D 03	0.29804946D 03	0.65017943D-02
0.35000000D 03	0.34707820D 03	0.83480108D-02
0.40000000D 03	0.39611834D 03	0.97041584D-02
0.44000000D 03	0.43583566D 03	0.94643982D-02
0.46000000D 03	0.45542672D 03	0.99419115D-02
0.48000000D 03	0.47490211D 03	0.10620547D-01
0.52000000D 03	0.51635801D 03	0.70038188D-02
0.52910000D 03	0.52910039D 03	-0.73371335D-06
0.55000000D 03	0.55250787D 03	0.98425335D-02
0.59044000D 03	0.58705607D 03	0.23438968D-02
0.60502000D 03	0.61152490D 03	-0.10754813D-01
0.63880000D 03	0.64409940D 03	-0.82958855D-02
0.68660000D 03	0.68471309D 03	0.27481916D-02
0.77944000D 03	0.78863804D 03	0.13858612D-01
0.82772000D 03	0.83404587D 03	-0.31805274D-01
0.92020000D 03	0.88688260D 03	0.23377245D-01
0.11900000D 04	0.11906470D 04	-0.54367036D-03
0.12929000D 04	0.13155399D 04	-0.17510924D-01
0.15650000D 04	0.15717583D 04	-0.43184257D-02
0.17450000D 04	0.16852745D 04	0.34223769D-01
0.18886000D 04	0.18586046D 04	0.10693323D-01
0.23740000D 04	0.24225598D 04	-0.20454626D-01

	PHI 0.46931246J-02	S E 0.13983807D-01	LAMBDA 0.100D 01	ESTIMATED PARTIALS USED
PTP INVERSE				
1 0.0	0.0	0.0	0.0	0.0
2 0.0	0.10000000D 01	0.0	0.0	0.0
3 0.0	0.0	0.10000000D 01	0.0	0.0
4 0.0	0.0	0.0	0.10000000D 01	0.0
5 0.0	0.0	0.0	0.0	0.10000000D 01
6 0.0	0.0	0.0	0.0	0.0
7 0.0	0.0	0.0	0.0	0.0
8 0.0	0.0	0.0	0.0	0.0
9 0.0	0.0	0.0	0.0	0.0
10 0.0	0.0	0.0	0.0	0.0
11 0.0	0.0	0.0	0.0	0.0
12 0.0	0.0	0.0	0.0	0.0
13 0.0	0.0	0.0	0.0	0.0
14 0.0	0.0	0.0	0.0	0.0
15 0.0	0.0	0.0	0.0	0.0
16 0.0	0.0	0.0	0.0	0.0
17 0.0	0.0	0.0	0.0	0.0
18 0.0	0.0	0.0	0.0	0.0
19 0.0	0.0	0.0	0.0	0.0
20 0.0	0.0	0.0	0.0	0.0
21 0.0	0.0	0.0	0.0	0.0
1 0.0	0.0	0.0	0.0	0.0
2 0.0	0.0	0.0	0.0	0.0
3 0.0	0.0	0.0	0.0	0.0
4 0.0	0.0	0.0	0.0	0.0
5 0.0	0.0	0.0	0.0	0.0
6 0.10000000D 01	0.0	0.0	0.0	0.0
7 0.0	0.10000000D 01	0.0	0.0	0.0
8 0.0	0.0	0.10000000D 01	0.0	0.0
9 0.0	0.0	0.0	0.10000000D 01	0.0
10 0.0	0.0	0.0	0.0	0.42193657D-01
11 0.0	0.0	0.0	0.0	0.0
12 0.0	0.0	0.0	0.0	0.0

[illegible]

19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	0.0	0.0	0.9024	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	0.0	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	0.0	0.0	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.0	0.0	0.0	1.0000	0.0	0.0	0.0	0.0	0.0	0.0
15	0.0	0.0	0.0	0.0	1.0000	0.0	0.0	0.0	0.0	0.0
16	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0	0.0	0.0
17	0.0	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0	0.0
18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0000	0.0	0.0
19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0000	0.0
20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0000
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	0.1083	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	0.4853	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	0.4045	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	0.2132	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

