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NUCLEAR EXPLOSION INTERACTION STUDIES

Volume II

Methods for Analysis of Thermal Phenomena

K. D. Pyatt, Jr., et al.

General Atomic Division
General Dynamics Corporation
Special Nuclear Effects Laboratory
San Diego, California
Contract AF 29(601)-7035

TECHNICAL REPORT NO. AFWL-TR-66-108, Vol. II

May 1967

AIR FORCE WEAPONS LABORATORY
Research and Technology Division
Air Force Systems Command
Kirtland Air Force Base
New Mexico

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FOREWORD

This report was prepared by General Atomic Division, General Dynamics Corporation, San Diego, California, under Contract AF29(601)-7035. The research was funded by DASA under Program Element 6.16.46.01D, Project 5710, Subtask 07.002, and by ARPA Order 313, Program Element 6.25.03.01.R.

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This final report on Nuclear Explosion Interaction Studies is being published in four volumes. The volume titles are as follows: Volume I, Methods for Analysis of Radiative Transfer; Volume II, Methods for Analysis of Thermal Phenomena; Volume III, Miscellaneous Code Development; and Volume IV, Phenomenology Studies (classified SECRET/RESTRICTED DATA).

The first three volumes are devoted, respectively, to theoretical studies and computer code development in radiative transfer, thermal phenomena, and miscellaneous efforts related to various other aspects of the work. The fourth volume, which is classified, contains the results of applications of these techniques, and of those previously developed, to the study of fireball growth and the interaction of laser radiation with materials.

The NEIS program is long-range, and most of the projects described in this report are in an incomplete state of development. This is due in part to the nature of the existing computer programs themselves, which continue in a state of development as long as they are in use, and in part to the time scale involved in bringing new programs to a state of capability for solving real problems.

General Atomic staff personnel contributing to the research include J.H. Alexander, C.R. Dismukes, R. Durstenfeld, R.S. Engelmores, B.E. Freeman, W.B. Lindley, J.T. Palmer, K.D. Pyatt, L.L. Reed, L.M. Schalit, J.R. Triplett, and numerous others. The cooperation of Col R.H. Pennington, Maj G.R. Spillman, Lt B.S. Chambers, III, Lt N.D. Morgan, Lt R.A. Howerton, Dr. P.V. Avizonis, and Mr. D.W. Lane of the Air Force Weapons Laboratory is gratefully acknowledged.

This report has been reviewed and is approved.


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ABSTRACT

Various analytic and numerical methods are described for the phenomena which take place when a high-energy-density source interacts with matter. The interaction usually begins with the transient heating of a solid surface for which analytical methods of study have been developed (Section I). The second phase of the interaction process is vaporization. Recent developments in numerical techniques for simulating vaporization are discussed in the context of the two-dimensional interaction code HECTIC (Section II). The third phase normally involves the nonsteady flow of ionized vapor, for which equations of state are required. A general numerical technique (EIONX) for evaluating internal energy and pressure for a given temperature and density has been developed and incorporated in the SPUTTER program (Section III). For computer programs, e.g., HECTIC, which use internal energy and density as the independent variables, numerical methods were developed to invert the equations of state generated by EIONX (Section IV). For relatively low energy-density sources, the vapor may be in a molecular phase for a significant part of the interaction process, thus requiring the development of special techniques for evaluating the molecular dissociation energy as a function of temperature and density. The calculations for one particular material--carbon--are discussed in detail (Section V).

(Distribution Limitation Statement No. 2)

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SECTION I

HEATING OF A SLAB BY A TIME-DEPENDENT SOURCE

1.1. INTRODUCTION

Analytic solutions of the heat conduction equation may often be used to advantage in the study of interaction phenomena (Ref. 1). Although the analytic treatment must in general neglect both temperature and position dependence of the thermal parameters of the material medium, it is at least not subject to the limitations of accuracy and stability which are encountered in the use of difference equations. The analytic method therefore serves both as a useful guide to the improvement of difference-equation methods and as a convenient check on the validity of particular computational results obtained by use of difference techniques.

1.2. SPECIFICATION OF THE HEAT CONDUCTION PROBLEM

In a typical interaction problem, a semi-infinite region $x > 0$ is occupied by a solid material which is heated by radiation incident upon its surface. The intensity of this source radiation will be denoted by $\dot{E}(t)$ ergs/cm²/sec, a defined function of time $t > 0$. The present discussion is concerned with the general problem of a source intensity which varies continuously with time. This entire class of problem is definitively treated by Carslaw and Jaeger (Ref. 2).

The absolute temperature of the material medium at position x , time t will be denoted by $T(x, t)$. The material parameters (assumed constant) are given by:

C = Specific heat,

ρ = Density,

- k = Thermal conductivity,
 $\alpha = \frac{k}{C\rho}$, Thermal diffusivity,
 T_B = Absolute temperature of fusion or sublimation,
 κ_L = Mass absorption coefficient for source radiation,
 $a = \rho\kappa_L$, Volumetric absorption coefficient for source radiation,
 R = Surface reflectivity for source radiation,
 ϵ = Total emissivity of surface.

