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INVISCID NONEQUILIBRIUM FLOW BEHIND BOW AND NORMAL SHOCK WAVES, PART III THE REVISED NORMAL SHOCK PROGRAM

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FOREWORD

The various program changes that are described in this report were completed as parts of several research efforts which had current needs for these refinements. The normal-shock correspondence method was supported under Contract No. DA-30-069-ORD-3443, ARPA Order No. 253-62. Both the revised Runge-Kutta integration scheme and the polynomial approximation to the thermodynamic properties (i.e., thermo-fit routine) were supported by NASA under Contract No. NASr-119. The change in dimensions of the kinetic model was completed under NASA Contract No. NAS 5-3976, Goddard Space Flight Center . Both the recoding of the program in Fortran IV and the preparation of the present report were supported by Cornell Aeronautical Laboratory.

It should be pointed out that this computing program has been developed to obtain specific results. It has proven to be successful and accurate within the range of application for which it was designed. However, individual application beyond the scope or intent of the present formulation will undoubtedly require meticulous checkout.

ABSTRACT

The investigation of the relaxation processes of multicomponent reacting gases behind normal and bow shock waves have been presented earlier in a two-part report, which provides a detailed discussion of the nonequilibrium shock wave programs developed at Cornell Aeronautical Laboratory. Since Parts I and II were written, a number of modifications have been introduced in the normal shock program and the present report (Part III) presents a discussion of the major changes and improvements to the normal shock program. The changes in the program itself are given in detail, including card additions, input-output format changes and complete flow diagrams of all modified subroutines.

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LIST OF SYMBOLS*

L' reference length in normal shock

M_o initial flow Mach number

MW' molecular weight of gas mixture; $MW = \frac{MW'}{MW_o'}$

p' pressure; $p = \frac{p'}{\rho_o'(U_o')^2}$

R_s' shock radius of curvature on centerline for bow shock

T' translational temperature; $T = \frac{T'}{T_o'}$

U' velocity; $U = \frac{U'}{U_o'}$

y' coordinate normal to shock; $y = \frac{y'}{R_s'}$ or $\frac{y'}{L'}$

ρ' density; $\rho = \frac{\rho'}{\rho_o'}$

x_i degree of nonequilibrium for i^{th} reaction

Subscript o indicates free stream conditions ahead of shock wave

Primes denote dimensional quantities

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*Definitions of symbols which appear in the Appendices and are not defined in this report are given in Parts I and II (Refs. 1 and 2).

I. INTRODUCTION

Investigations of the nonequilibrium thermodynamic and chemical phenomena occurring in the shock layer around the nose of hypersonic vehicles have led to the development of numerical methods of solution utilizing high-speed computers. Parts I and II of this report (Refs. 1 and 2) describe in detail two computer programs developed at CAL for the purpose of investigating the thermal and chemical relaxation of a complex mixture of reacting gases behind strong shock waves. The normal shock program concerns the relaxing flow behind a plane shock wave, while the bow shock program utilizes the inverse method to determine the inviscid, nonequilibrium flow around the blunt nose of an axisymmetric hypersonic vehicle. Part I of the report, General Analysis and Numerical Examples, discusses the development of the equations involved in the analysis and presents numerical solutions for both normal and bow shock waves. Part II, The IBM 704 Computer Programs presents a detailed description of the Fortran II programs.

Since Parts I and II were written, the programs have been in general use at CAL and from time to time they have been modified to meet the requirements of a new problem. This is particularly true of the normal shock program, which has proven to be an extremely versatile tool for the investigation of reacting gas flows. It is felt that the general usefulness of these improvements in the normal shock program warrants their publication as Part III of the overall report. The revised normal shock program differs from the original, as described in Refs. 1 and 2, in five major respects, which will be described in the present report. These changes are as follows:

1. The program has been changed to Fortran IV language for use on the IBM 7044 computer.

2. The maximum dimensions of the kinetic model used to describe the overall relaxation process have been changed from 20 species and 40 reactions to 15 species and 65 reactions. This change was prompted by a study of ionization phenomena behind shock waves, where a large group of ionization reactions was employed to describe electron formation in the relaxation zone at high temperatures.

3. A modified Runge-Kutta method of numerical integration, developed by C. E. Treanor[3], has been incorporated in the revised normal shock program. Coupled differential equations which describe the simultaneous relaxation of different components at greatly different rates present a difficulty in numerical integration, since the integration interval is determined by the fastest rate, and the extent of the region of integration is determined by the slowest rate. In problems of high temperature air flows, for example, the chemical rate equations sometimes have this character, involving both fast and slow chemical rates in some regions of integration. Difficulties arising with maximum integration step size, discussed in Refs. 1 and 2, have been greatly alleviated with this technique, enabling the numerical solutions to proceed without oscillations generated by the usual Runge-Kutta procedure in the approach to equilibrium. For a detailed presentation of this modified Runge-Kutta technique, reference should be made to Ref. 3.

4. The revised normal shock program can use the computed properties to predict the flow properties along a bow shock stagnation streamline, and to compute the nonequilibrium bow shock standoff distance. This involves the use of the "correspondence" method, which is described in detail by Gibson and Marrone in Ref. 4. Although the analysis of the method is given in Ref. 4, the technique of numerical solution of the pertinent equations has never been presented in a unified manner. This will be discussed in Section II of the present report.

5. The generality of the thermodynamic model has been extended by Joss[5], through the use of "thermo-fit" polynomials to describe the enthalpy and free energy of complex species. The original model allowed for a mixture of reacting ideal gases, the species being either monatomic or diatomic, and their vibrational energy described as that of simple harmonic oscillators. The use of thermo-fit polynomials in the revised program now allows for mixtures containing complex species (i.e., CO_2, H_2O) as well as diatomic species described either as simple oscillators or through thermo-fits. A discussion of this thermo-fit procedure is presented in Section 3 of this report.

It should be pointed out that in converting and revising the original normal shock program the model of vibration-dissociation coupling utilizing preferential dissociation from excited vibrational levels has been deleted. The revised deck discussed in this report includes the nonpreferential (or CVDV) vibration-dissociation coupling model along with the usual options of

uncoupled vibration and dissociation, or vibrational equilibrium during dissociation. For computations involving the preferential model, recourse should be made to the original program (Refs. 1 and 2).

It is the purpose of this report primarily to describe the changes in programming involved in the above revisions, and the modifications to program input and output. Consequently, Appendix I presents a list of new subroutines, new input cards, and detailed flow diagrams of all additions and modifications to the original program.

2. CORRESPONDENCE EQUATIONS

The analysis presented in Ref. 4 describes an approximate solution for complex chemistry for inviscid, blunt-body flows. The solution is derived from a correspondence between the chemical relaxation zone along a streamline and that behind a normal shock. Since a detailed description of the correspondence method is given in Ref. 4, only a discussion of the application of this method to the normal shock program will be given here.

The normal shock solutions are transformed to streamline solutions utilizing a new coordinate ζ (which is designated as χ in Ref. 4), as

$$\zeta = \rho_0' U_0' \int_0^y \frac{\rho}{U} \, dy \tag{1}$$

where primes denote dimensional quantities. The variable y is the distance behind the normal shock. Thus, at the shock,

$$y = 0 \text{ and } \zeta = 0,$$

and for the stagnation streamline case, at the body stagnation point (where equilibrium exists),

$$z \rightarrow \infty, \quad \text{since} \quad U \rightarrow 0.$$

The integral in Eq. (I) is programmed as a differential equation and the value of z is actually computed from

$$\frac{dz}{dy} = \rho_0' U_0' \frac{P}{U} \tag{2}$$

and is updated at each value of y in the numerical solution, using the Runge-Kutta method. For the special case of the stagnation streamline, additional equations are solved step by step along with Eq. (2). From the assumptions employed for the pressure and velocity near the stagnation region, (see Ref. 4), the following equation is obtained

$$\varphi_\ell^2(z) + B_\ell \frac{d\varphi_\ell(z)}{dz} = \frac{2}{\rho} \quad (\text{at} \quad z = 0, \ \varphi = 1), \tag{3}$$

where $\varphi(z)$ is used in defining the velocity component parallel to the body, and

$$B_\ell = \rho_0' U_0' [P_0] R_{s_\ell}' \tag{4}$$

The value of $[P_0]$ is the pressure immediately behind the shock wave, and R_{s_ℓ}' is the shock radius on the centerline, in centimeters. The running subscript ℓ is used to denote the fact that five separate input values of shock radii (i.e., ℓ runs from 1 through 5) can be used (see Appendix I), so that five corresponding flows can be obtained for each normal shock calculation. Equation (3) is solved in a manner similar to Eq. (I), that is

$$\frac{d\varphi_\ell(z)}{dz} = \frac{\left[\frac{2}{\rho} - \varphi_\ell^2(z)\right]}{B_\ell} \tag{5}$$

and

$$\frac{d\varphi_\ell}{dy} = \frac{\left[\frac{2}{\rho} - \varphi_\ell^2\right]}{B_\ell} \frac{dz}{dy}. \tag{6}$$

φ_ℓ is obtained from Eq. (6) and is updated at each value of y in the numerical solution.

The distance from the shock wave along the stagnation streamline is given in nondimensional form as C_ℓ (again ℓ is the running subscript 1....., 5). To compute this distance another integral is used

$$\hat{f}_\ell = \int_0^z \varphi_\ell \, dz \, , \tag{7}$$

and is written as

$$\frac{d\hat{f}_\ell}{dy} = \varphi_\ell \frac{dz}{dy} \qquad (\hat{f}_\ell = 1 \quad at \quad z = 0) \, , \tag{8}$$

and is updated in the solution. The value of C_ℓ is then computed and, for generality, to make the calculation applicable to either two-dimensional ($\nu = 0$) or axisymmetric ($\nu = 1$) bodies, one obtains

$$(C_\ell)_\nu = \frac{1}{B_\ell} \int_0^z \frac{1}{\rho} \exp\left(-\frac{(\nu+1)}{B_\ell} \int_0^{z'} \varphi_\ell \, dz''\right) dz' \tag{9}$$

for $\nu = 0$, or 1.

Equation (9) is rewritten as

$$\frac{d(C_\ell)_\nu}{dy} = \frac{1}{B_\ell} \frac{1}{\rho} \exp\left(-\frac{(\nu+1)}{B_\ell} \hat{f}_\ell\right) \frac{dz}{dy} \qquad \left((C_\ell)_\nu = 0 \text{ at } z = 0\right), \tag{10}$$

and is also updated in the numerical integration. The above-mentioned equations can be seen in the flow chart for Subroutine DER, page 2 of LG02 in Appendix I. Thus, the distance from the shock along the stagnation streamline is computed as the integration proceeds. At some point in the solution the variables get sufficiently close to equilibrium so that they remain essentially constant the rest of the way in to the stagnation point (program checks are used to determine this point, such as the value of χ_i for all chemical

reactions, i, for example). At this point, if all variables are assumed constant, a closed form integration from the last value of ζ to $\zeta \rightarrow \infty$ is computed and this value is added to the $(C_\ell)_\nu$ at this last value of ζ to obtain the overall shock-standoff distance. Depending on the value of R'_{s_ℓ}, this "almost equilibrium" point may occur near the shock (large body) or near the body for small values of R'_{s_ℓ}. If $\tilde{\zeta}$ is considered as the last value of ζ, and $(\tilde{C}_\ell)_\nu$ is the distance at this point, the nondimensionalized standoff distance δ/R'_{s_ℓ} is obtained from,

$$\frac{\delta}{R'_{s_\ell}} = \tilde{C}_\ell + \frac{1}{\sqrt{8\tilde{\rho}}}\left\{(1-\tilde{\lambda}_\ell)\exp\left(\frac{-2\tilde{\hat{f}}_\ell}{B_\ell}\right)\right\} \quad \text{for } \nu = 1, \tag{11}$$

and

$$\frac{\delta}{R'_{s_\ell}} = \tilde{C}_\ell + \frac{1}{\sqrt{8\tilde{\rho}\tilde{\lambda}_\ell}}\left\{(1-\tilde{\lambda}_\ell)\ln\left(\frac{1+\sqrt{\tilde{\lambda}_\ell}}{1-\sqrt{\tilde{\lambda}_\ell}}\right)\exp\left(-\frac{\tilde{\hat{f}}_\ell}{B_\ell}\right)\right\} \tag{12}$$

for $\nu = 0$.

The term $\tilde{\lambda}_\ell$ is given as

$$\tilde{\lambda}_\ell = \frac{\tilde{\varphi}_\ell - \sqrt{\frac{2}{\tilde{\rho}}}}{\tilde{\varphi}_\ell + \sqrt{\frac{2}{\tilde{\rho}}}} \tag{13}$$

where it is understood that all of these variables are evaluated at the last computation point. These equations can be seen in the flow chart for Subroutine STOP, LG09 in Appendix I.

The correspondence technique is very useful for the rapid investigation of hypersonic flow fields. As shown in Ref. 4 and in the extensive study presented in Ref. 6, streamline mapping using this technique has proven very successful, and nonequilibrium standoff distances computed using this

technique compare with exact bow-shock solutions with discrepancies of less than 5%.

A description of input and output modifications involved in this correspondence calculation are given in Appendix I.

3. THERMO-FIT METHOD

The original normal-shock program utilized a model for the thermodynamic description of diatomic species as simple harmonic oscillators (Refs. I and 2). With this model the reacting gas could be a mixture of monatomic and diatomic species. To generalize the model to allow for complex molecular species, a thermo-fit method has been added to the program. The following discussion of this modification, is based on the description given in Ref. 5 by Joss.

Under the conditions of vibrational equilibrium, the enthalpy and free energy of complex molecules are functions of the translational temperature of the gas. A curve representing these data, based on experiment, can be fitted by polynomial equations. This procedure has been named thermofitting. The problem of defining the thermodynamic properties of a complex species is thus reduced to one of obtaining the proper coefficients to be used in the thermofit equations. The use of this method for a given component involves the assumption that the component is in vibrational equilibrium with the translational temperature in the relaxation zone behind the shock wave. For the case of a diatomic species in vibrational nonequilibrium, the simple-

harmonic oscillator technique is used, with the vibrational energy defined by a vibrational temperature, T_V, different from the translational temperature.

For any gaseous species, a relationship exists between the enthalpy and free energy, since both are functions of the temperature. Both quantities can be defined, in a nondimensional form, by the same set of thermo-fit coefficients. The two nondimensional quantities, enthalpy H_j and free energy F_j, to which curves are to be fitted are presented below.

Enthalpy:

$$H_j = \frac{h_j' - h_j^{o'}}{R_o' T'} \tag{14}$$

Free Energy:

$$F_j = \frac{F_j^{o'} - h_j^{o'}}{R_o' T'} \tag{15}$$

where

h_j' = static enthalpy of jth species

$h_j^{o'}$ = heat of formation of jth species

$F_j^{o'}$ = free energy of jth species

R_o' = universal gas constant

T' = temperature

The polynomial equations which are to be fitted to thesequantities are

$$H_j = (A_1)_j + (A_2)_j (T') + (A_3)_j (T')^2 + (A_4)_j (T')^3 + (A_5)_j (T')^4 \tag{16}$$

and

$$F_j = (A_1)_j (1 - \ln T') - (A_2)_j (T') - (A_3)_j (T')^2 - (A_4)_j (T')^3 - (A_5)_j (T')^4 - k_j \tag{17}$$

where

$(A_{1 \rightarrow 5})_j$ = thermo-fit coefficients

k_j = constant which makes the nondimensional free energy, F_j, compatible with the nondimensional enthalpy, H_j.

Fits are made over two temperature ranges. The first encompasses the temperature ahead of the shock and only the coefficients A_1 through A_5 are required as inputs since the free energy ahead of the shock is not calculated. The second covers the temperature range behind the shock and the program requires k_j as well as the five coefficients (called $B_{1 \rightarrow 5}$ for this range) as inputs.