S	STD	ONE - PARAMETER		SUPPORT PLANE	
	ERRR	LOWER	UPPER	LOWER	UPPER
1	0.13983807-01	-0.136083940 01	-0.130490410 01	-0.139540920 01	-0.127033440 01
2	0.13983807-01	0.405808390 00	0.902743610 00	0.872238510 00	0.997313440 00
3	0.13983807-01	-0.217042660 02	-0.217133320 02	-0.218030370 02	-0.216707690 02
4	0.13983807-01	0.740419960 00	0.796355140 00	0.705850090 00	0.830445060 00
5	0.13983807-01	-0.979825610 00	-0.923891390 00	-0.101439650 01	-0.889321510 00
6	0.13983807-01	-0.335671680 02	-0.335114320 02	-0.336014370 02	-0.336768630 02
7	0.13983807-01	-0.152470160 00	-0.969349530-01	-0.187440050 00	-0.023650840-01
8	0.13983807-01	0.143460240 01	0.149053760 01	0.149000320 01	0.152210750 01
9	0.13983807-01	0.110843030 03	0.110898970 03	0.110808460 03	0.110933340 03
10	0.287262700-02	-0.343262760-01	-0.228385640-01	-0.414293060-01	-0.157373300-01
11	0.13983807-01	-0.645761610 00	-0.589820340 00	-0.680331440 00	-0.555230610 00
12	0.13983807-01	-0.544290680 02	-0.543691320 02	-0.544596370 02	-0.543345030 02
13	0.144523750 04	-0.214460080 04	0.558626400 04	-0.700357230 04	0.103531000 05
14	0.13983807-01	0.125497720 05	0.125498280 05	0.125497730 05	0.125498630 05
15	0.13983807-01	0.100959000 07	0.100959000 07	0.100958990 07	0.100959000 07
16	0.100637170 07	-0.130393920 07	0.272154760 07	-0.379161040 07	0.520994330 07
17	0.13983807-01	0.156416000 07	0.156416000 07	0.156415990 07	0.156416000 07
18	0.13983807-01	0.230770000 09	0.230770000 09	0.230770000 09	0.230770000 09
19	0.13983807-01	0.520976240 01	0.526569760 01	0.517519250 01	0.530626750 01
20	0.140816050 01	0.100846810 02	0.177223230 02	0.537244890 01	0.224395550 02
21	0.276175300-01	0.377923630-01	0.148262480 00	-0.3044819270-01	0.216536770 00

NONLINEAR CONFIDENCE LIMITS

PHI CRITICAL = 0.86040610-02

PARAMETER	LOWER PHI	UPPER B	UPPER PHI
1 PARAMETER NOT USED			
2 PARAMETER NOT USED			
3 PARAMETER NOT USED			
4 PARAMETER NOT USED			
5 PARAMETER NOT USED			
6 PARAMETER NOT USED			
7 PARAMETER NOT USED			
8 PARAMETER NOT USED			
9 PARAMETER NOT USED			
10 -0.301131380-01	0.857547680-02	-0.270659720-01	0.860406100-02
11 PARAMETER NOT USED			
12 PARAMETER NOT USED			
13 0.165945620 04	0.853914930-02	0.17321000	0.860406100-02
14 PARAMETER NOT USED			
15 PARAMETER NOT USED			

16	0.680476200 06	0.856406420-02	0.737129010 06	0.860406840-02
17	PARAMETER NOT USED			
18	PARAMETER NOT USED			
19	PARAMETER NOT USED			
20	0.138987530 02	0.502145740-02	0.139375430 02	0.106023320-01
21	0.914104530-01	0.120746620-01	0.941286000-01	0.820225060-02

Appendix F

OUTPUT FROM APPROX

CRITICAL TEMPERATURE 0.7360500 03		CRITICAL PRESSURE 0.3600300 02		CRITICAL VOLUME 0.7240000 01	
0.1603330 02		0.1466070 00		0.4200000 01	
FTC(1) -0.1342450 01		FTC(2) 0.0055370 00		FTC(3) -0.1747460 00	
A(1) -0.1743750 01		A(2) 0.1099910 01		A(3) -0.3917890 00	
B(1) 0.6116580 00		B(2) -0.2813220 00		B(3) -0.1021540 00	
C(1) -0.1406340 02		C(2) -0.0700000 00		C(3) 0.2128010 02	
				FTC(4) -0.6034860 02	
				FTC(5) 0.7497260 04	
				FTC(6) 0.4229580 07	
				A(4) -0.1964100 00	
				A(5) 0.1541960 06	
				A(6) -0.7698160 01	
				E(4) 0.3226690 00	
				B(5) -0.1559390 06	
				B(6) 0.6174500 08	
				C(4) -0.8822180 01	
				C(5) 0.6162000 06	
				C(6) 0.1298150 10	