In addition, T_0 denotes the initial absolute temperature of the material, T_A denotes the effective blackbody temperature of the external region ($x < 0$), and σ is the Stefan-Boltzmann constant.

The surface fluxes associated with source radiation, thermal radiation, and conduction, are, respectively,

$$\varphi_S(0, t) = (1 - R)\dot{E}(t) \quad (1)$$

$$\varphi_T(0, t) = -\epsilon\sigma \left[T(0, t)^4 - T_A^4 \right] \quad (2)$$

$$\varphi_C(0, t) = -k \left. \frac{\partial T}{\partial x} \right|_{x=0} \quad (3)$$

The general boundary condition for the heat conduction problem is

$$-\varphi_T(0, t) + \varphi_C(0, t) = \varphi_S(0, t) \quad (4)$$

Within the solid material, account will be taken of the conductive and source fluxes only, since the measured values of conductivity presumably include a first order contribution from radiative diffusion, and the high order contributions are presumably not more significant than the temperature dependence of the conductivity which is being ignored. If the attenuation of the source flux within the material can be described by a single coefficient a , as in the case of a laser source,

$$\varphi_S(x, t) = (1 - R)\dot{E}(t) e^{-ax} \quad (5)$$

The heat conduction equation is then

$$\frac{\partial \varphi_C}{\partial x} + \frac{\partial \varphi_S}{\partial x} + \rho C \frac{\partial T}{\partial t} = 0 \quad (6)$$

or

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha} \frac{\partial T}{\partial t} = - (1 - R) \frac{a}{k} \dot{E}(t) e^{-ax} \quad (7)$$

The initial condition

$$T(x, 0) = T_0, \quad x > 0 \quad (8)$$

then completes the specification of the problem.

1.3. EXAMPLE: HEATING OF A METALLIC SLAB BY A PULSED SOURCE

In a medium with relatively high conductivity and low transparency for source radiation, the conductive flux will dominate not only the thermal radiative flux at the surface but also the source flux inside the medium; i. e., at times of interest the characteristic depth of the conductive front $\sqrt{\alpha t}$ will be large compared with the characteristic depth of penetration of the source radiation $1/a$. The equation to be solved is then the homogeneous heat transfer equation

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha} \frac{\partial T}{\partial t} = 0, \quad x > 0, t > 0 \quad (9)$$

with boundary condition

$$-k \left. \frac{\partial T}{\partial x} \right|_{x=0} = (1 - R) \dot{E}(t), \quad t > 0 \quad (10)$$

and initial condition (8).

We note first that, with the aid of Duhamel's Theorem, this problem can be reduced to a simpler problem in which the boundary condition is that the flux be a constant. That is, let

$$T(x, t) = \frac{\partial}{\partial t} \int_0^t \theta(x, t - t_0, t_0) dt_0 \quad (11)$$

Then $\theta(x, t, t_0)$ is a solution of the equation

$$\frac{\partial^2 \theta}{\partial x^2} - \frac{1}{\alpha} \frac{\partial \theta}{\partial t} = 0 \quad (12)$$

with

$$-k \left. \frac{\partial \theta}{\partial x} \right|_{x=0} = (1 - R) \dot{E}(t_0) \quad (13)$$

and

$$\theta(x, 0, t_0) = T_0 \quad (14)$$

Assume a solution of form

$$\theta = C_0 t^{n/2} f_n \left(\frac{x}{\sqrt{4\alpha t}} \right) + T_0 \quad (15)$$

Then, from Eq. (12), $f_n(z)$ must be a solution of the equation

$$\frac{d^2 f}{dz^2} + 2z \frac{df}{dz} - 2n f = 0 \quad (16)$$

or

$$f_n(z) = i^n \operatorname{erfc}(z) \quad (17)$$

where the functions $i^n \operatorname{erfc}(z)$ satisfy the relations

$$i^n \operatorname{erfc}(z) = \int_z^\infty i^{n-1} \operatorname{erfc}(s) ds \quad (18)$$

$$i^{-1} \operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} e^{-z^2} \quad (19)$$

$$2n i^n \operatorname{erfc}(z) = i^{n-2} \operatorname{erfc}(z) - 2z i^{n-1} \operatorname{erfc}(z) \quad (20)$$

$$i^n \operatorname{erfc}(0) = \frac{1}{2^n \Gamma\left(\frac{n}{2} + 1\right)} \quad (21)$$