The curve-fitting is done by a least squares program developed by F. E. Butler at CAL, which provides the five coefficients and k_j for a given molecule and temperature range. Since the program for this calculation is described in Appendix II, only a brief discussion of the method will be presented here. The input for the curve-fit program is a table of temperature (T), enthalpy (H(T)), and free energy (F(T)); experience has shown that seven data points yield accurate fits. The fit program actually computes two slightly different sets of coefficients for each temperature range; one set by fitting the enthalpy and one by fitting the free energy. The coefficients found by fitting the enthalpy are then used to compute values of the free energy for the selected temperatures. Similarly, the coefficients found by fitting the free energy are used to compute values of the enthalpy at the given temperatures. The one set of coefficients which fits both the free energy and enthalpy most accurately is then selected. Generally, the coefficients found by fitting the enthalpy give the best overall results.

As was mentioned previously, the curves are fit to the data in the form H_j and F_j, given by Eqs. (14) and (15). However, due to frequent use of the JANAF tables (Ref. 7), the curve-fit program was modified to permit the input of enthalpy and free energy data as tabulated therein. If

this option is chosen, the program converts the data to the proper form before fitting. (The conversion of the data from the JANAF tables is accomplished as indicated in Appendix II.)

This curve fit program has been used, for example, to produce thermo-fit data for the species present in high temperature air. A listing of the coefficients for a fourteen-species model used in shock-wave computations can be found in Ref. 8.

A detailed description of the input and output formats for the curve-fit program is given in Appendix II.

4. REFERENCES

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2. Garr, L.J. and Marrone, P.V., Inviscid, Nonequilibrium Flow Behind Bow and Normal Shock Waves, Part II. The IBM 704 Computer Programs. CAL Report No. QM-1626-A-12(II) (May 1963)

3. Treanor, C.E., A Method for the Numerical Integration of Coupled First-Order Differential Equations with Greatly Different Time Constants. CAL Report No. AG-1729-A-4 (January 1964)

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5. Joss, W.W., The Thermo-Fit Method. CAL Internal Memo (November 1963)

6. Gibson, W.E. and Marrone, P.V., Nonequilibrium Scaling Criterion for Inviscid Hypersonic Airflows. CAL Report No. QM-1626-A-8 (November 1962)

7. JANAF Thermochemical Tables. Compiled by the Thermal Research Laboratory, Dow Chemical Company, Midland, Michigan

8. Marrone, P.V., Normal Shock Waves in Air: Equilibrium Composition and Flow Parameters for Velocities from 26,000 to 50,000 ft/sec. CAL Report No. AG-1729-A-2 (August 1962)

APPENDIX I

REVISIONS AND MODIFICATIONS TO THE NORMAL SHOCK DECK

This section of the report presents a detailed discussion of all modifications to the normal shock deck in the following order:

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I. I INPUT CHANGES

A. Changes to existing cards

1. Second Card: When entering values for P_o', T_o', ρ_o', MW_o', enter values for only three of the four quantities. The program computes the value of the missing (blank) quantity from the equation of state. Also, when entering values for M_o, U_o', enter only one of the two quantities. The program computes the missing (blank) quantity.

2. Third Card:

   (a) $TEST_2$ is now an indicator for the optional output of rate of production of species j from reaction i, Q_{ij}, on utility tape 3. o indicates no. I indicates yes.

   (b) $TEST_4$: Maximum allowable running time in seconds.

   (c) Change $TEST_5$ to read "Test on loss of significant figures in subtraction for equation $P = -\left(\frac{f_3 - f_2}{y_3 - y_2}\right)$ used in modified Runge-Kutta integration method".

   See Ref. 3, page 5, i.e.,

   $$P = -\left(\frac{f_3 - f_2}{y_3 - y_2}\right) = -\left(\frac{f_3 - f_2}{f_2 - f_1}\right)\frac{2}{h}$$

   If $\left|\frac{f_3 - f_2}{f_2}\right|$ or $\left|\frac{f_2 - f_1}{f_1}\right| \leq TEST_5$, revert to original Runge-Kutta method.

   We have used $TEST_5 = 5 \times 10^{-4}$.

3. Fourth Card:

   (a) Add to $TEST_6$ the statement "When all values of $|x_i| \leq TEST_6$, program terminates".

(b) Add $TEST_8$. "Allowable relative change in χ_i when $|\chi_i| > TEST_6$ (i.e., when χ_i out of band-width around zero)".

(c) Add $TEST_9$. An indicator for the optional thermodynamic and chemistry print out. 0 indicates no. I indicates yes.

(d) Add $TEST_{10}$. "Species identification number (j) for electrons; used in calculation of electrons/c.c."

B. Additional input cards required for the modified normal shock program (see Fig. 3).

1. Card containing the five values of bow shock radii (cm) used for the normal shock-bow shock correspondence calculation (see Ref. 4). This card is placed immediately behind the fifth card in the input deck (i.e., behind the card containing $TEST_{11}$ through $TEST_{15}$). If a correspondence solution is not desired, the new sixth card should be left blank, but it must always be included. If a correspondence solution is desired, all five values of the bow-shock radii must be nonzero to avoid division by zero.

2. Thermo-fit cards.

   These two cards contain the coefficients used for an empirical description of the species thermodynamics.

   The cards are placed immediately behind the original group of four cards describing each species. The card with the coefficients for the low-temperature range is placed ahead of the

card with the coefficients for the high-temperature range. These cards must be included for every species. For those species not utilizing the thermo-fit method, the cards may be left blank.

3. Thermo-fit indicator card.

   This card is placed immediately behind the cards defining the initial species concentrations. The first 15 spaces are used to indicate which of the species in a particular problem will be handled by the thermo-fit method and which will be handled by the harmonic oscillator method. A number I in a space indicates that the species will be thermo-fit; a number zero or a blank space indicates that the species will utilize the harmonic oscillator technique.

RUN DESCRIPTION

RUN #	s	r	f	g	c	I.C.	E.E.	DUMP IND	$\Delta y'_{START}$	y'_{STOP}

AMBIENT CONDITIONS ; SHOCK VELOCITY

p'_o	ρ'_o	T'_o	γ_o	M_o	U'_o	MW'_o	L'

$TEST_i$ CONSTANTS $i = 1,15$

NO. OF RESULT PARAGRAPHS PER PAGE	Q_{ij} OPTIONAL OUTPUT 0 = NO 1 = YES	MAXIMUM RELATIVE CHANGE IN T OVER Δy INTERVAL	ALLOWABLE RUNNING TIME ~ SEC	TEST ON SIGNIFICANT FIGURES - MRK
BAND WIDTH FOR X_i TESTING	MAXIMUM ABSOLUTE CHANGE IN X_i WHEN IN BAND	MAXIMUM RELATIVE CHANGE IN X_i WHEN OUT OF BAND	THERMO. AND CHEM. OUTPUT 0 = NO 1 = YES	SPECIES NUMBER FOR e^-
NO. OF SUCCESSFUL STEPS BEFORE C (Δy)	c FOR c Δy	MAXIMUM RELATIVE ERROR IN H_o FOR SHOCK ITERATION	MINIMUM Δy ALLOWED	MAXIMUM Δy ALLOWED

INITIAL SPECIE CONCENTRATIONS (USE ONLY THOSE CARDS THAT CONTAIN THE S ENTRIES)

$\gamma'_{1,0}$	$\gamma'_{2,0}$	$\gamma'_{3,0}$	$\gamma'_{4,0}$	$\gamma'_{5,0}$
$\gamma'_{6,0}$	$\gamma'_{7,0}$	$\gamma'_{8,0}$	$\gamma'_{9,0}$	$\gamma'_{10,0}$
$\gamma'_{11,0}$	$\gamma'_{12,0}$	$\gamma'_{13,0}$	$\gamma'_{14,0}$	$\gamma'_{15,0}$

I.C.
INITIAL CONDITIONS
(POST SHOCK)
1 ITERATE
0 COMPUTE

E.E.
ELECTRONIC EXCITATION
0 NO
1 YES

DUMP IND.
0 NO DUMP
1 DUMP FIRST R-K CALCULATION IN INTERVAL
4 DUMP ALL R-K CALCULATIONS IN INTERVAL

Figure 1 REVISED NORMAL SHOCK PROGRAM: INPUT CARD FORMAT

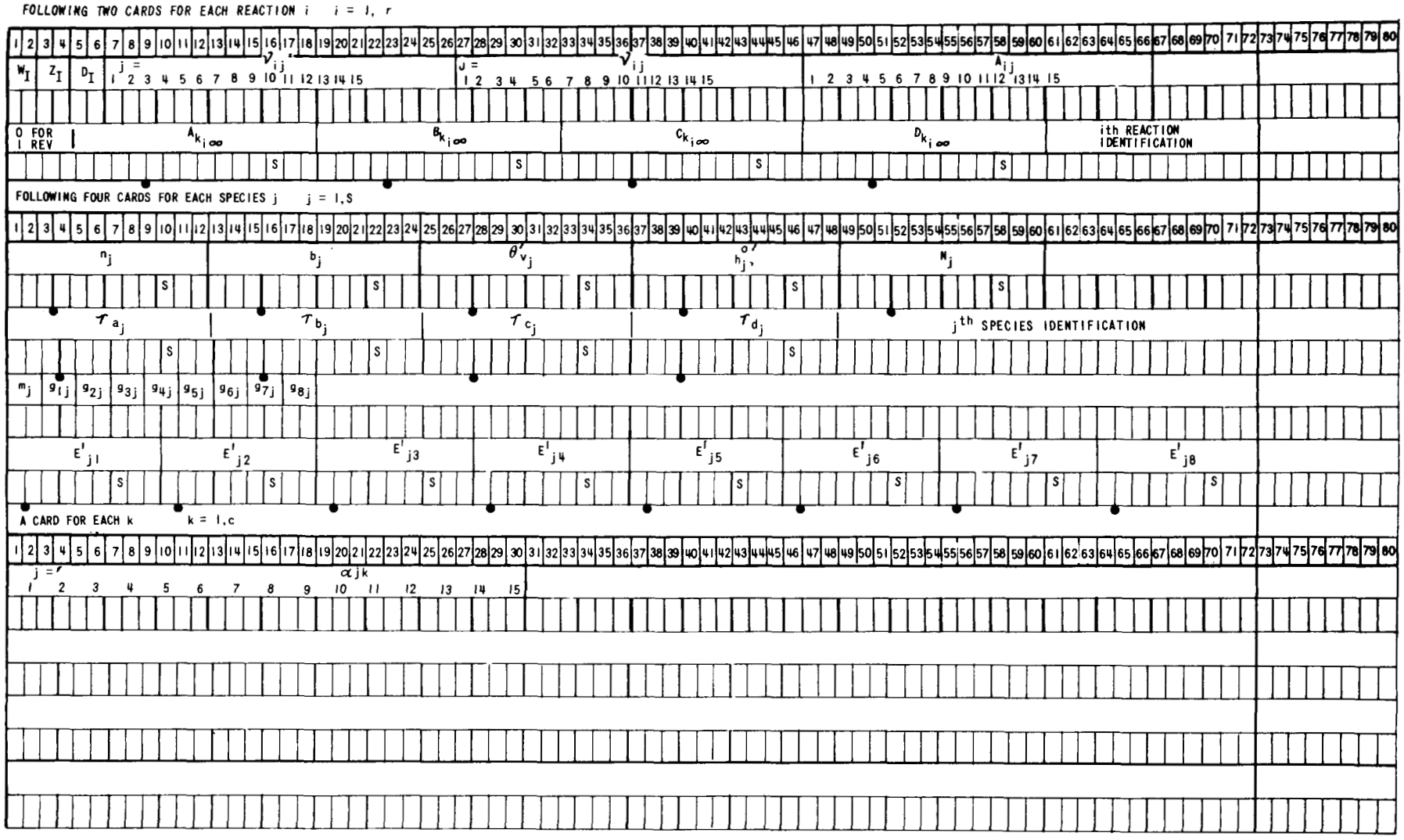


Figure 2 REVISED NORMAL SHOCK PROGRAM: INPUT CARD FORMAT (CHEMISTRY AND THERMODYNAMICS)

CORRESPONDENCE CALCULATION: FORMAT FOR CARD NO. 6 (THE FIVE BOW SHOCK RADII)

R(1)	R(2)	R(3)	R(4)	R(5)

THERMO-FIT CARD FORMAT: FINAL TWO (OUT OF SIX) CARDS FOR EACH SPECIE

A_1	A_2	A_3	A_4	A_5
B_1	B_2	B_3	B_4	B_5	k

THERMO-FIT INDICATOR

J = 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

0 = HARMONIC OSC 1 = THERMO FIT

Figure 3 ADDITIONAL INPUT CARDS FOR REVISED NORMAL SHOCK

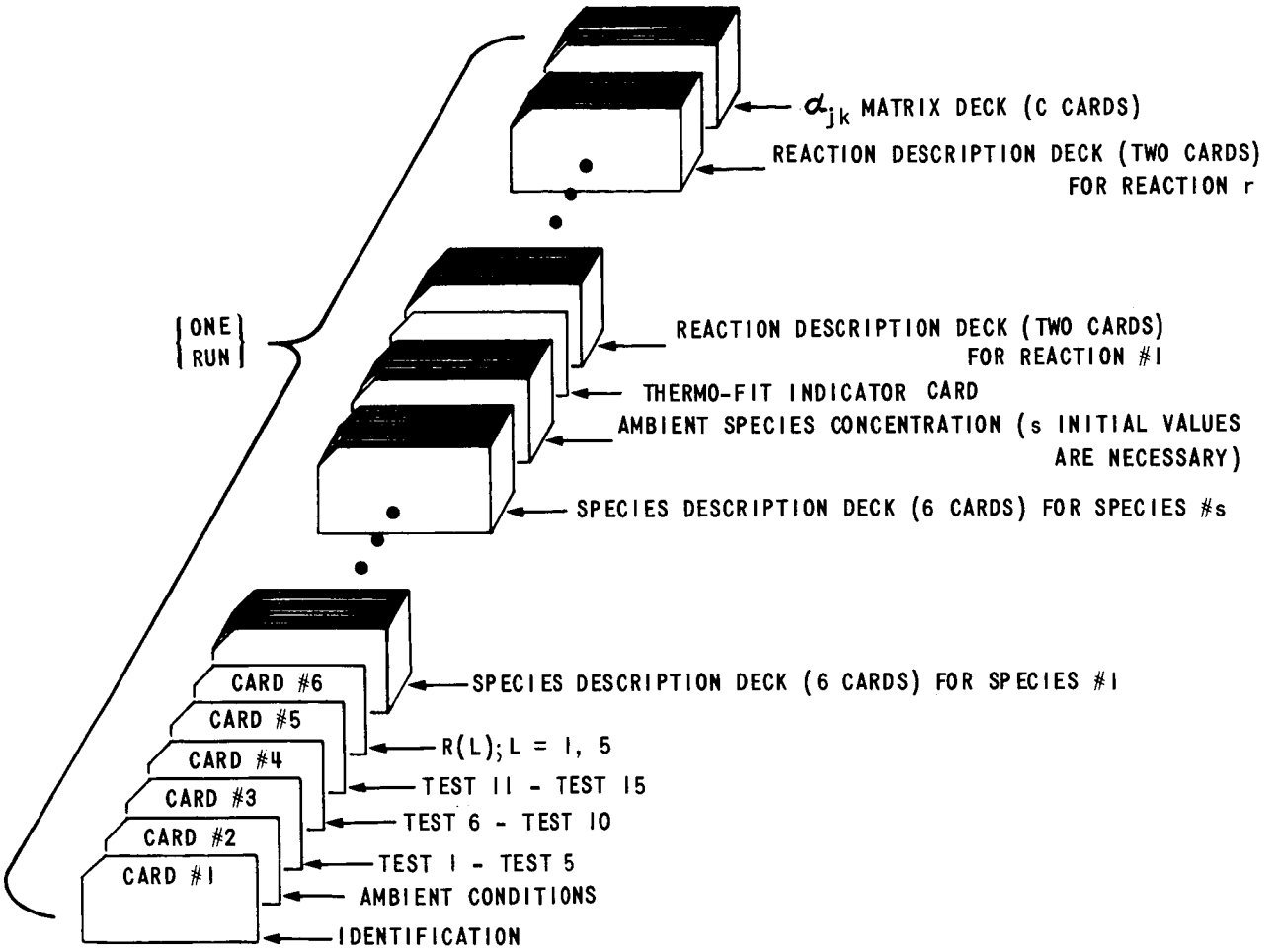


Figure 4 REVISED NORMAL SHOCK PROGRAM: CARD ORDER FOR DATA INPUT DECK

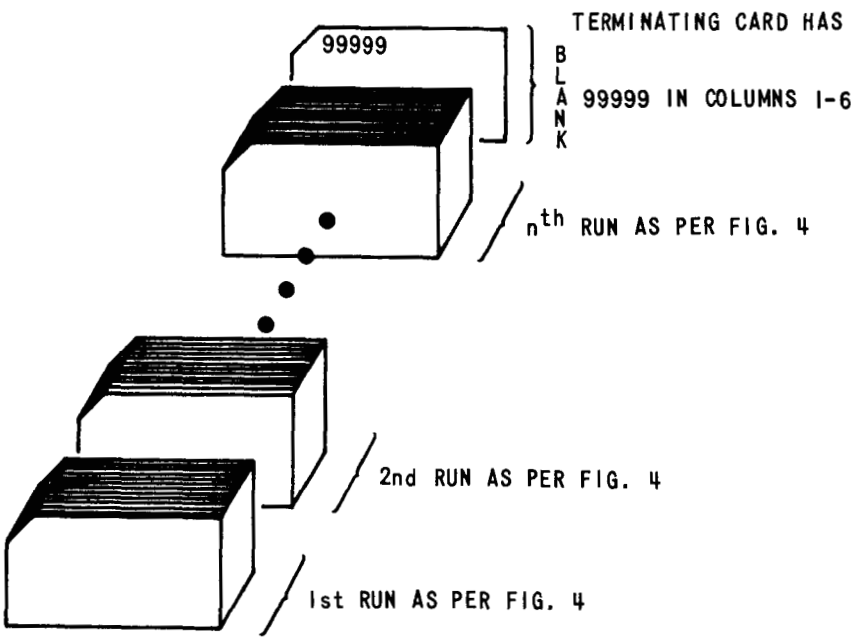


Figure 5 REVISED NORMAL SHOCK PROGRAM: INPUT DECK ORDER FOR SUCCESSIVE RUNS

I.2 OUTPUT MODIFICATIONS

The program output has been modified as follows:

1. The five values of shock radius of curvature used in the correspondence solution are printed directly beneath the controls-and-constants paragraph.
2. An indicator is printed after each species name denoting whether that species' thermodynamic properties were thermo-fit (T-F) or computed by the harmonic oscillator technique (H-O).
3. When a correspondence solution is performed, each output paragraph includes the correspondence-mapping variable, defined as χ in Ref. 4, as well as values of y'/R_s' denoting where, along the stagnation streamline, the properties in the particular paragraph apply. The final nondimensional stand-off distance is printed below the last output paragraph.

I.3 FORTRAN PAUSE INSTRUCTIONS

Pause 77777	Pause in subroutine SAVE(I). Press start to continue.

I.4 TAPE UTILIZATION

Tape	Usage
1	Checkpoint device for save-and-restart procedure
2	Optional thermodynamic and chemistry when $TEST_9 = 1$ and $RKIND \leq DUMP_{IND}$.
3	Optional Q_{ij} output when $TEST_2 = 1$
5	System input tape
6	System output tape

I. 5 POSSIBLE REASONS FOR PROGRAM TERMINATION

1. $y \geqslant y_{STOP}$; $YSTOP = \frac{y'_{STOP}}{L'}$, where y'_{STOP} and L' are input parameters.

2. $|x_i| \leqslant$ TEST(6) for i = 1, ISR. TEST(6) is an input parameter. (This run termination will indicate that the run is "near" equilibrium.)

3. If the diagnostic "DETERMINANT = 0, NO SOLUTION" appears on the output, there is probably an error in the α_{jk} matrix input data.

4. Pause 77777. This pause occurs after the program has been saved on utility tape 1 by subroutine SAVE. Press start to continue.

5. Running time exceeded the allowable time specified in TEST (4). The program will be saved on utility tape 1 and stops on pause 77777.

6. If the diagnostic "EXP (EQ. OR GT. 80)" appears on the output, then one of the radii for the correspondence solution is too small.

7. $\Delta y \leqslant \Delta y_{min}$ = TEST (14). TEST (14) is an input parameter.

8. Run number = $\begin{bmatrix} \text{B} \\ \text{L} \\ \text{A} \quad 99999 \\ \text{N} \\ \text{K} \end{bmatrix}$, which designates end of data, gives Fortran stop which returns control to the monitor system.

I. 6 DESCRIPTION OF UTILITY SUBROUTINES USED IN THE REVISED NORMAL SHOCK PROGRAM

1. SUBROUTINE HOLRTH (6H. . . . . , A)

   Places the six specified hollerith characters in location A.

2. SUBROUTINE SAVE (1)

   Saves program on utility tape 1. Program may be continued at a later date by using $RESTART card. Details available in the following manual:

   IBM 7040/7044 Operating System (16/32K)
   Programmer's Guide
   File No. 7040-36
   Form C-28-6318-4

3. SUBROUTINE COPY (I)

Copies one Fortran file from utility I onto system output unit.

4. SUBROUTINE TYPEST

Writes message on the on-line typewriter. The calling sequence is as follows:

```
      CALL TYPEST
YYYY WRITE (6, XXXX) LIST
XXXX FORMAT (          )
```

A call to subroutine TYPEST modifies Fortran statement YYYY so that the list according to format XXXX appears on the on-line typewriter.

5. SUBROUTINE TIME (NTIME, IND)

Gives the running time in seconds for a current run. The first call to TIME should have IND = 0 to initialize the clock setting. Then set IND = I to get elapsed time in seconds in location NTIME.

Subroutine HOLRTH is included in the deck. Subroutines SAVE, COPY (I), TYPEST, TIME are MAP routines and therefore not included in the deck. Instead, dummy routines are included in the deck.

6. SUBROUTINE DVCHK(J)

J is set to: I if the Divide Check indicator is on, or 2 if it is off. The indicator is left in the off condition.

Details available in the following manual:

IBM 7040/7044 Operating System (16/22K)
Fortran IV Language

File No. 7040-25
Form C-28-6329-3

I.7 THE REVISED NORMAL SHOCK PROGRAM

CORRESPONDENCE OF FORTRAN AND REPORT SYMBOLS

(SUPPLEMENT TO LIST IN REF. 2, P. 74)

CI	(5,2)	$(\tilde{C}_1)_0$ $(\tilde{C}_1)_1$ $(\tilde{C}_2)_0$ $(\tilde{C}_2)_1$ $(\tilde{C}_3)_0$ $(\tilde{C}_3)_1$ $(\tilde{C}_4)_0$ $(\tilde{C}_4)_1$ $(\tilde{C}_5)_0$ $(\tilde{C}_5)_1$	$(\tilde{C}_\ell)_\nu$; $\ell=1,5$; $\nu=0$ AND $\nu=1$. (NON-DIMENSIONAL DISTANCE IN FROM SHOCK) $\nu=0$ {2-DIMENSIONAL, 2ND FORTRAN SUBSCRIPT = 1} $\nu=1$ {AXISYMMETRIC, 2ND FORTRAN SUBSCRIPT = 2}	INITIAL CONDITIONS FOR A RUNGE-KUTTA INTEGRATION INTERVAL
FI	(5)	$\tilde{f}_\ell(z)$	$\ell=1,5$ $\int_0^\chi \varphi_\ell(\xi')d\xi'$ OF EQ (13), REF. 4	
ZI		$\tilde{z}$	χ SHOCK MAPPING VARIABLE	
PHII	(5)	$\tilde{\varphi}_\ell(z)$	$\ell=1,5$ SEE EQS. (11), (12); REF. 4	
CT	(5,2)	$(C_1)_0$ $(C_1)_1$ $(C_2)_0$ $(C_2)_1$ $(C_3)_0$ $(C_3)_1$ $(C_4)_0$ $(C_4)_1$ $(C_5)_0$ $(C_5)_1$	$(C_\ell)_\nu$; $\ell=1,5$; $\nu=0$ AND $\nu=1$ (NON-DIMENSIONAL DISTANCE IN FROM SHOCK) $\nu=0$ {2-DIMENSIONAL, 2ND FORTRAN SUBSCRIPT = 1} $\nu=1$ {AXISYMMETRIC, 2ND FORTRAN SUBSCRIPT = 2}	INCREMENTAL AND/OR UPDATED VALUES FOR THE FOUR COLLOCATION POINTS IN A RUNGE-KUTTA INTERVAL
FT	(5)	$f_\ell(z)$	$\ell=1,5$ $\int_0^\chi \varphi_\ell(\xi')d\xi'$ OF EQ (13), REF. 4	
ZT	(5)	z	χ SHOCK MAPPING VARIABLE	
PHIT	(5)	$\varphi_\ell(z)$	$\ell=1,5$ SEE EQS. (11), (12); REF. 4	

DCT (5,2)	$d(C_\ell)_\nu/dy$	$\ell=1,5$; $\nu=0$ AND $\nu=1$
DF (5)	$df_\ell(z)/dy$	$\ell=1,5$
DZ	dz/dy	
DPHI (5)	$d\varphi_\ell(z)/dy$	$\ell=1,5$
YB (5)	B_ℓ	$\ell=1,5$; $B_\ell=\rho_0'U_0'R_{S_\ell}'\,p_{[0]}$ (SEE EQ.(12), REF.4)
R (5)	R_{S_ℓ}'	$\ell=1,5$; SHOCK RADII AT CENTER LINE
XNEW9 (15,4)	U,ρ,p	
XNEW8 (15,4)	γ_j	$j=1,s$
XNEW7 (15,4)	ϵ_j	$j=f+1,g$
XNEW6 (15,4)	z	
XNEW5 (15,4)	φ_ℓ	$\ell=1,5,1$
XNEW4 (15,4)	f_ℓ	$\ell=1,5,1$
XNEW3 (15,4)	$(C_\ell)_{\nu=0}$	$\ell=1,5,1$
XNEW2 (15,4)	$(C_\ell)_{\nu=1}$	$\ell=1,5,1$
XNEW9D (15,4)	$\frac{dU}{dy}\ \frac{d\rho}{dy}\ \frac{dp}{dy}$	
XNEW8D (15,4)	$d\gamma_j/dy$	$j=1,s$
XNEW7D (15,4)	$d\epsilon_j/dy$	$j=f+1,g$
XNEW6D (15,4)	dz/dy	
XNEW5D (15,4)	$d\varphi_\ell/dy$	$\ell=1,5,1$

STORAGE FOR THE APPROPRIATE FUNCTIONS AT THE FOUR COLLOCATION POINTS IN A RUNGE-KUTTA INTERVAL

STORAGE FOR THE APPROPRIATE DERIVATIVES AT THE FOUR COLLOCATION POINTS IN A RUNGE-KUTTA INTERVAL

XNEW4D (15,4)	df_ℓ/dy	$\ell = 1,5,1$
XNEW3D (15,4)	$d(C_\ell)_{\nu=0}/dy$	$\ell = 1,5,1$
XNEW2D (15,4)	$d(C_\ell)_{\nu=1}/dy$	$\ell = 1,5,1$
TFIND (15)		HARMONIC OSCILLATOR OR THERMO-FIT INDICATOR, ONE FOR EACH SPECIES; 0 → HARMONIC OSCILLATOR 1 → THERMO-FIT
TFBCDI (2,15)		2 WORD IDENTIFICATION FOR THERMO-FIT INPUT DATA, ONE FOR EACH SPECIES
TFC (6,15,2)		THERMO-FIT COEFFICIENTS
	$(A_{1\to5})_j$	FIVE COEFFICIENTS AHEAD OF THE SHOCK $\left[\begin{array}{l} TFC(m,j,1) = (A_m)_j \\ TFC(m,j,2) = (B_m)_j \end{array}\right\} m=1,5$
	$(B_{1\to5})_j$, k_j	SIX COEFFICIENTS BEHIND THE SHOCK $\left.\begin{array}{l} TFC(6,j,2) = k_j \end{array}\right]$
Z1		BCD (bGAMMA)
Z3		BCD (bbbEPS)
Z4		BCD (bbbTWJ)
Z5		BCD (bbbCHI)
Z6		BCD (bbbbbQ)
Z7		BCD (bbbbbP)
Z8		BCD (bbbRHØ)
Z9		BCD (bbbVEL)
SQQQ1		BCD (bITER.)
SQQQ2		BCD (bCØMP.)

SQQQ4	BCD (bbbbNØ)
SQQQ5	BCD (bbbYES)
SQQQ6	BCD (FØRWBb)
SQQQ7	BCD (REVbbb)
SQQQ8	BCD (bbbT-F)
SQQQ9	BCD (bbbH-O)
BLNK	BCD (bbbbbb)
NTIME	RUNNING TIME IN SECONDS SINCE CALL TIME WITH IND=0.
IND	INDICATOR FOR SUBROUTINE TIME. 0→INITIALIZE TIME READING. 1→INITIALIZATION HAS TAKEN PLACE.

I. 8 LIST OF SUBROUTINES

NEW SUBROUTINES

Deckname	Subroutine Name
LG00	MAIN PROGRAM
LG01	MAIN
LG22	SUB 11(i)
LG23	SUB 12
LG28	MRK (J1, J2, F, FDØT, DELF)
LG29	MRK1 (J1, J2, FDØT, DELF)
LG21	CØMMØN AND DIMENSIØN STATEMENTS (No flow chart)

REF. 2 SUBROUTINES THAT WERE RETAINED

Ref. 2 Deckname	New Deckname	Subroutine Name	Flow Chart (Ref. 2)
A16	LG 16	SUB2	p 67
A15	LG 15	SUB4	p 66
A13	LG 13	LCØUNT	p 64
A12	LG 12	MATRIX	p 62
A04	LG 04	TEST 2	p 54

REF. 2 SUBROUTINES THAT WERE CHANGED

Ref. 2 Deckname	New Deckname	Subroutine Name
A02	LG02	DER
A03	LG03	TEST I
A05	LG05	READIN
A06	LG06	SUB 10
A07	LG07	INICØN
A08	LG08	WRITE 2
A09	LG09	STØP
A10	LG10	SUB 6(j)
A11	LG11	SUB 5
A14	LG14	SUB I
A17	LG17	START
A18	LG18	WRITE I
A19	LG19	SIMSØL (SINGLE PRECISIØN)

I. 9 SYNOPSIS OF NEW SUBROUTINES

LG00 MAIN PROGRAM

Calls subroutine MAIN

LG01 Subroutine MAIN

Original main program, which has been modified and changed into a subroutine

LG22 Subroutine SUB 11(i)

Computes enthalpy for all the species

LG23 Subroutine SUB 12

Computes enthalpy, vibrational energy, specific heat and chemical potential for all the species

LG28 Subroutine MRK (J1, J2, F, FDØT, DELF)

Computes the increment for a dependent variable corresponding to a change in the independent variable (step size) according to Eq. (9) of Ref. 3

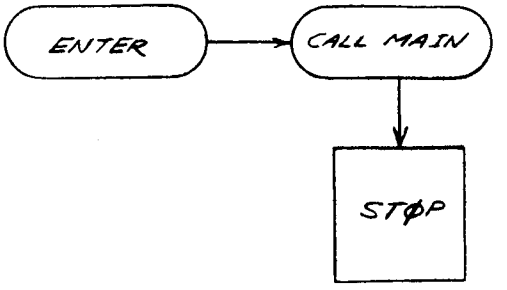
LG29 Subroutine MRK I (J1, J2, FDØT, DELF)

Computes the increment for a dependent variable corresponding to a change in the independent variable (step-size) according to Eq. (11) of Ref. 3