TEMP.	VOLUME	PRESSURE (EXPT.)	PRESSURE (CALC.)	PERCENT DIFF.
399.690	0.7353000 02	0.1000000 01	0.9986690 00	-0.1331250 00
419.690	0.7742000 02	0.1000000 01	0.9967170 00	-0.3282970 00
439.690	0.8092000 02	0.1000000 01	0.9956570 00	-0.3433440 01
459.690	0.8462000 02	0.1000000 01	0.9949380 00	-0.6241070 02
479.690	0.8836000 02	0.1469600 02	0.1463590 02	-0.4090000 00
479.690	0.5797000 01	0.1469600 02	0.9996990 00	-0.3013640 01
479.690	0.1495000 01	0.5000000 02	0.1465010 02	-0.3125510 00
499.690	0.9215000 02	0.1000000 01	0.9983330 02	-0.3334500 00
499.690	0.0067000 01	0.1000000 01	0.9989020 00	-0.1098350 00
499.690	0.1601000 01	0.1469600 02	0.1466520 02	-0.2092960 00
519.690	0.9574000 02	0.5000000 02	0.4987740 02	-0.2451600 00
519.690	0.0337000 01	0.1000000 01	0.1000220 01	0.2185020 01
519.690	0.1701000 01	0.1469600 02	0.1467170 02	-0.1650300 00
539.690	0.9963000 02	0.5000000 02	0.4991210 02	-0.1757160 00
539.690	0.6604000 01	0.1000000 01	0.1000410 01	0.4116500 01
539.690	0.1790000 01	0.1469600 02	0.1467830 02	-0.1207400 00
539.690	0.7742000 00	0.5000000 02	0.4995420 02	-0.9163810 01
559.690	0.1031000 03	0.1000000 01	0.9930110 02	-0.6988610 00
559.690	0.6669000 01	0.1000000 01	0.1000770 01	0.7650370 01
559.690	0.1889000 01	0.1469600 02	0.1468360 02	-0.8407650 01
559.690	0.6367000 00	0.5000000 02	0.4995660 02	-0.8642380 01
579.690	0.1068000 03	0.1000000 03	0.9956840 02	-0.4316380 00
579.690	0.7133000 01	0.1000000 01	0.1000800 01	0.7571860 01
579.690	0.1972000 01	0.1469600 02	0.1468680 02	-0.6290230 01
579.690	0.8541000 00	0.5000000 02	0.4998750 02	-0.2497020 01
599.690	0.1103000 03	0.1000000 03	0.9974300 02	-0.2569810 00
599.690	0.7390000 01	0.1469600 02	0.1000210 01	0.8137090 01
599.690	0.2066000 01	0.5000000 02	0.1468840 02	-0.5170990 01
599.690	0.9480000 00	0.1000000 03	0.4998850 02	-0.2276460 01
599.690	0.5041000 00	0.1500000 03	0.9985590 02	-0.1441420 00
619.690	0.1142000 03	0.1000000 01	0.1491650 03	-0.5566030 00
619.690	0.7667000 01	0.1000000 01	0.1000820 01	0.8179350 01
619.690	0.2152000 01	0.1469600 02	0.1467220 02	-0.1617070 00
619.690	0.9993000 00	0.5000000 02	0.4999350 02	-0.1295100 01
619.690	0.0071000 00	0.1000000 03	0.9992910 02	-0.7091010 01
619.690	0.4004000 00	0.1500000 03	0.1495530 03	-0.2579100 00
639.690	0.1172000 03	0.2000000 03	0.1981620 03	-0.9188840 00
639.690	0.7919000 01	0.1000000 01	0.1001660 01	0.1661220 00
639.690	0.2237000 01	0.1469600 02	0.1468690 02	-0.3381650 01
639.690	0.1048000 01	0.5000000 02	0.4998750 02	-0.2509990 01
639.690	0.6468000 00	0.1000000 03	0.1000250 03	0.2541480 01
639.690	0.4390000 00	0.1500000 03	0.1497780 03	-0.1480760 00
639.690	0.3033000 00	0.2000000 03	0.1990740 03	-0.4632370 00
659.690	0.1216000 03	0.2500000 03	0.2469280 03	-0.1228720 01
659.690	0.8179000 01	0.1000000 01	0.1000800 01	0.7595100 01
659.690	0.2320000 01	0.1469600 02	0.1468990 02	-0.4183780 01
659.690	0.1090000 01	0.5000000 02	0.4999690 02	-0.6162810 02
659.690	0.6840000 00	0.1000000 03	0.1000280 03	0.2831170 01
659.690	0.4731000 00	0.1500000 03	0.1499300 03	-0.4681720 01
659.690	0.3404000 00	0.2000000 03	0.1995970 03	-0.2013280 00
659.690	0.2402000 00	0.2500000 03	0.2485760 03	-0.5655180 00
679.690	0.1253000 03	0.3000000 03	0.2957600 03	-0.1413330 01
679.690	0.8430000 01	0.1000000 01	0.1000780 01	0.7806620 01
679.690	0.2402000 01	0.1469600 02	0.1469030 02	-0.3863240 01
679.690	0.1141000 01	0.5000000 02	0.5000460 02	0.9253120 02
679.690	0.7194000 00	0.1000000 03	0.9999680 02	-0.3169340 02
679.690	0.3044000 00	0.1500000 03	0.1500220 03	0.1497730 01