The functions $i^0 \text{erfc}$ and $i^1 \text{erfc}$ are written as erfc and ierfc , respectively. On imposing the condition (13), one notes first that $n = 1$, and also that

$$-k \frac{C_0}{\sqrt{4\alpha}} f_1'(0) = (1 - R) \dot{E}(t_0) \quad (22)$$

or, using Eqs. (18) and (21) to show that $f_1'(0) = -1$,

$$\theta(x, t, t_0) = \frac{2}{\sqrt{kC\rho}} (1 - R) \dot{E}(t_0) t^{1/2} \text{ierfc}\left(\frac{x}{\sqrt{4\alpha t}}\right) + T_0 \quad (23)$$

From Duhamel's Theorem, Eq. (11), and using also Eqs. (20) and (19),

$$\begin{aligned} T(x, t) &= \frac{2(1 - R)}{\sqrt{kC\rho}} \frac{\partial}{\partial t} \int_0^t \dot{E}(t_0) (t - t_0)^{1/2} \text{ierfc}\left[\frac{x}{\sqrt{4\alpha(t - t_0)}}\right] dt_0 + T_0 \\ &= \frac{1 - R}{\sqrt{kC\rho}} \int_0^t \frac{\dot{E}(t_0)}{\sqrt{t - t_0}} \left[\text{ierfc}\left(\frac{x}{\sqrt{4\alpha(t - t_0)}}\right) + \right. \\ &\quad \left. \frac{x}{\sqrt{4\alpha(t - t_0)}} \text{erfc}\left(\frac{x}{\sqrt{4\alpha(t - t_0)}}\right) \right] dt_0 + T_0 \\ &= \frac{1 - R}{\sqrt{rkC\rho}} \int_0^t \frac{\dot{E}(t_0)}{\sqrt{t - t_0}} e^{-[x^2/4\alpha(t - t_0)]} dt_0 + T_0 \quad (24) \end{aligned}$$

A pulse shape $\dot{E}(t)$ which has been found useful is

$$\begin{aligned} \dot{E}(t) &= \frac{(m + 1) E}{2t_1^{m+1}} t^m, & 0 < t < t_1 \\ &= \frac{(m + 1) E}{2t_1^{m+1}} (2t_1 - t)^m, & t_1 < t < 2t_1 \\ &= 0 & t > 2t_1 \end{aligned} \quad (25)$$

That is, $\dot{E}$ rises as the m^{th} power of the time to a maximum at time t_1 , then decreases in a symmetric manner to zero at time $2t_1$. The width of the pulse at half maximum, Δ , is given by

$$\Delta = 2(1 - 2^{-1/m}) t_1$$

The constant E is the time integral of $\dot{E}$ over the entire pulse, in ergs/cm^2 .

An explicit solution is readily derived for the time interval $0 < t < t_1$, the rising portion of the pulse. In general, for

$$\dot{E}(t) = At^{n/2} \quad (26)$$

where n is an integer not less than -1 ,

$$T(x, t) = T_0 + A(1-R) (k\rho C)^{-1/2} \Gamma(\frac{1}{2}n + 1) (4t)^{\frac{1}{2}n + \frac{1}{2}} i^{n+1} \text{erfc} \frac{x}{\sqrt{4\alpha t}} \quad (27)$$

The surface temperature is given by

$$T(0, t) = T_0 + A(1 - R) (\pi k \rho C)^{-\frac{1}{2}} B(\frac{1}{2}n + 1, \frac{1}{2}) t^{\frac{1}{2}n + \frac{1}{2}} \quad (28)$$

where $B(p, q) = \Gamma(p) \Gamma(q) / \Gamma(p + q)$ is the beta function.

Returning to the pulse shape, Eq. (25), the surface temperature may be obtained by substituting Eq. (25) into Eq. (24), setting $x = 0$, and evaluating the integrals; for $m = 4$,

$$T(0, t) = T_0 + (\pi k \rho C)^{-\frac{1}{2}} (1 - R) At_1^{9/2} I(s) \quad (29)$$

where $s = t/t_1$

$$\begin{aligned} I(s) &= \int_0^s \dot{E}(\sigma) (s - \sigma)^{-\frac{1}{2}} d\sigma \\ &= \frac{256}{315} s^{9/2} - \frac{32}{105} (s - 1)^{3/2} (24s^2 - 48s + 59) H(s-1) \\ &\quad - \frac{256}{315} (s-2)^{9/2} H(s-2) \end{aligned} \quad (30)$$

$$H(x) = 0, \quad x < 0$$

$$= 1, \quad x \geq 0$$

and

$$A = \frac{(m+1)E}{2t_1^{m+1}} = \frac{5E}{2t_1^5}$$

The dimensionless quantities

$$I(s) = \frac{(\pi k \rho C)^{\frac{1}{2}}}{(1-R)At_1^{9/2}} \left[T(0,t) - T_0 \right] \text{ and } \frac{\dot{E}(s)}{At_1^4}$$

are plotted as functions of s in Fig. 1. The temperature rises as the $9/2$ power of the time from $t = 0$ to $t = t_1$ and reaches a maximum at approximately $1.10 t_1$. This result has been closely reproduced by difference equation solutions to the heat conduction equation.