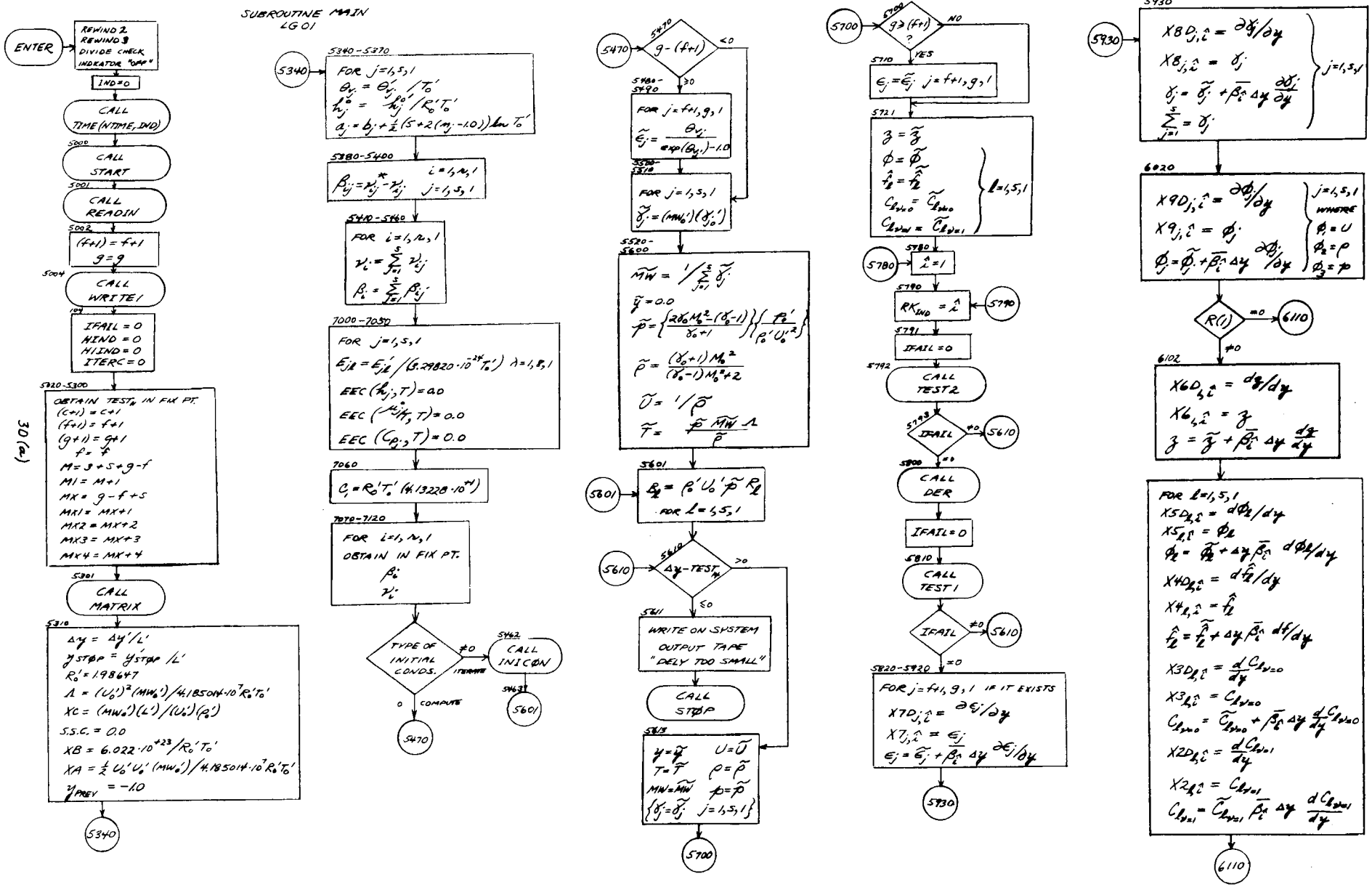
I.10 FLOW CHARTS

Flow charts for the new and the modified subroutines are given on pages 29 to 47.