679.690	0.3680000 00	0.2000000 03	0.1998860 03	-0.5865340 01
679.690	0.2771000 00	0.2500000 03	0.2507580 03	0.5032940 00
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1259.690	0.2308000	01	0.1000000	03	0.9996740	02	-0.3262120	-01
1259.690	0.1533000	01	0.1500000	03	0.1499160	03	-0.5601470	-01
1259.690	0.1145000	01	0.2000000	03	0.1999450	03	-0.2737230	-01
1259.690	0.9123000	00	0.2500000	03	0.2499990	03	-0.4648200	-03
1259.690	0.7574000	00	0.3000000	03	0.3000160	03	0.5228880	-02
1259.690	0.6464000	00	0.3500000	03	0.3499940	03	-0.1615800	-02
1259.690	0.5664000	00	0.4000000	03	0.3998790	03	-0.3034390	-01
1259.690	0.5366000	00	0.4200000	03	0.4198600	03	-0.3331940	-01
1259.690	0.5114000	00	0.4400000	03	0.4399370	03	-0.1423340	-01
1259.690	0.4886000	00	0.4600000	03	0.4598380	03	-0.3518200	-01
1259.690	0.4676000	00	0.4800000	03	0.4798360	03	-0.3408050	-01
1259.690	0.4484000	00	0.5000000	03	0.4997120	03	-0.5751590	-01
1259.690	0.4307000	00	0.5200000	03	0.5195590	03	-0.8479070	-01
1259.690	0.4142000	00	0.5400000	03	0.5395420	03	-0.8486070	-01
1259.690	0.3989000	00	0.5600000	03	0.5595030	03	-0.8877990	-01
1259.690	0.3847000	00	0.5800000	03	0.5794050	03	-0.1025990	00
1259.690	0.3714000	00	0.6000000	03	0.5993820	03	-0.1030200	00
1259.690	0.3590000	00	0.6200000	03	0.6192970	03	-0.1133540	00
1259.690	0.3474000	00	0.6400000	03	0.6391730	03	-0.1292930	00
1259.690	0.3366000	00	0.6600000	03	0.6588580	03	-0.1715650	00
1259.690	0.3263000	00	0.6800000	03	0.6788250	03	-0.1728230	00
1259.690	0.3167000	00	0.7000000	03	0.6985550	03	-0.2064650	00
1259.690	0.2948000	00	0.7500000	03	0.7482030	03	-0.2395910	00
1259.690	0.2757000	00	0.8000000	03	0.7977100	03	-0.2862470	00
1259.690	0.2599000	00	0.8500000	03	0.8467620	03	-0.3809790	00
1259.690	0.2441000	00	0.9000000	03	0.8959860	03	-0.4459710	00
1259.690	0.2308000	00	0.9500000	03	0.9451010	03	-0.5156700	00
1259.690	0.2189000	00	0.1000000	04	0.9939280	03	-0.6071950	00
1259.690	0.1985000	00	0.1100000	04	0.1090790	04	-0.8375170	00
1259.690	0.1814000	00	0.1200000	04	0.1188250	04	-0.9790830	00
1259.690	0.1554000	00	0.1400000	04	0.1376710	04	-0.1663400	01
1259.690	0.1360000	00	0.1600000	04	0.1564570	04	-0.2214520	01
1259.690	0.1213000	00	0.1800000	04	0.1749410	04	-0.2810720	01
1259.690	0.1098000	00	0.2000000	04	0.1933830	04	-0.3308460	01
1259.690	0.8995000	-01	0.2500000	04	0.2409500	04	-0.3620140	01
1259.690	0.7748000	-01	0.3000000	04	0.2948520	04	-0.1716130	01
1259.690	0.6905000	-01	0.3500000	04	0.3588160	04	0.2518830	01
1309.690	0.2418000	03	0.1000000	01	0.1000050	01	0.5368740	-02
1309.690	0.1645000	02	0.1469600	02	0.1468640	02	-0.6507630	-01
1309.690	0.4821000	01	0.5000000	02	0.4995560	02	-0.8769840	-02
1309.690	0.2403000	01	0.1000000	03	0.9997920	02	-0.2082680	-01
1309.690	0.1597000	01	0.1500000	03	0.1499640	03	-0.2420900	-01
1309.690	0.1194000	01	0.2000000	03	0.1999620	03	-0.1903250	-01
1309.690	0.9521000	00	0.2500000	03	0.2500120	03	0.4934500	-02
1309.690	0.7911000	00	0.3000000	03	0.3000120	03	0.4102750	-02
1309.690	0.6762000	00	0.3500000	03	0.3499890	03	-0.3059410	-02
1309.690	0.5402000	00	0.4000000	03	0.3997570	03	-0.3120640	-01
1309.690	0.5614000	00	0.4200000	03	0.4199280	03	-0.1794360	-01
1309.690	0.5354000	00	0.4400000	03	0.4398470	03	-0.3478910	-01
1309.690	0.5117000	00	0.4600000	03	0.4597300	03	-0.5875410	-01
1309.690	0.4898000	00	0.4800000	03	0.4797760	03	-0.4666570	-01
1309.690	0.4693000	00	0.5000000	03	0.5001990	03	0.3973880	-01
1309.690	0.4513000	00	0.5200000	03	0.5196260	03	-0.7189170	-01
1309.690	0.4342000	00	0.5400000	03	0.5395400	03	-0.8517910	-01