1.4. THE RADIATION BOUNDARY CONDITION

If the temperature of the surface of the target becomes sufficiently high before sublimation or melting occurs, the blackbody radiation from the surface can no longer be neglected. In the transient regime this radiation condition can become of major importance for the case of refractory non-metal targets (for a good conductor the conductive flux would still overwhelmingly predominate) when the total energy delivered by the source is near the ablation threshold.

We consider again the homogeneous problem (Eq. (9)) in which the source deposition is assumed to occur only at the surface. The boundary condition is, from Eq. (4),

$$-k \frac{\partial T}{\partial x} \Big|_{x=0} + \epsilon \sigma \left[T(0,t)^4 - T_A^4 \right] = (1-R) \dot{E}(t) \quad (31)$$

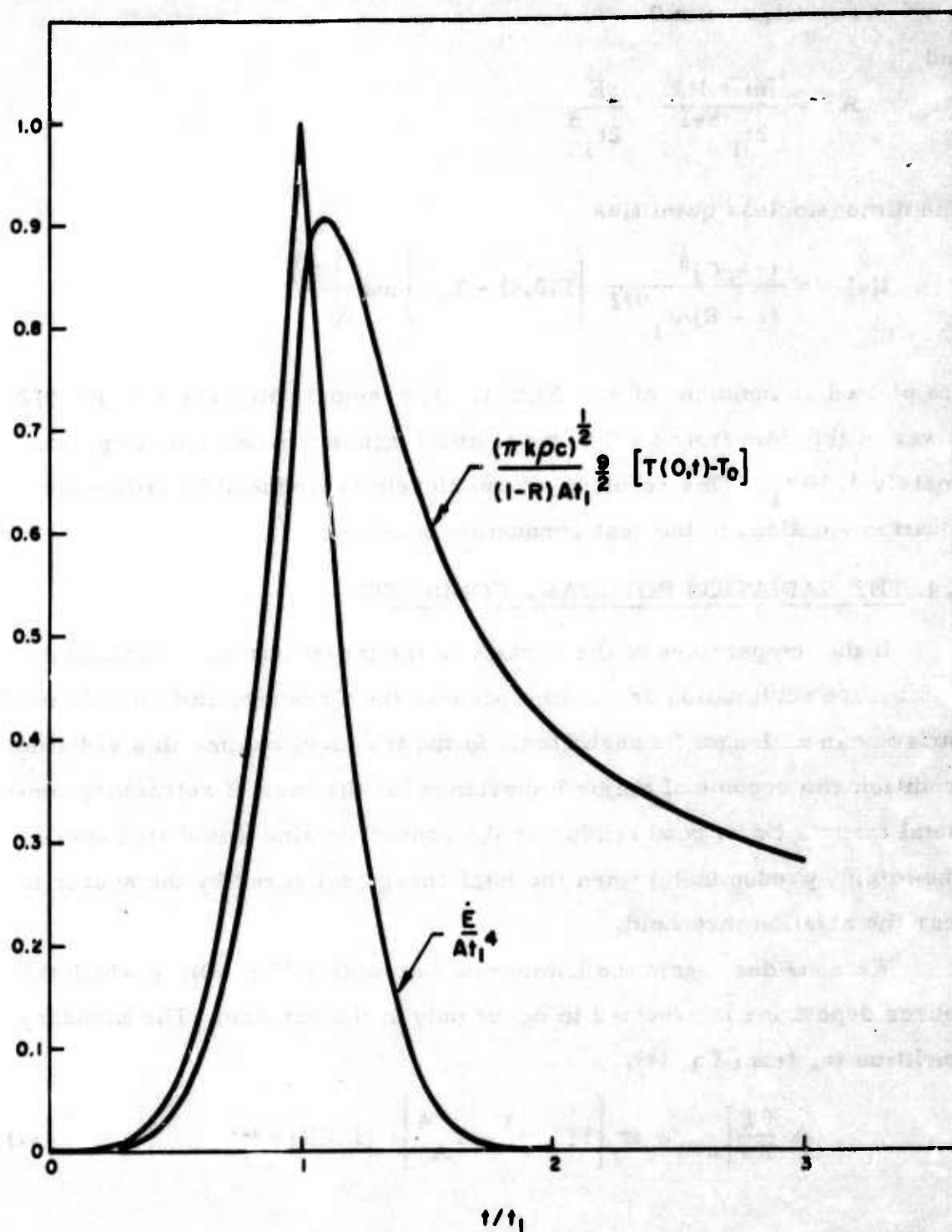


Figure 1. Relative Temperature and Source Intensity versus Time (Dimensionless Plot)

Since this condition is nonlinear in T , some artifice must be employed in order to obtain a solution. Two will be considered:

1. Implicit solution.
2. Linearization.

Linearization is appropriate when the total change of surface temperature during the time of interest is relatively small. However, for refractory materials, which can be heated over a large temperature range, this assumption is not always particularly good. An implicit method which solves the problem with the exact nonlinear boundary condition will therefore be described first. The method is essentially that of Jaeger (Ref. 3).