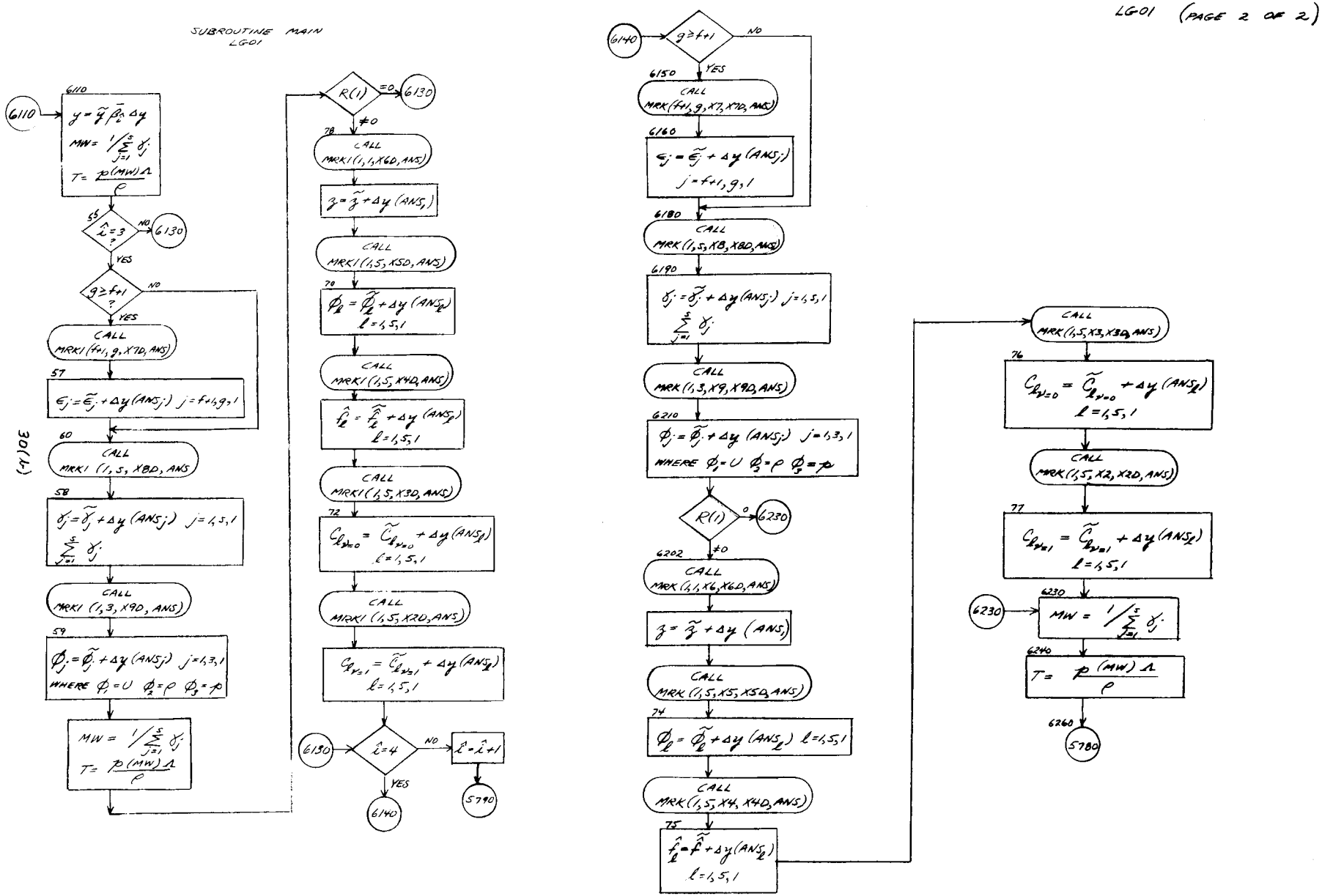
MAIN PROGRAM
LG00



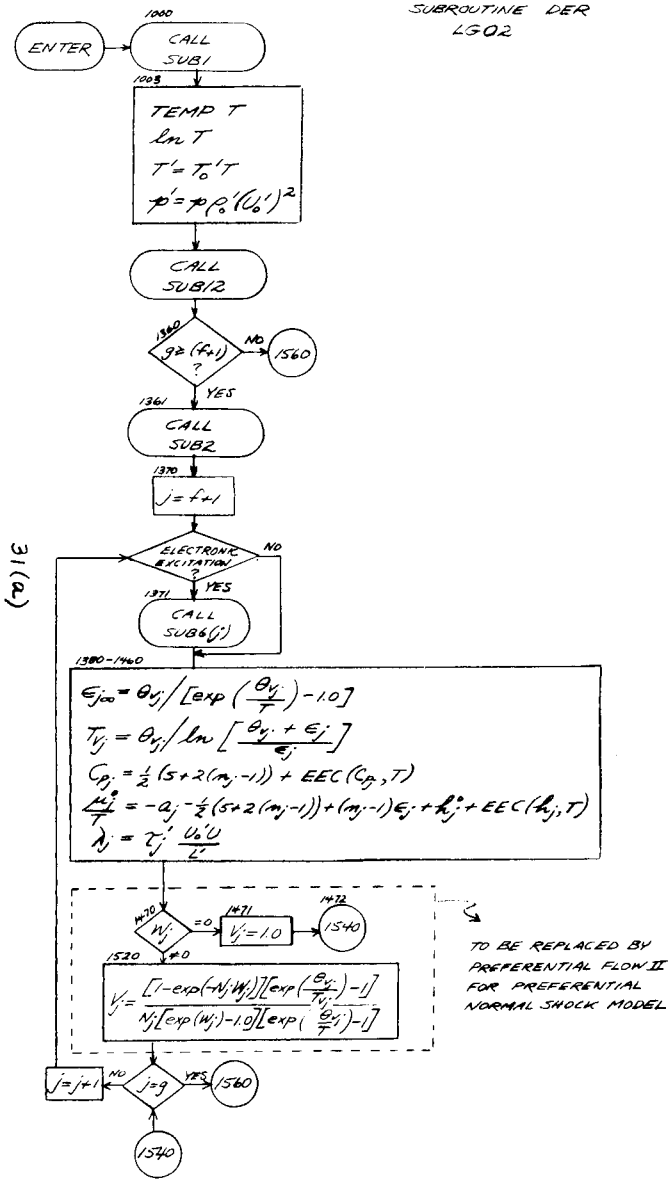
SUBROUTINE MAIN
LG01



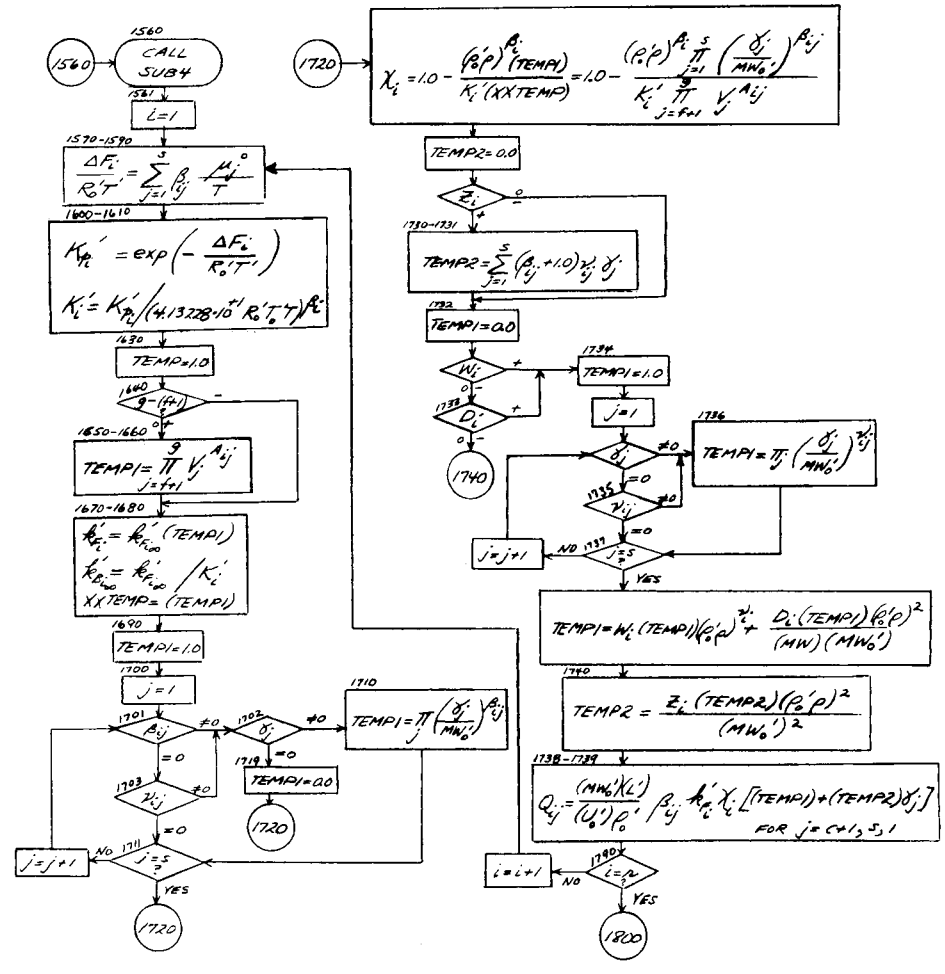
SUBROUTINE MAIN
LG01



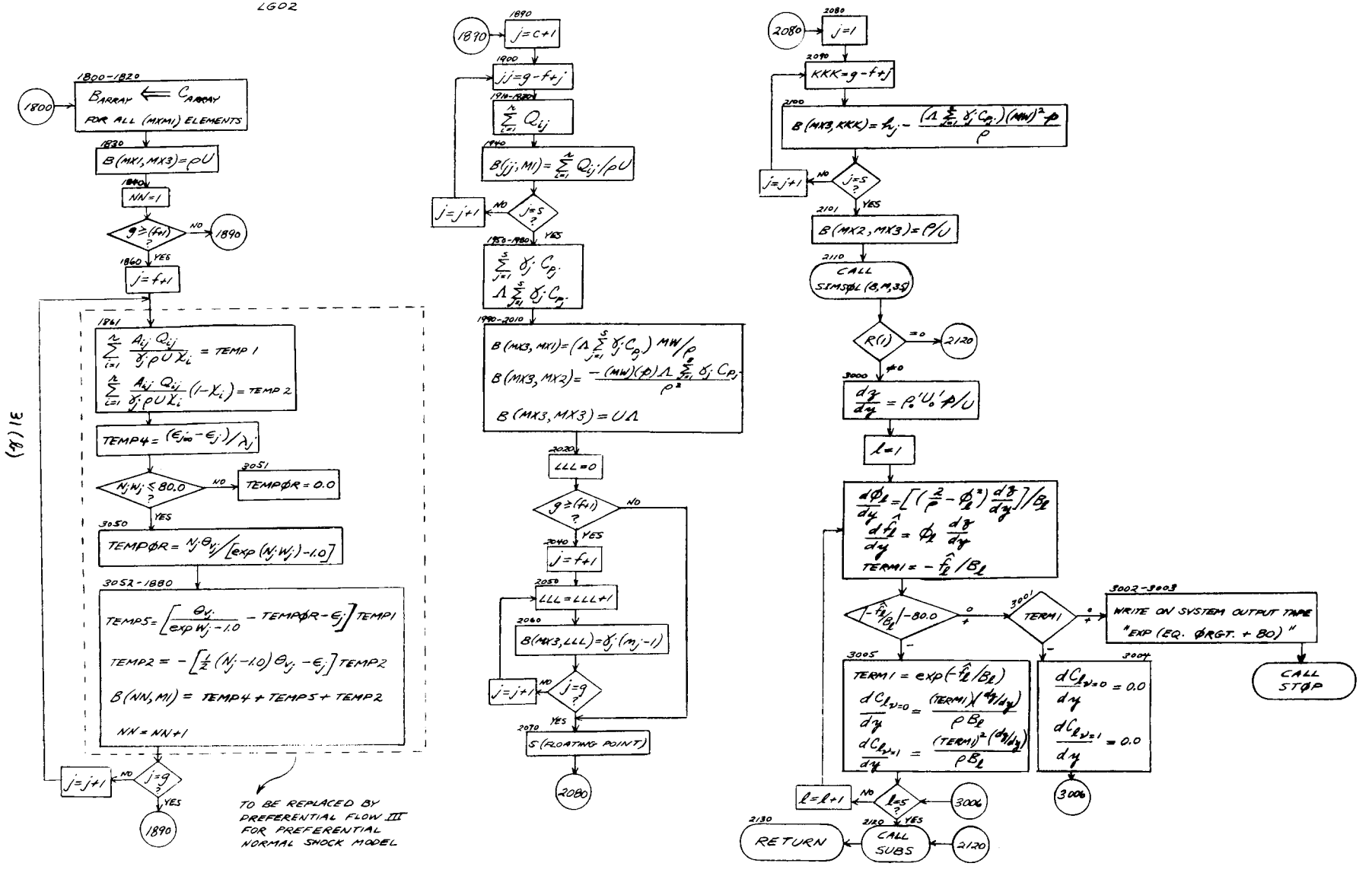
SUBROUTINE DER
LG02



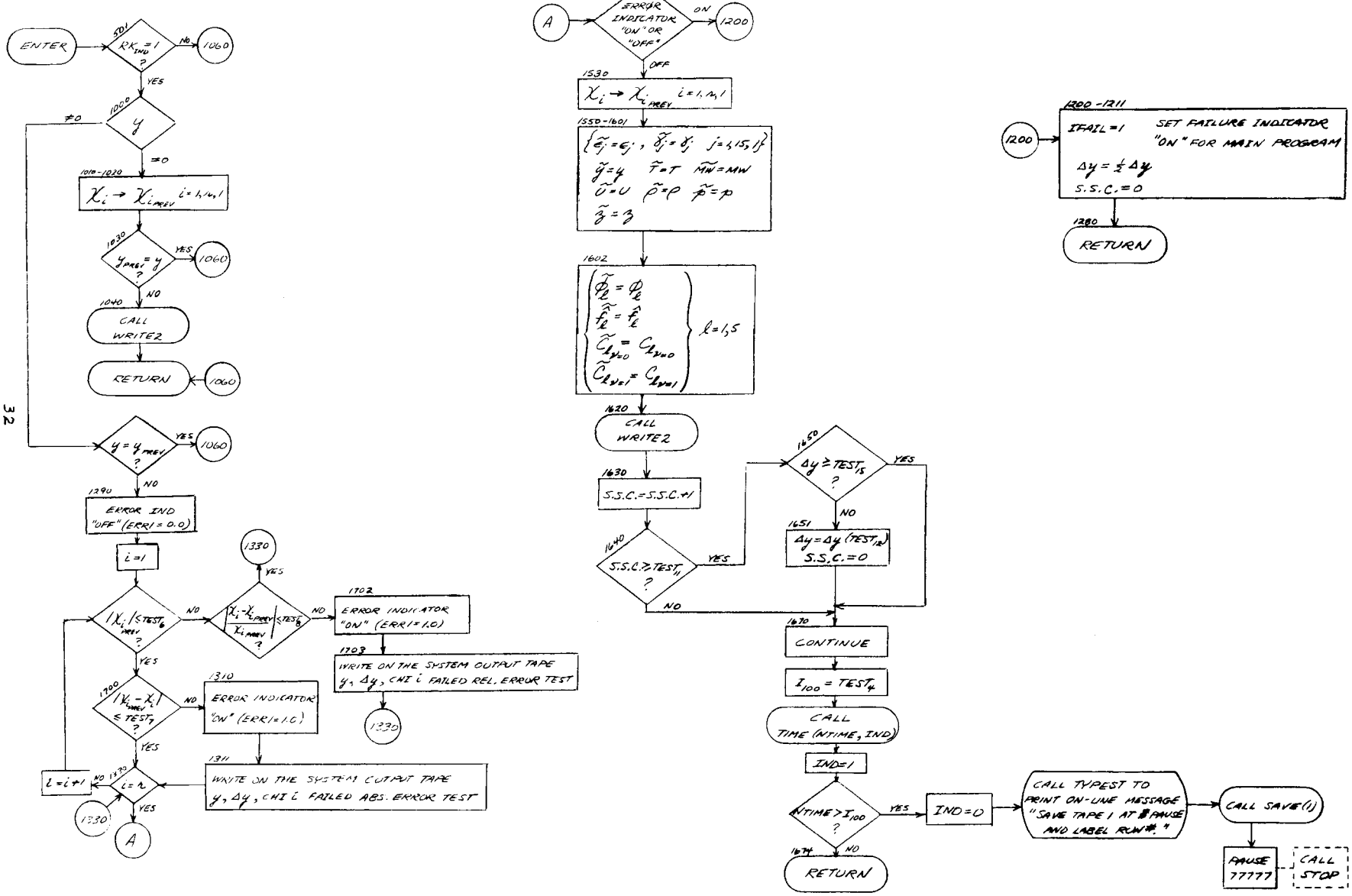
TO BE REPLACED BY PREFERENTIAL FLOW II FOR PREFERENTIAL NORMAL SHOCK MODEL



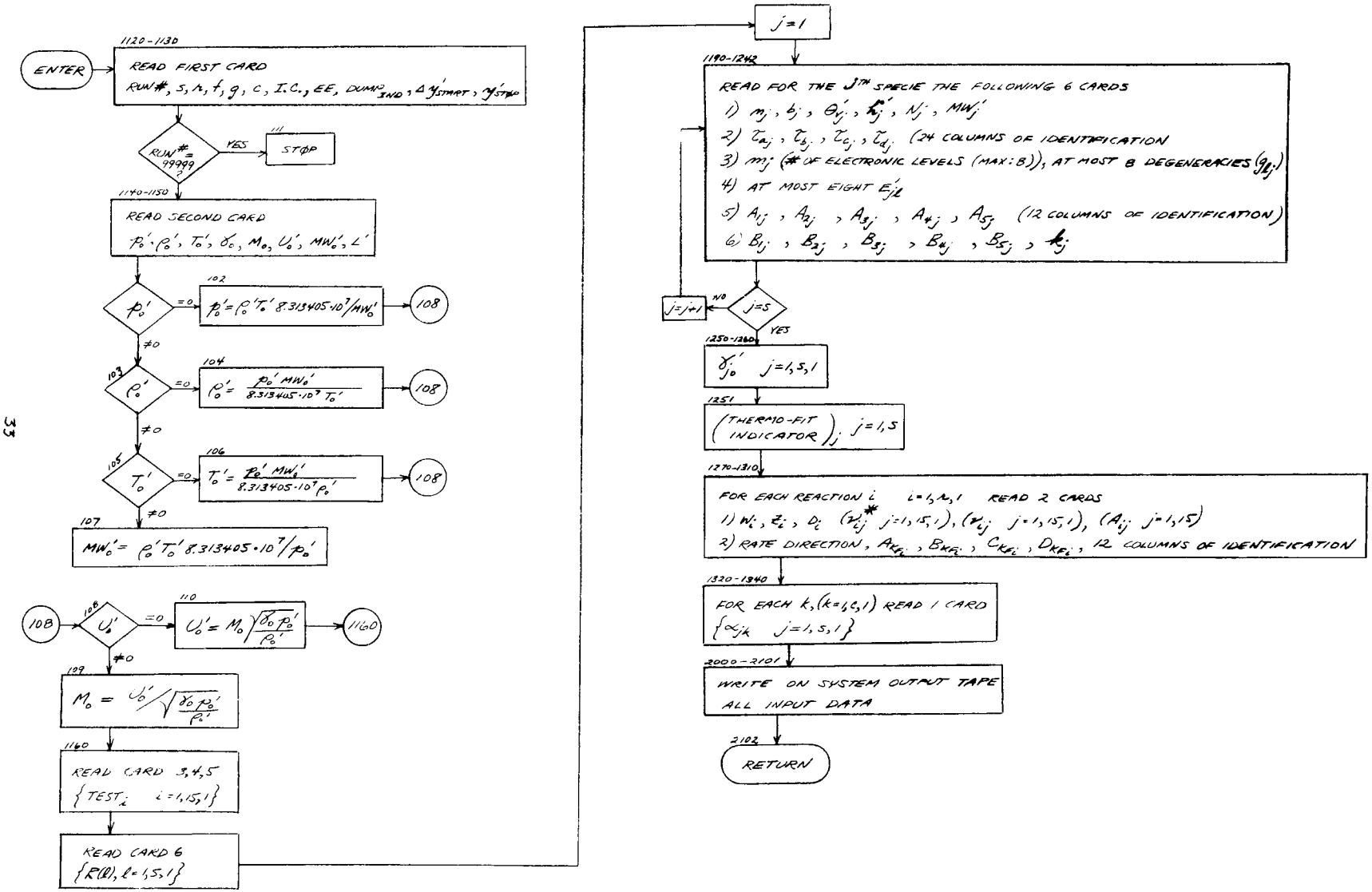
SUBROUTINE DER
LG02



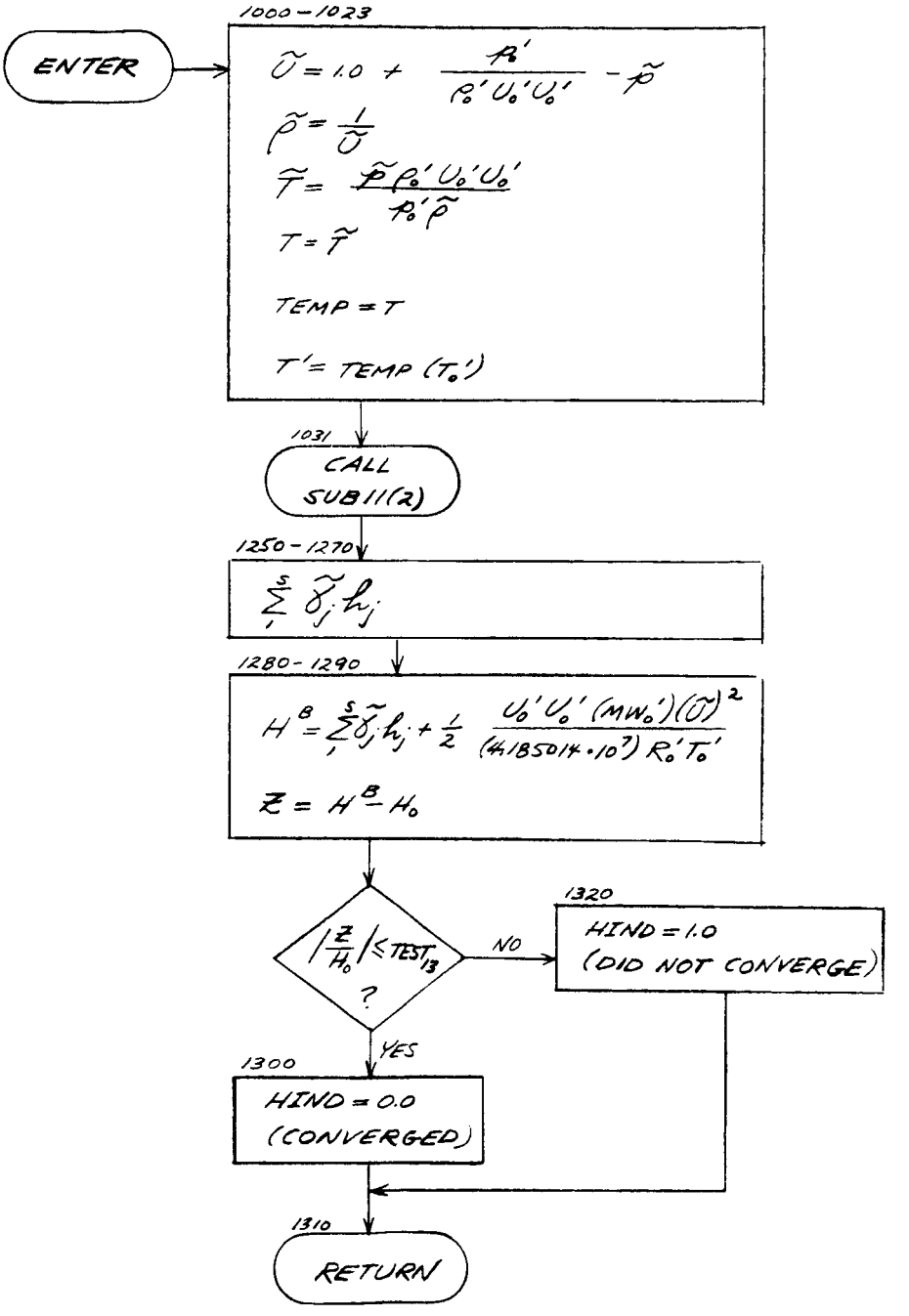
SUBROUTINE TEST1
LG03



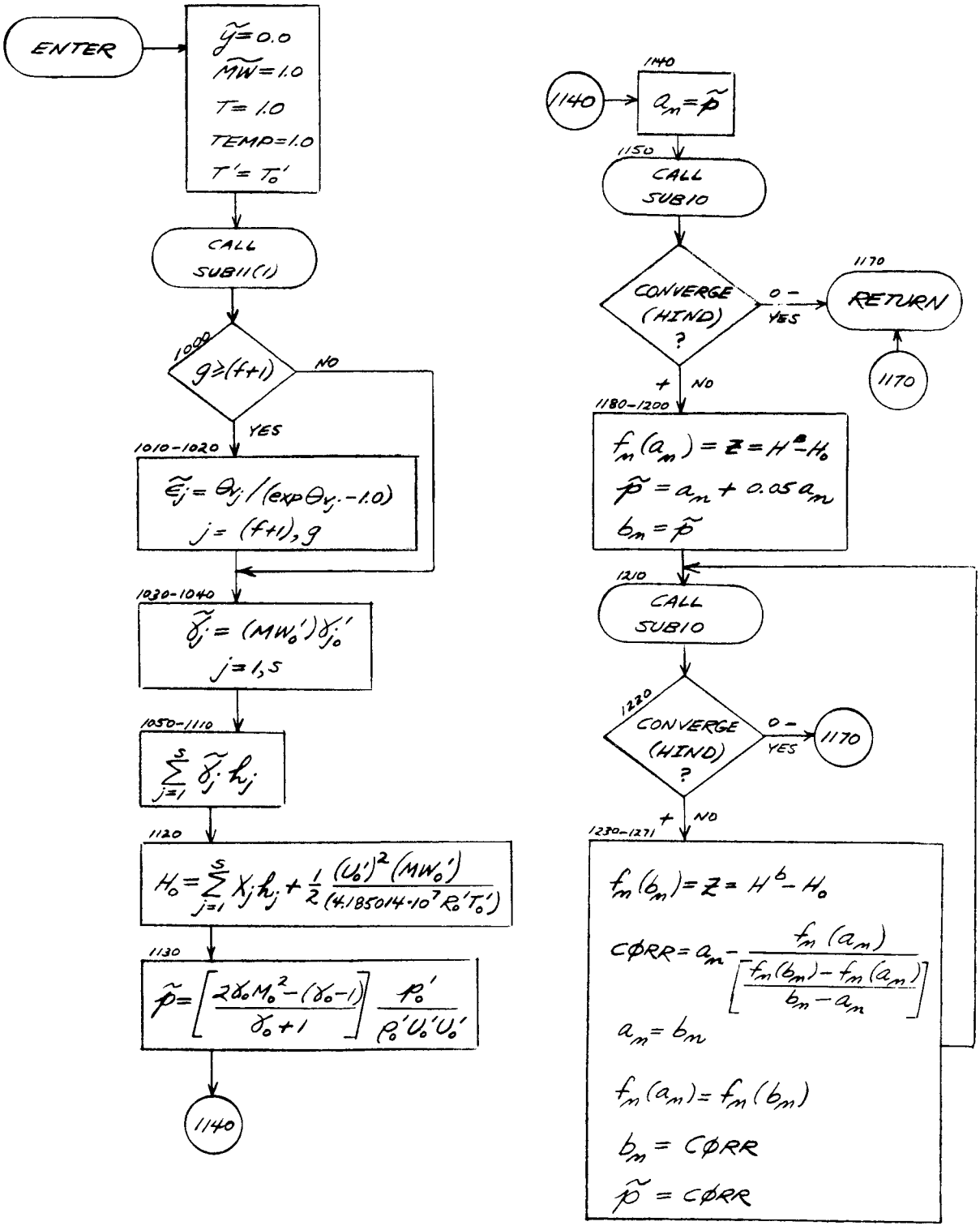
SUBROUTINE READIN
LG05



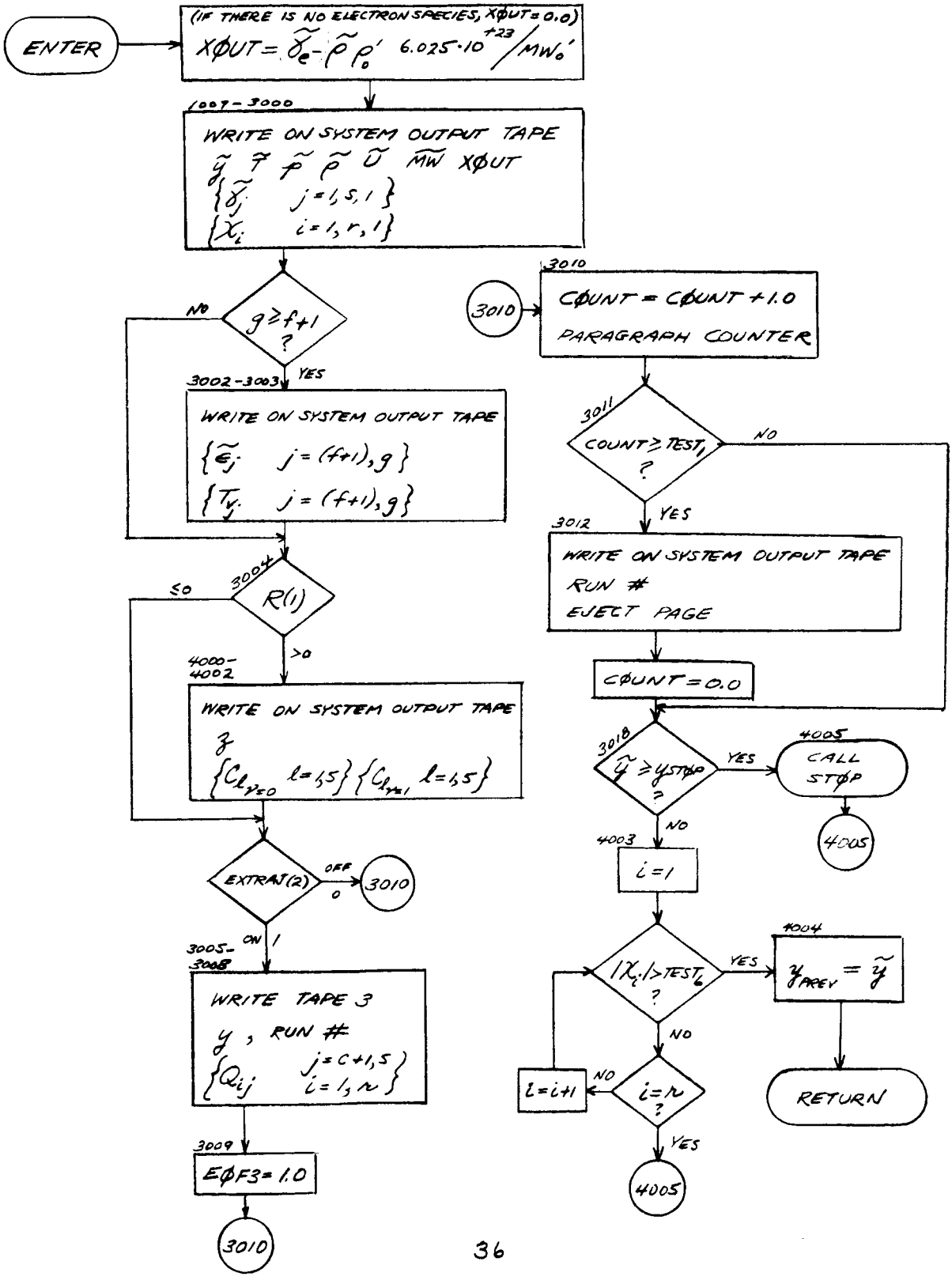
SUBROUTINE SUB10