1309.690	0.4132000 00	0.5600000 03	0.5596130 03	-0.6905540-01
1309.690	0.4035000 00	0.5800000 03	0.5791260 03	-0.9903910-01
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1309.690	0.3758000 00	0.6200000 03	0.6192680 03	-0.1181160 00
1309.690	0.3647000 00	0.6400000 03	0.6391970 03	-0.1254750 00
1309.690	0.3534000 00	0.6600000 03	0.6590100 03	-0.1499420 00
1309.690	0.3428000 00	0.6800000 03	0.6787540 03	-0.1832060 00
1309.690	0.3328000 00	0.7000000 03	0.6985040 03	-0.2136540 00
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1309.690	0.2727000 00	0.8500000 03	0.8468520 03	-0.3703810 00
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1309.690	0.2434000 00	0.9500000 03	0.9449920 03	-0.5271550 00
1309.690	0.2310000 00	0.1000000 04	0.9938350 03	-0.6165370 00
1309.690	0.2097000 00	0.1100000 04	0.1090900 04	-0.8270400 00
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1309.690	0.12220000-01	0.3500000 04	0.3497030 04	-0.8484870-01
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1309.690	0.6158000 00	0.4000000 03	0.3999570 03	-0.1068310-01
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1309.690	0.3943000 00	0.6200000 03	0.6192780 03	-0.1164110 00
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