Assume that $T(0, t)$, $T(0, t)^4$, and $E(t)$ may all be expanded in powers of the variable $z = t^{1/2}$:

$$T(0, t) = T_0 \sum_{n=0}^{\infty} \frac{f_n}{n!} t^{n/2} \equiv T_0 f(z) \quad (32)$$

$$T(0, t)^4 = T_0^4 \sum_{n=0}^{\infty} \frac{g_n}{n!} t^{n/2} \equiv T_0^4 g(z) \quad (33)$$

$$E(t) = A \sum_{n=0}^{\infty} \frac{h_n}{n!} t^{n/2} \quad (34)$$

The application of the initial condition (8) then provides at once

$$f_0 = 1 \quad \text{and} \quad g_0 = 1 \quad (35)$$

The first step in the solution is the derivation of the relations between the g_n and the f_n . Since $g(z) = f(z)^4$,

$$f(z)g'(z) - 4f'(z)g(z) = 0 \quad (36)$$

Differentiating Eq. (36) n times, setting $z = 0$, and noting that $f^{(r)}(0) = f_r$, $g^{(r)}(0) = g_r$, one obtains

$$\sum_{r=0}^n \binom{n}{r} (f_r g_{n-r+1} - 4f_{r+1} g_{n-r}) = 0 \quad (37)$$

Equations (35) and (37) may readily be solved explicitly for the g_n :

$$\begin{aligned} g_0 &= 1 \\ g_1 &= 4f_1 \\ g_2 &= 12f_1^2 + 4f_2 \\ &\text{etc.} \end{aligned} \quad (38)$$

The second step is the solution of the heat conduction equation (9) for the temperature $T_n(x, t)$ when the surface value is a prescribed function of time: $T_n(0, t) = V_n t^{n/2}$, where $V_n = T_0^n / n!$. The Laplace transform of Eq. (9) may be written

$$\frac{d^2 S}{dx^2} - q^2 S = 0, \quad x > 0 \quad (39)$$

where

$$S(x) = \int_0^\infty T_n(x, t) e^{-pt} dt \quad (40)$$

and

$$q^2 = p/\alpha \quad (41)$$

The boundary condition at $x = 0$ is that S shall be the transform of $V_n t^{n/2}$, namely,

$$S(0) = V_n \Gamma(1 + n/2) p^{-1-n/2} \quad (42)$$

The solution of Eq. (39) which satisfies this condition and is regular at infinity is

$$S(x) = S(0) e^{-qx} \quad (43)$$

The inverse transformation then yields the desired result for the temperature:

$$T_n(x, t) = V_n \Gamma(1 + n/2) (4t)^{n/2} i^n \operatorname{erfc}\left(\frac{x}{\sqrt{4\alpha t}}\right) \quad (44)$$

Linear superposition of the contributions given by Eq. (44) for each n , as in Eq. (32), then yields the complete solution $T(x, t)$:

$$T(x, t) = T_0 \left[1 + \sum_{n=1}^{\infty} \frac{f_n}{n!} \Gamma(1 + n/2) (4t)^{n/2} \operatorname{erfc} \left(\frac{x}{\sqrt{4\alpha t}} \right) \right] \quad (45)$$

It remains to determine the coefficients f_n using the boundary condition (31). The conductive flux at the surface is, from Eqs. (18), (21), and (45),

$$\begin{aligned} -k \frac{\partial T}{\partial x} \Big|_{x=0} &= k\alpha^{-1/2} T_0 \sum_{n=1}^{\infty} \frac{\Gamma(1 + n/2)}{n! \Gamma(1/2 + n/2)} f_n t^{(n-1)/2} \\ &= k\alpha^{-1/2} T_0 \sum_{n=0}^{\infty} \frac{\Gamma\left(\frac{3}{2} + \frac{n}{2}\right)}{(n+1)! \Gamma(1 + n/2)} f_{n+1} t^{n/2} \end{aligned} \quad (46)$$

Substituting Eqs. (46), (33), and (34) into Eq. (31), one finds for $n = 0$

$$k\alpha^{-1/2} T_0 \frac{\sqrt{\pi}}{2} f_1 + \epsilon\sigma(T_0^4 - T_A^4) = (1 - R) Ah_0 \quad (47)$$

and for $n > 0$

$$k\alpha^{-1/2} T_0 \frac{\Gamma\left(\frac{3}{2} + \frac{n}{2}\right)}{(n+1)! \Gamma(1 + n/2)} f_{n+1} + \epsilon\sigma T_0^4 g_n = (1 - R) Ah_n$$

or for $n \geq 2$

$$k\alpha^{-1/2} T_0 \frac{\Gamma\left(1 + \frac{n}{2}\right)}{n! \Gamma\left(\frac{1}{2} + \frac{n}{2}\right)} f_n = (1 - R) Ah_{n-1} - \epsilon\sigma T_0^4 g_{n-1} \quad (48)$$

The solution, Eq. (45), is thus completely specified. With the coefficients h_n given, one finds first f_1 from Eq. (47), then g_1 from Eq. (38), f_2 from Eq. (48), g_2 from Eq. (38), etc.