LG06



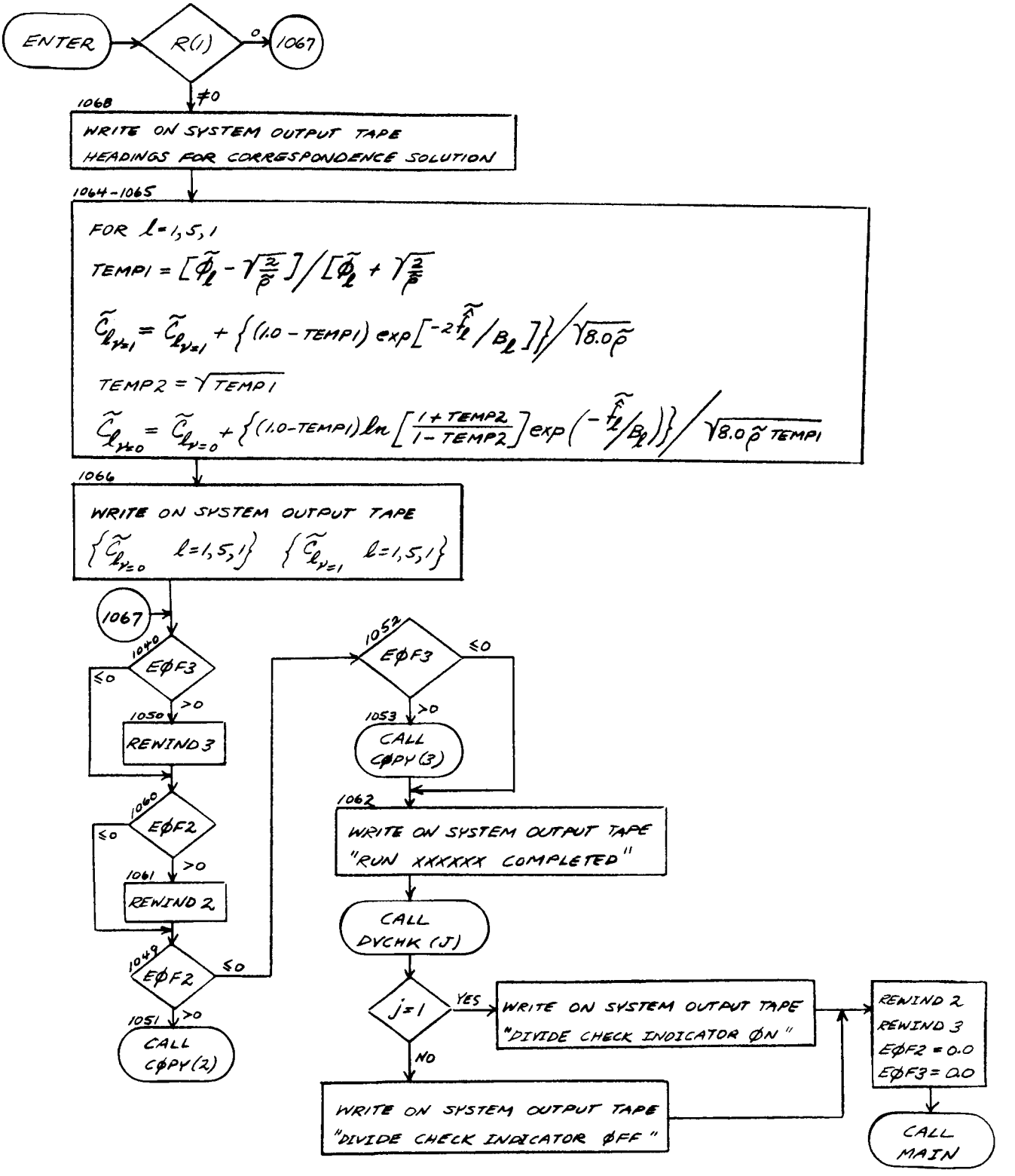
SUBROUTINE INICØN
LG07



SUBROUTINE WRITE 2
LG08



SUBROUTINE STØP
LG09



SUBROUTINE SUB6(j)
LG10

ENTER

1010 – 1110

$$\sum_{l=1}^{m_j} g_{jl} \exp\left[-\frac{E_{jl}}{T}\right] = TT2$$

$$\sum_{l=1}^{m_j} g_{jl} E_{jl} \exp\left[-\frac{E_{jl}}{T}\right] = TT1$$

$$\sum_{l=1}^{m_j} g_{jl} E_{jl}^2 \exp\left[-\frac{E_{jl}}{T}\right] = TT3$$

1120 – 1140

$$EEC(h_j; T) = TT1/TT2$$

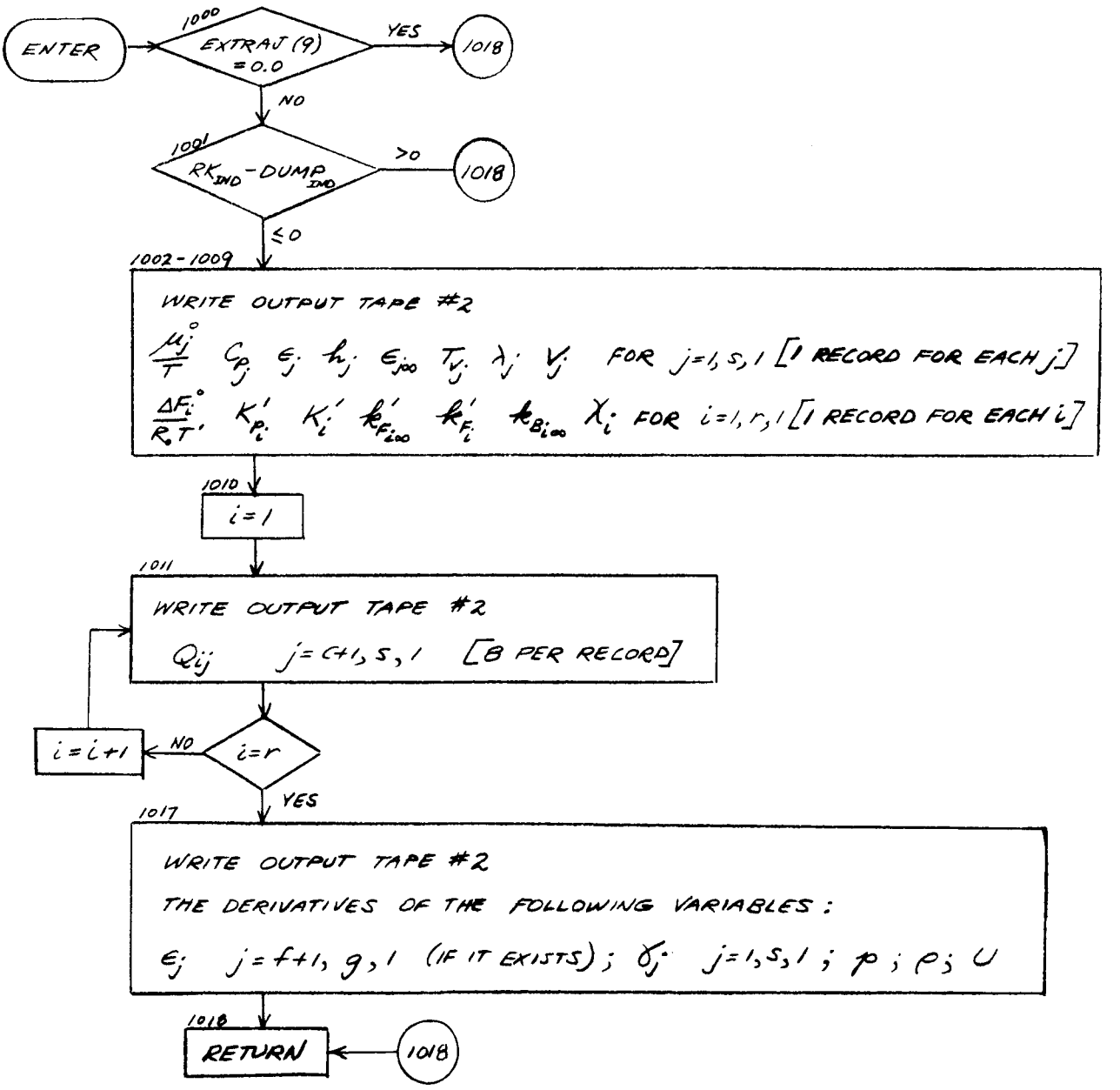
$$EEC\left(\mu_j^\circ/T; T\right) = \ln \frac{TT2}{g_{j1}}$$

$$EEC\left(C_{p_j}; T\right) = \frac{TT2 \cdot TT3 - TT1 \cdot TT1}{T^2 (TT2)^2}$$