An alternative approach to the above is to specify a linearized radiation boundary condition in place of Eq. (31):

$$- \frac{\partial T}{\partial x} \Big|_{x=0} + h [T(0, t) - T_A] = \frac{1 - R}{k} \dot{E}(t) \quad (49)$$

where in some sense

$$h(T - T_A) \sim \frac{\epsilon\sigma}{k} (T^4 - T_A^4) \quad (50)$$

is an adequate approximation for the problem at hand. For problems in which $|T(0, t) - T_A|/T_A \ll 1$ at all times of interest, a good fit is obtained by defining

$$h = h_1 = 4 \epsilon \sigma T_A^3 / k \quad (51)$$

Equation (51) underestimates the radiative cooling rate for $T(0, t) > T_A$. A second alternative is

$$h = h_2 = \frac{\epsilon \sigma}{k} (T_B^4 - T_A^4) / (T_B - T_A) \quad (52)$$

which is correct for $T(0, t) = T_A$ and $T(0, t) = T_B$, but overestimates the cooling rate at all intermediate temperatures. A third alternative, intermediate between h_1 and h_2 in value, is defined by

$$h = h_3 = \frac{\epsilon \sigma}{k} \left[\frac{2}{5} (T_B - T_A)^3 + 2T_A (T_B - T_A)^2 + 4T_A^2 (T_B - T_A) + 4T_A^3 \right] \quad (53)$$

This yields the correct total radiated energy between $T = T_A$ and $T = T_B$, if $T(0, t)$ is a linear function of the time; in this sense it gives an approximately correct mean cooling rate over this interval.

With the initial condition

$$T_0 = T(x, 0) = T_A \quad (54)$$

and the boundary condition (49), the general solution is

$$T(x, t) - T_A = \frac{2}{\sqrt{\pi}} (1 - R) \int_0^\infty e^{-hy} dy \int_{\frac{x-y}{\sqrt{4\alpha t}}}^\infty \dot{E} \left(t - \frac{(x+y)^2}{4\alpha z^2} \right) e^{-z^2} dz \quad (55)$$

(see Ref. 2, p. 74). Other formulas involving the linearized radiation boundary condition are presented in the following section.

1.5. INTERNAL SOURCE DEPOSITION

We consider next the case in which the depth of penetration of the source radiation is not negligible; i. e., at times of interest $\sqrt{\alpha t}$ is not large compared with $1/a$. The source flux must then appear in the differential

equation rather than in the boundary condition. For simplicity, we adopt the initial condition (54) and define $\theta(x, t) = T(x, t) - T_0$. Then the equation to be solved is (7), or in the present notation,

$$\frac{\partial \theta}{\partial t} - \alpha \frac{\partial^2 \theta}{\partial x^2} = (1 - R) \frac{a\alpha}{k} \dot{E}(t) e^{-ax}, \quad x > 0 \quad (56)$$

with the linearized radiation boundary condition

$$\frac{\partial \theta}{\partial x} = h\theta, \quad x = 0 \quad (57)$$

and initial condition

$$\theta(x, 0) = 0 \quad (58)$$

The general solution of this problem may be written in the form

$$\theta(x, t) = (1 - R) \frac{a\alpha}{k} \int_0^t dt_0 \dot{E}(t_0) \int_0^\infty dx_0 e^{-ax_0} G(x, t | x_0, t_0) \quad (59)$$

where $G(x, t | x_0, t_0)$ is the temperature rise at x, t due to a unit source at $x_0, t_0 < t$. Several forms of this Green's function may be written, the choice being one of computational convenience. We introduce first the infinite medium heat conduction kernel

$$U(x, t | x_0, t_0) = \frac{1}{\pi} \int_0^\infty e^{-\beta^2 \alpha (t - t_0)} \cos \beta (x - x_0) d\beta \quad (60a)$$

$$= \left[4\pi\alpha(t - t_0) \right]^{1/2} \exp \left[-\frac{(x - x_0)^2}{4\alpha(t - t_0)} \right] \quad (60b)$$

which satisfies the equation

$$\frac{\partial U}{\partial t} - \alpha \frac{\partial^2 U}{\partial x^2} = 0, \quad -\infty < x < \infty, \quad t > t_0$$

with initial condition

$$U(x, t_0 | x_0, t_0) = \delta(x - x_0)$$

and

$$U \rightarrow 0 \text{ as } |x| \rightarrow \infty \text{ and as } t \rightarrow +\infty$$

This kernel is itself the Green's function for the infinite medium. For our semi-infinite medium, the Green's function may be found by the method of images (Ref. 4):

$$G(x, t | x_0, t_0) = U(x, t | x_0, t_0) + U(x, t | -x_0, t_0) - 2h \int_{-\infty}^{-x_0} U(x, t | y, t_0) e^{h(x_0+y)} dy \quad (61)$$

$$= \frac{1}{\pi} \int_0^\infty d\beta e^{-\beta^2 \alpha(t-t_0)} \left[\cos \beta(x - x_0) + \cos \beta(x + x_0) - 2h \int_{x_0}^\infty e^{-h(y-x_0)} \cos \beta(x+y) dy \right] \quad (62)$$

$$= \left[4\pi\alpha(t-t_0) \right]^{-1/2} \left\{ \exp \left[-\frac{(x-x_0)^2}{4\alpha(t-t_0)} \right] + \exp \left[-\frac{(x+x_0)^2}{4\alpha(t-t_0)} \right] - 2he^{hx_0} \int_{x_0}^\infty dy \exp \left[-hy - \frac{(x+y)^2}{4\alpha(t-t_0)} \right] \right\} \quad (63)$$

$$= \left[4\pi\alpha(t-t_0) \right]^{-1/2} \left\{ \exp \left[-\frac{(x-x_0)^2}{4\alpha(t-t_0)} \right] + \exp \left[-\frac{(x+x_0)^2}{4\alpha(t-t_0)} \right] - h \exp \left[h(x+x_0) + h^2\alpha(t-t_0) \right] \operatorname{erfc} \left[\frac{x+x_0 + 2h\alpha(t-t_0)}{\sqrt{4\alpha(t-t_0)}} \right] \right\} \quad (64)$$

Equation (59) has the form of a Laplace convolution, so that if the Laplace transforms of $\theta(t)$, $\dot{E}(t)$, and $G(t-t_0)$ are denoted, respectively, by $\theta(p)$, $\bar{E}(p)$, and $\bar{G}(p)$, then

$$\bar{\theta}(x, p) = (1 - R) \frac{a\alpha}{k} \bar{E}(p) \int_0^\infty \bar{G}(p) e^{-ax_0} dx_0 \quad (65)$$

The transform of the Green's function is

$$\bar{G}(p) = \frac{1}{2\alpha q} \left(e^{-|x-x_0|q} + e^{-(x+x_0)q} \right) - \frac{he^{-(x+x_0)q}}{\alpha q(q+h)} \quad (66)$$

where $q^2 = p/\alpha$ as before. Therefore,

$$\int_0^\infty dx_0 e^{-ax_0} \bar{G}(p) = \frac{pe^{-ax} - a\alpha q e^{-qx}}{p^2 - a^2\alpha p} - \frac{he^{-qx}}{\alpha q [q^2 + (h+a)q + ha]} \quad (67)$$

and the general result is thus

$$\theta(x, t) = (1-R) \frac{a}{2\pi ik} \int_{c-i\infty}^{c+i\infty} dp \bar{E}(p) e^{pt} \left[-\frac{ae^{-qx}}{q(q^2 - a^2)} - \frac{he^{-qx}}{q(q+h)(q+a)} \right] \quad (68)$$

Although this expression involves only a single quadrature, it is not necessarily easier to evaluate than (59), even when $h = 0$. Numerical methods based upon either form are certainly possible and are worth investigating.

1.6. CONCLUSIONS

The analytic approach offers some significant advantages over purely numerical methods of solving difference equations representing the flow of heat. It is not subject to numerical instability difficulties or to truncation error, and simple problems may be solved with far less computational effort than the numerical approach demands. Furthermore, many features of the solution, such as the existence and location of maxima and minima, the leading terms of power series expansions of the solution, and perturbation coefficients which describe the effects of small changes in the parameters of the problem, may be derived directly. Many of these features can be obtained only with considerable difficulty from a numerical treatment.

On the other hand, it must be recognized that the numerical approach is potentially far more powerful and versatile. Temperature-dependent conductivity, the radiation boundary condition, complex time and space dependence of the problem characteristics, and two- or three-dimensional geometry can all be handled within the scope of a practicable calculation

effort. One can, in effect, solve the real problem with which one is presented, rather than some idealized problem which bears an imperfectly known relation to the real problem.

The use of analytic methods within the framework of a basically numerical approach remains to be considered. For example, in a two- or three-dimensional calculation it might be preferable to use a numerical approach based upon the integral formulation (Eq. (59)) rather than the difference equations. Even where the difference equations are entirely adequate, it may require less computer time to evaluate an analytic formula for those cases in which one is available. Purely analytic and purely numerical methods are merely the extremes of a "spectrum" of available approaches; for the majority of problems the most practical techniques probably involve some combination of the two.