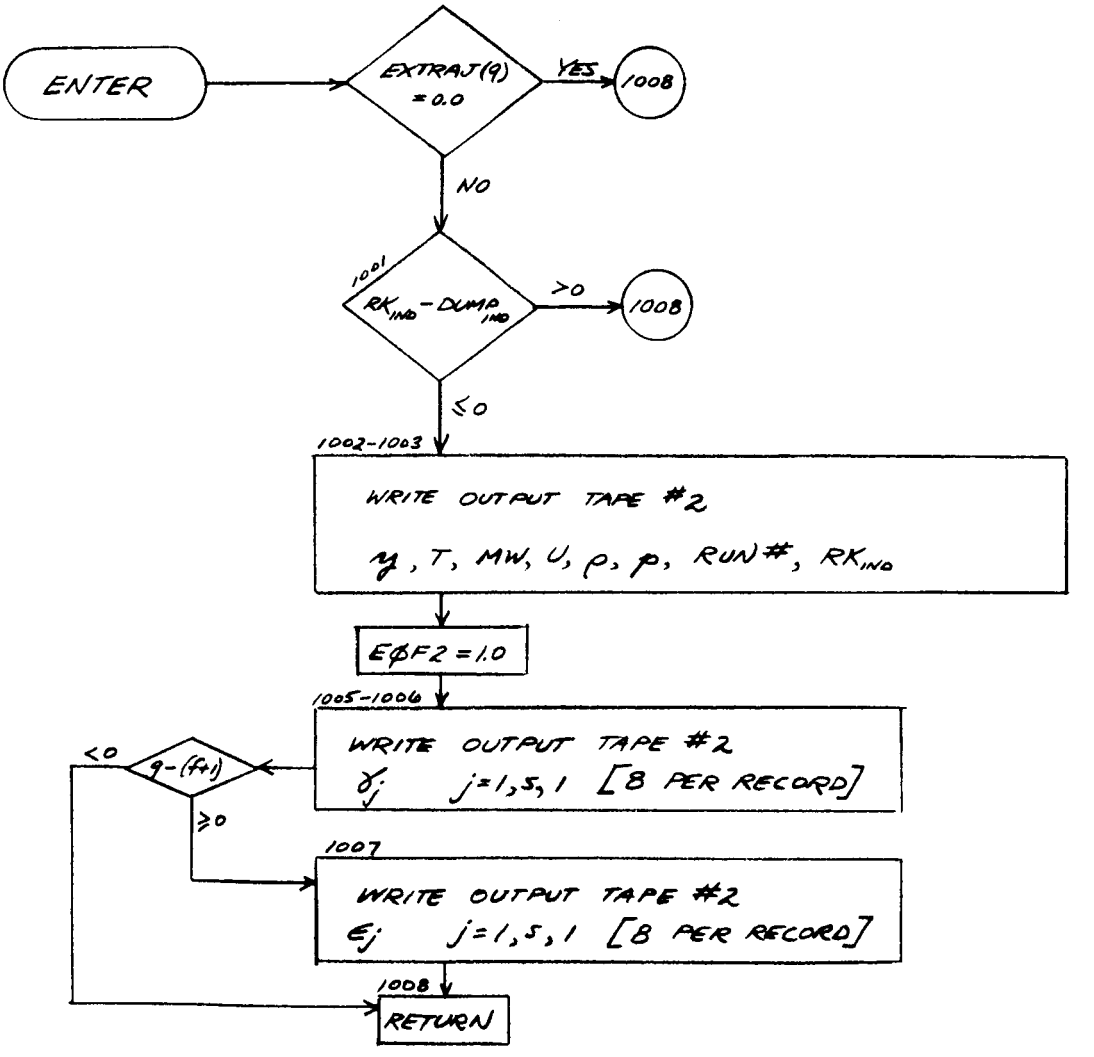
1150

RETURN

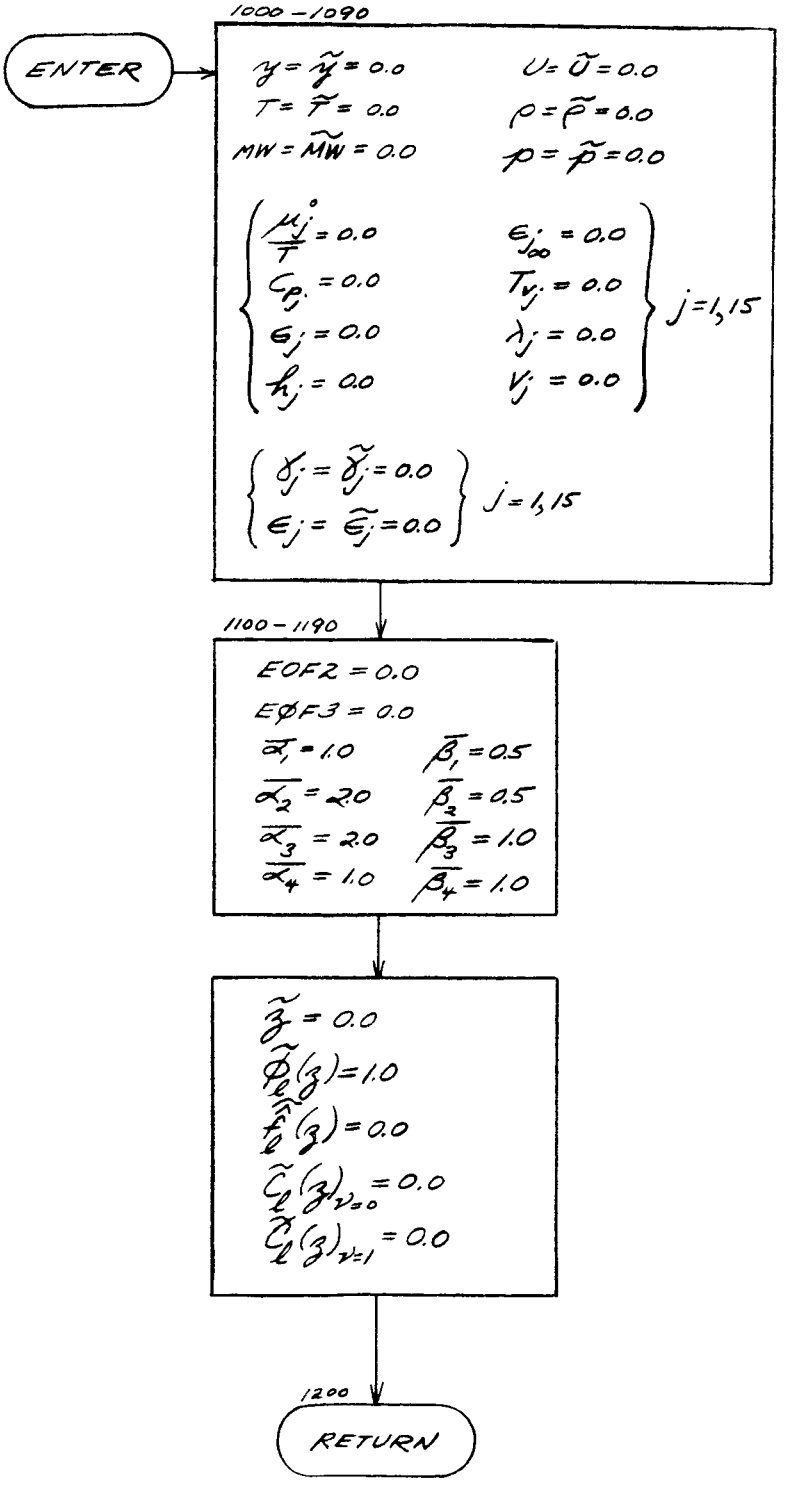
SUBROUTINE SUBS
LG11



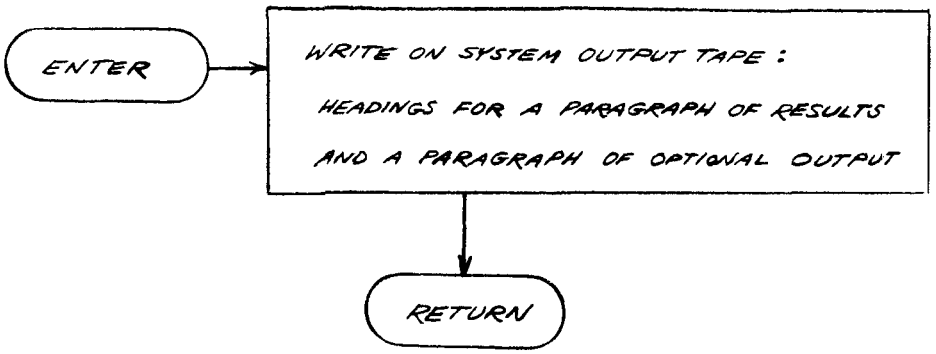
SUBROUTINE SUB1
LG-14



SUBROUTINE START
LG17



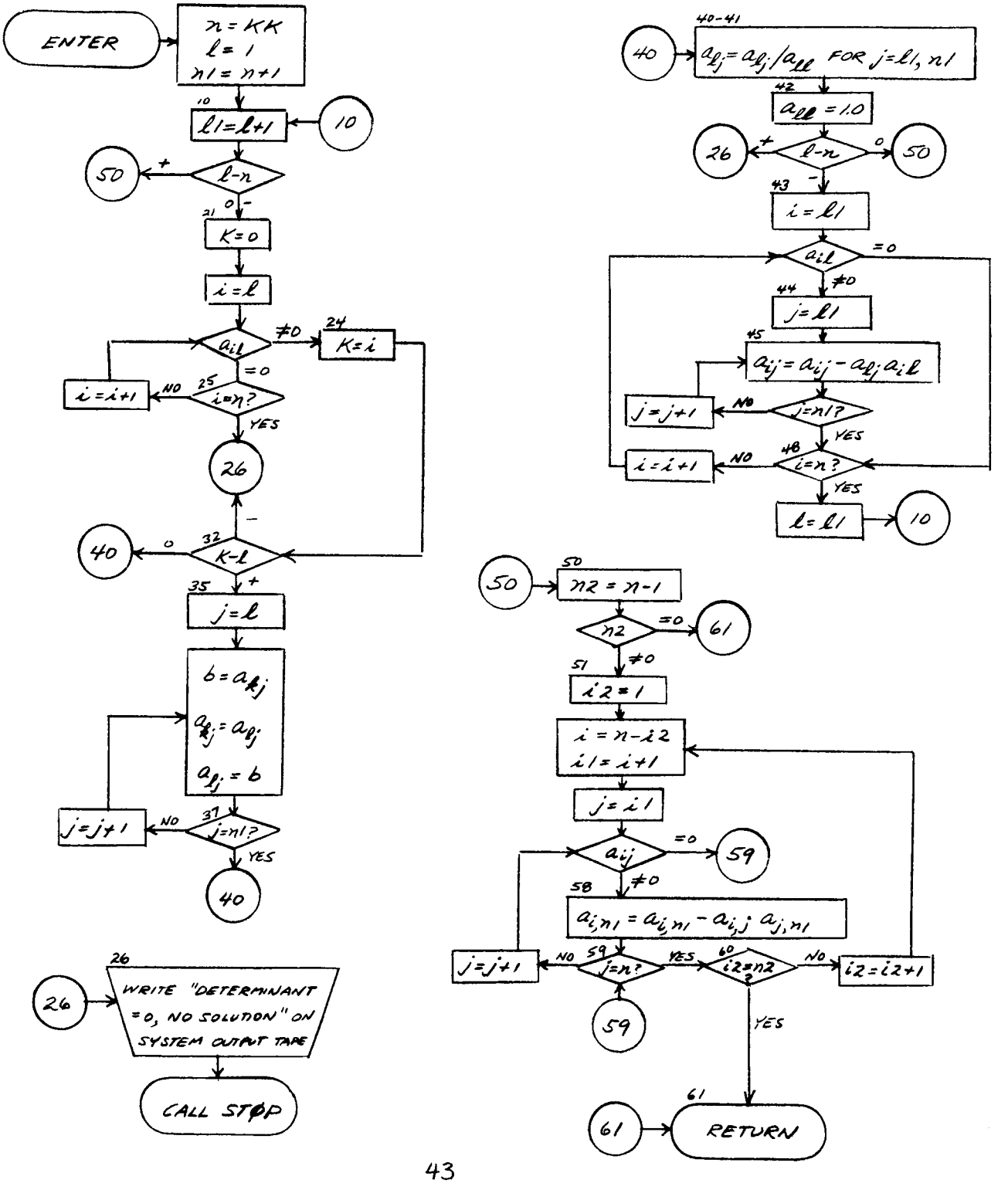
SUBROUTINE WRITE1
LG18



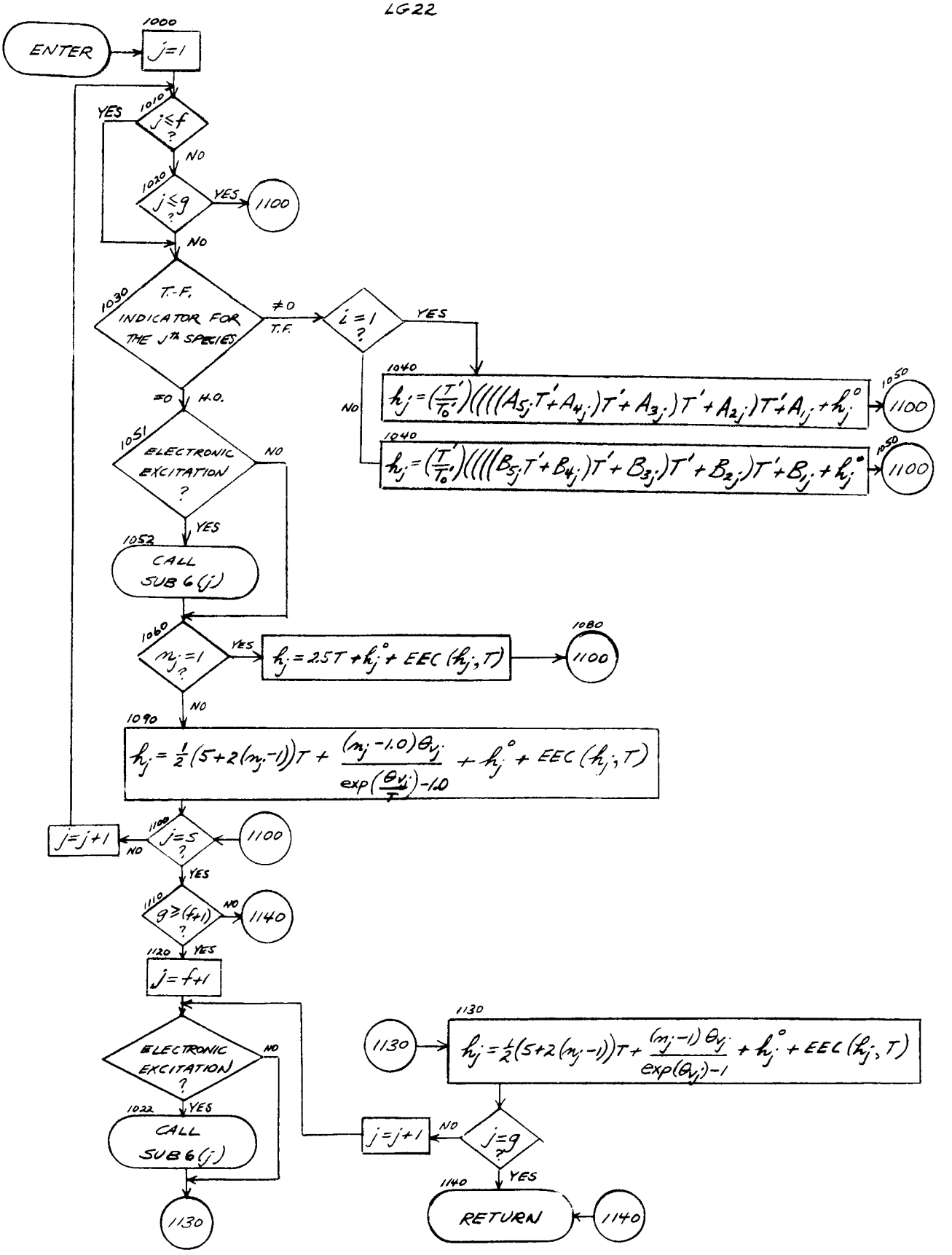
SUBROUTINE SIMSØL (A, KK, LL)

LG19

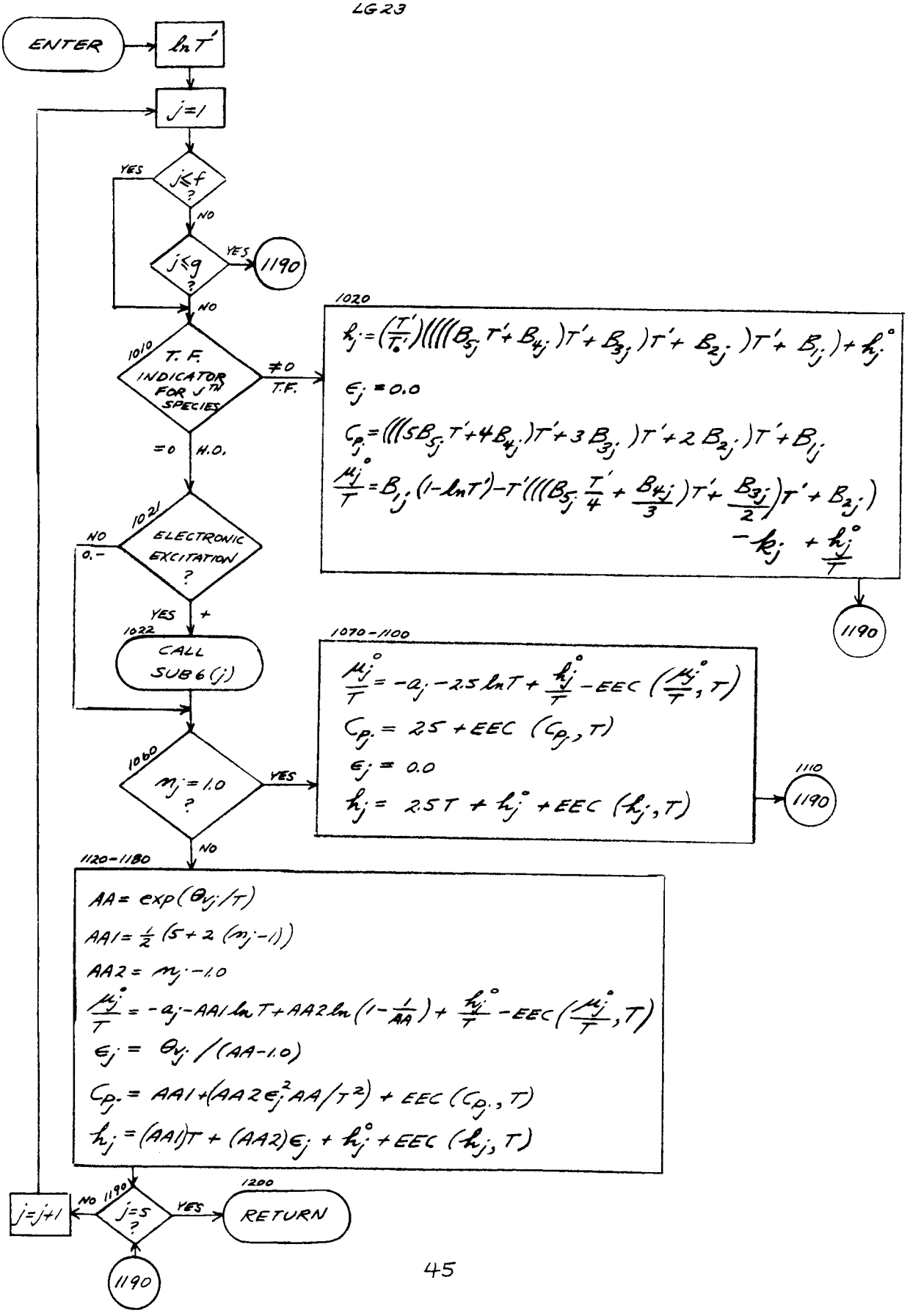
SINGLE PRECISION



SUBROUTINE SUB11 (i)
LG22



SUBROUTINE SUB12
LG23



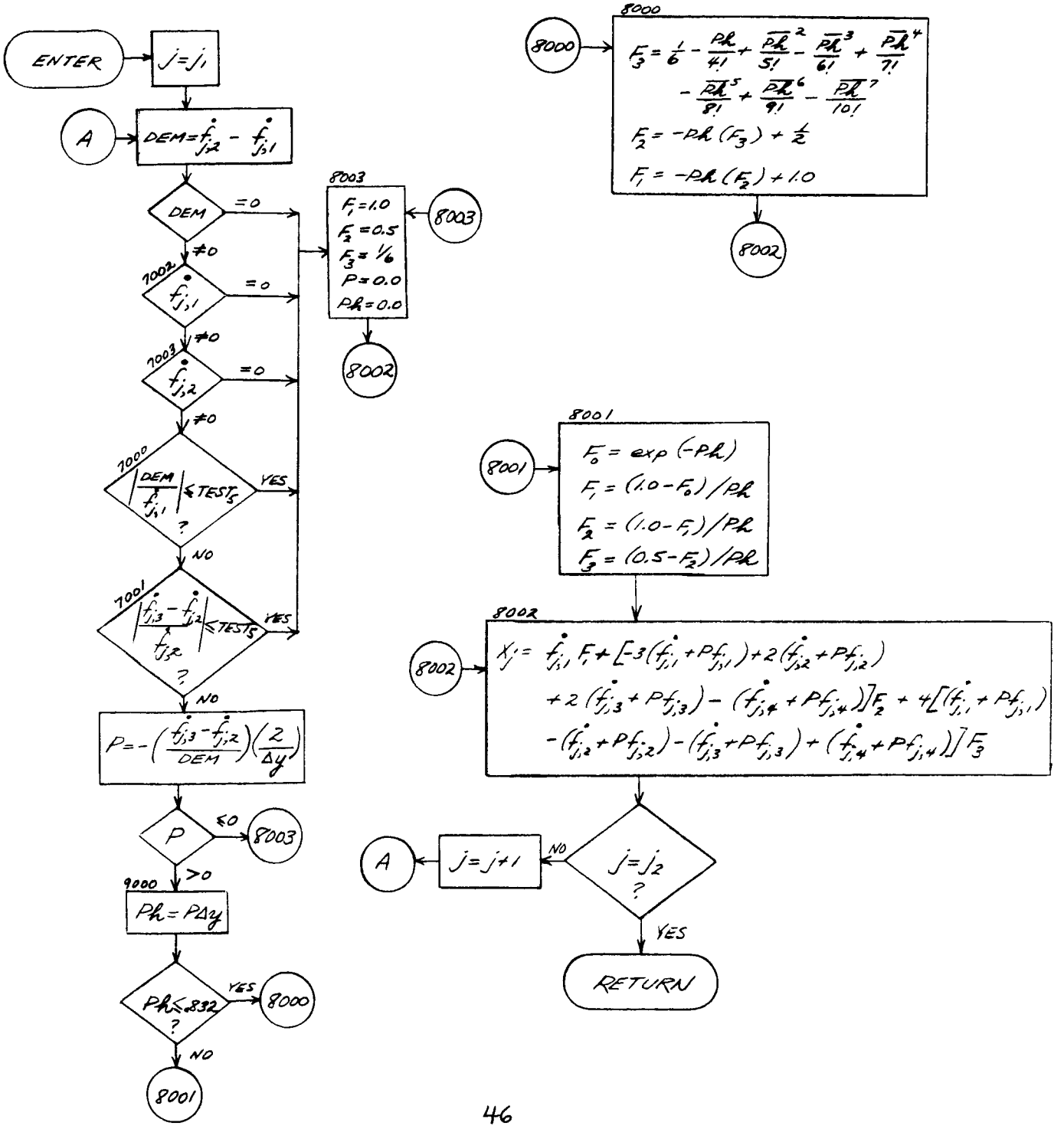
SUBROUTINE MRK $(j_1, j_2, f_{j,i}, \dot{f}_{j,i}, X_j)$
LG28

WHERE j_1, j_2 ARE THE RANGE OF THE INDEX j

$f_{j,i}$ IS THE VALUE OF THE jth VARIABLE AT THE FOUR R.K. LOCATIONS $(i=1,2,3,4)$ IN AN INTERVAL

$\dot{f}_{j,i}$ IS THE DERIVATIVE OF THE jth VARIABLE AT THE FOUR R.K. LOCATIONS $(i=1,2,3,4)$ IN AN INTERVAL

X_j IS THE INCREMENT FOR THE jth VARIABLE

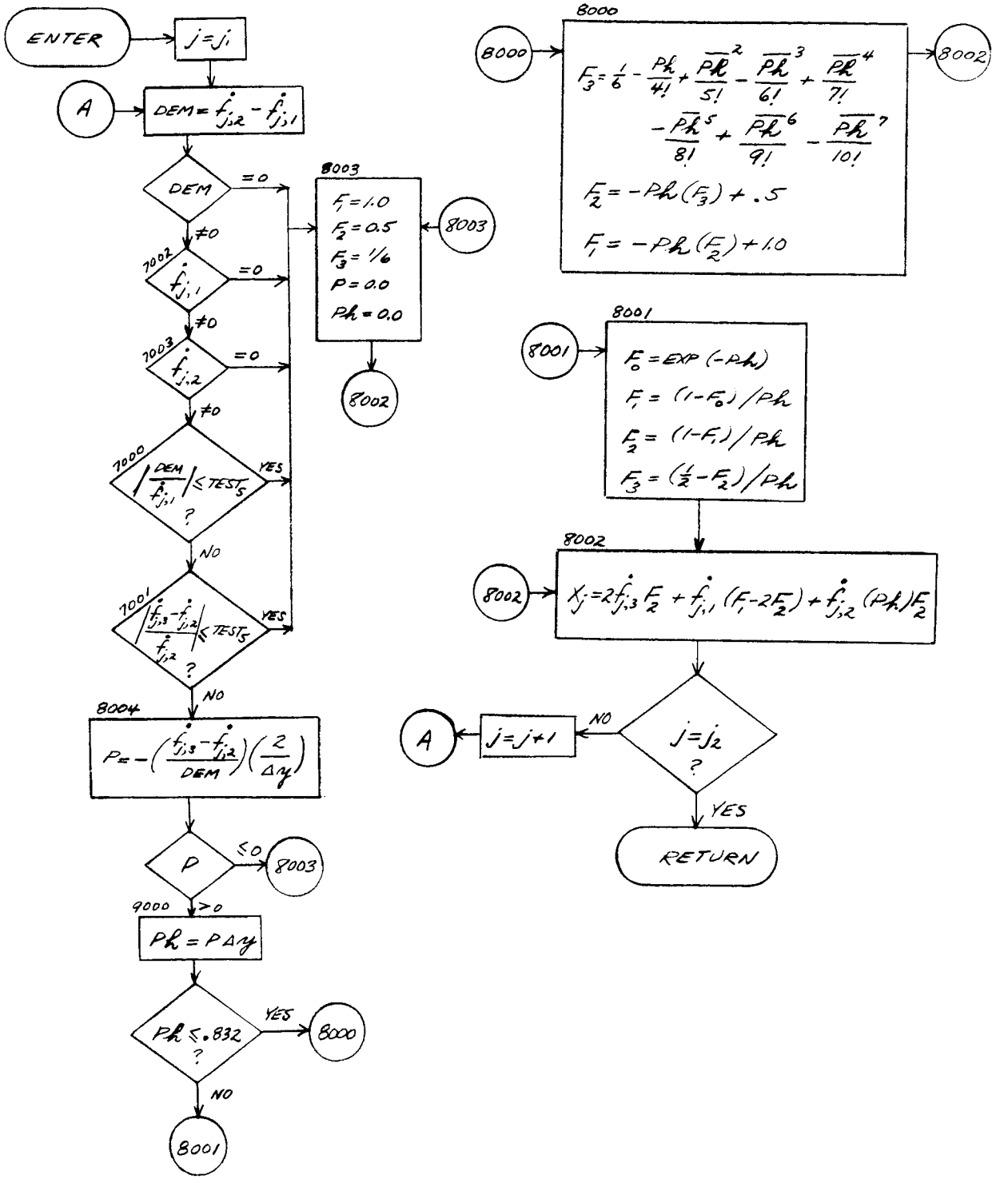


SUBROUTINE MRK1 $(j_1, j_2, \dot{f}_{j,i}, X_j)$
LG29

WHERE j_1, j_2 ARE THE RANGE OF THE INDEX j

$\dot{f}_{j,i}$ IS THE DERIVATIVE OF THE jth VARIABLE AT THE FOUR R.K. LOCATIONS $(i=1,2,3,4)$ IN AN INTERVAL

X_j IS THE INCREMENT FOR THE jth VARIABLE



APPENDIX II

CURVE-FIT PROGRAM

		Page
II. 1	INPUT DATA AND CARD FORMATS	49
II. 2	CONVERSION OF JANAF DATA	51
II. 3	CURVE-FIT PROGRAM PROCEDURE AND OUTPUT FORMAT	53

II. I INPUT DATA AND CARD FORMATS

The input format for the curve-fit program is given by Fig. 6. The first card is for the purpose of identification. The second card indicates how many data points are to be provided and the maximum temperature in the range. It also includes an indicator (NJ), which is 0 when the data on the following cards is in the form given by Eqs. (14) and (15), and 1 when the data is in the form given by the JANAF tables (see page 51). In the latter case, the value of $(\mathcal{H}_j)_{T'=0}$ must be supplied on the second card. The following cards convey the temperature, enthalpy and free energy for each data point. (When JANAF data is used directly, care should be taken to use the proper signs and units, as $\mathcal{H}$ is given in kilocalories/mole and (- $\mathcal{F}$) is tabulated.)

IF A NUMBER IS WRITTEN USING A DECIMAL POINT RATHER THAN AN EXPONENT, IT MAY BE PLACED ANYWHERE IN ITS FIELD.

	1–72	73–80
12	TITLE CARD	12A6
11	IF NJ=0, LEAVE BLANK. IF NJ=1, PUT IN $(\mathcal{H}_j)_{T=0}$ (CAL/MOLE)	MAXIMUM TEMPERATURE (°K)	NJ {0 OR 1}	NUMBER OF DATA POINTS	3E20.8, 2I6
0	TEMPERATURE (°K)	IF NJ=0, PUT IN H_j; IF NJ=1, PUT IN $\mathcal{H}_j$ (CAL/MOLE)	IF NJ=0, PUT IN F_j; IF NJ=1, PUT IN $(F-\mathcal{F}_j)$ (CAL/MOLE DEG)	3E20.8
1				
2				
3				
4				
5				
6				
7				
8				
9				

ONE CARD FOR EACH DATA POINT

Figure 6 CURVE-FIT PROGRAM: INPUT FORMAT

II. 2 CONVERSION OF JANAF DATA

Enthalpy:

The JANAF data is in the form

$$\mathcal{H} \equiv (H^{\circ} - H^{\circ}_{298})_{\substack{\text{JANAF}\\ \text{NOTATION}}} = (h'_j - h'_{j\,298})_{\substack{\text{PRESENT}\\ \text{NOTATION}}}$$

where h'_j is the static enthalpy of the jth species (calories/mole).

The thermo-fit data must be in the form

$$H = \frac{h'_j - h^{\circ\prime}_j}{R'_o T'}$$

where $h^{\circ\prime}_j$ is the heat of formation of the jth species, R'_o is the universal gas constant and T' is the temperature (°K).

Therefore

$$H = \frac{1}{R'_o T'}\left\{(h'_j - h'_{j298}) + (h_{j298} - h^{\circ\prime}_j)\right\}$$

$$= \frac{1}{R'_o T'}\left\{\mathcal{H} + (h'_{j298} - h^{\circ\prime}_j)\right\}$$

At $T' = 0$

$$H R'_o T' = 0 = (\mathcal{H})_{T'=0} + (h'_{j298} - h^{\circ\prime}_j)$$

Therefore

$$(h'_{j298} - h^{\circ\prime}_j) = -(\mathcal{H})_{T'=0}$$

and finally

$$H = \frac{1}{R'_o T'}\left\{\mathcal{H} - (\mathcal{H})_{T'=0}\right\}$$

Free Energy:

The JANAF data is in the form

$$-\mathcal{F} = -\frac{1}{T}(F^{\circ} - H^{\circ}_{298})_{\substack{\text{JANAF}\\ \text{NOTATION}}} = -\frac{1}{T'}(F^{\circ\prime}_j - h'_{j\,298})_{\substack{\text{PRESENT}\\ \text{NOTATION}}}$$

where $F^{\circ\prime}_j$ is the free energy of the jth species (calories/mole).

The thermo-fit data must be in the form

$$F = \frac{F_j^{\circ\prime} - h_j^{\circ\prime}}{R_o' T'}$$

Therefore

$$F = \frac{1}{R_o'}\left(\mathcal{F} + \frac{h_{j298}'}{T'} - \frac{h_j^{\circ\prime}}{T'}\right)$$

$$= \frac{1}{R_o'}\left[\mathcal{F} - \frac{1}{T'}(\mathcal{H})_{T'=0}\right]$$

The following table illustrates the procedure as applied to ozone;

with $R_o' = 1.98647 \frac{\text{cal}}{\text{mole - °K}}$

	k-cal / mole			cal / mole - °K		
T'(°K)	$\mathcal{H}$	$\mathcal{H} - \mathcal{H}_{T'=0}$	H	$\mathcal{F}$	$-\frac{\mathcal{H}_{T'=0}}{T'}$	F
2000	21.959	24.433	6.150	-69.413	1.237	-34.320
2500	28.959	31.433	6.329	-71.933	0.990	-35.713
3000	36.023	38.497	6.460	-74.084	0.825	-36.879

II. 3 CURVE-FIT PROGRAM PROCEDURE AND OUTPUT FORMAT

Given: T', $H(T')$, $F(T')$

(Either direct input or derived from input JANAF data)

Procedure: (Ref to Fig. 7)

1. Fit polynomial Eq. (16) to the $H(T')$ data and thus determine one set of thermo-fit coefficients, $A_{1 \rightarrow 5}$ (1st line of output, labelled "Eq. (16)").
2. Using these coefficients in Eq. (16), calculate $H(T')$ for each input value of T' (3rd column of output, labelled "H(Eq. 16)").
3. Using the same coefficients in Eq. (17), calculate $\left[F(T') + k\right]_{CALC}$ for each input value of T'
4. From the formula
   $$\left[F(T') + k\right]_{CALC} - \left[F(T')\right]_{INPUT} = k,$$
   calculate k for each input value of T' (last column of output, labelled "K")
5. Average this set of k's to get a single value to accompany $A_{1 \rightarrow 5}$ as determined in Item I above. (Last item in first line of output)
6. Using the now-completed, first set of constants (based on Eq. (16) and comprising the first line of output) in Eq. (17), calculate $F(T')$ for each input value of T' (6th column of printout, labelled "F(Eq. 16)")

7. Fit polynomial Eq. (17) to the $F(T')$ input data and thus determine a second set of thermo-fit constants, $A_{1 \rightarrow 5}$ and (2nd line of output, labelled "Eq. (17)")

8. Using this complete set of constants, calculate $F(T')$ for each input value of T' (7th column of output, labelled "F(Eq. (17)")

9. Using the same coefficients in Eq. (16), calculate $H(T')$ for each input value of T' (4th column of output, labelled "H(Eq. (17)").

TITLE

	A(1)	A(2)	A(3)	A(4)	A(5)	K	
EQ. (16)							
EQ. (17)							

TEMP	H(INPUT)	H(EQ.16)	H(EQ.17)	F(INPUT)	F(EQ.16)	F(EQ.17)	K

Figure 7 CURVE-FIT PROGRAM: OUTPUT FORMAT