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SECTION II

VAPORIZATION AND HEAT CONDUCTION IN HECTIC2.1. INTRODUCTION

In a two-dimensional geometry the phenomena of vaporization and heat conduction are considerably more complex than in one dimension, and the simplest approaches to the calculations, employing explicit differencing of the partial differential equations involved, are even less feasible than in the one-dimensional case. The approach taken in the effort to develop a two-dimensional Eulerian interaction code has therefore been to concentrate on the analytic description of the physical processes involved in more or less typical applications, rather than on the most general possible solution of the equations. For this reason the approach is essentially one-dimensional.

2.2. VAPORIZATION

The following equations are employed in the description of vaporization at the surface:

Continuity

$$\dot{m} = \rho_o u_a \quad (69)$$

$$\dot{m} = \rho_1 c_1 \quad (70)$$

Equation of motion

$$P_1 + \dot{m}c_1 = P_o + \dot{m}u_a \quad (71)$$

Energy conservation

$$\dot{m}(H_1 + c_1^2/2 - H_0 - u_a^2/2) = \phi_{SV} \quad (72)$$

Vapor equation of state

$$P_1 = (\gamma-1) H_C' \rho_1 \quad (73)$$

Hugoniot pressure in solid⁽¹⁾

$$P_0 = \frac{\alpha^2(1 - \rho_s/\rho_0)}{\rho_s - \beta(1 - \rho_s/\rho_0)^2} \quad (74)$$

These six equations involve seven unknown quantities:

- $\dot{m}$ Mass ablation rate,
- ρ_0 Density on solid side of solid-vapor interface,
- ρ_1 Density on vapor side of solid-vapor interface,
- c_1 Magnitude of vapor velocity at solid-vapor interface, relative to the interface,
- u_a Magnitude of ablation velocity, i.e., velocity of solid relative to the interface,
- P_0 Pressure on solid side of solid-vapor interface,
- P_1 Pressure on vapor side of solid-vapor interface.

The equations also involve seven material parameters, assumed to be known:

- H_C Specific internal energy of solid at the vaporization temperature,
- H_V Specific internal energy of vaporization,
- ρ_s Normal solid density,

H'_C Specific random internal energy of vapor at the interface,

γ Polytropic index of vapor,

α, β Constants in empirical low-pressure state equation for solids:

$$P = \alpha u_p + \beta u_p^2, \text{ where } u_p \text{ is the particle velocity (Ref. 1).}$$

The specific enthalpies of vapor and solid at the interface are defined, respectively, by

$$H_1 = H_C + H_V + P_1 / \rho_1 \quad (75)$$

$$H_0 = H_C + P_0 / \rho_0 \quad (76)$$

Finally, the net energy flux at the interface available for producing vapor, φ_{SV} , is assumed known. In effect,

$$\varphi_{SV} = \dot{E} - \varphi_c \quad (77)$$

where $\dot{E}$ is the total incident flux on the interface and φ_c is the loss due to heat conduction into the interior of the solid. The latter term is treated in detail in Section 2.3. All quantities defined above are non-negative; vector quantities are represented by their magnitudes, since relative orientations are determined by the model assumed. The evaluation of the solid pressure on the Hugoniot replaces the more complete equations of state and motion for the solid, which are not needed for the analysis of many interaction processes. This remains, however, a limitation of the model which may require further developmental effort in the future.

Since the number of equations is one less than the number of unknowns, an additional condition is necessary. The velocity c_1 of the vapor at the interface, relative to the interface, must be such that

$$u_a \leq c_1 \leq \sqrt{\gamma(\gamma-1)H'_C} \quad (78)$$

That is, it cannot be less than the constant density limit, in which $\rho_1 = \rho_0$, nor greater than the Chapman-Jouguet limit, namely, the local sound speed, for which the entropy is a maximum. If c_1 lies between these limits, the pressure P_1 on the vapor side of the interface is obtainable from the conditions in the external vapor field, for example, by integration back from an exterior boundary condition. In any of these three cases, the additional condition is determined by the hydrodynamic coupling of the vapor at the interface to that beyond the interface. The constant density limit should theoretically be instead a constant pressure limit; i.e., with a more detailed state equation treatment in both vapor and solid, the lower limit of c_1 would appear naturally from the formulation as a condition involving constant pressure across the interface rather than constant density. In the absence of such a more detailed and algebraically involved treatment, the constant density assumption is a reasonable and convenient artifice.

Case 1. Assume first that ϕ_{SV} is sufficiently small that $c_1^2 = \gamma(\gamma - 1)H'_C$, the Chapman-Jouguet case. Then using Eqs. (69), (70), (71), (73), (75), and (76), Eq. (72) may be written in the form

$$\dot{m} \left[H_V + c_1^2 (1 - u_a/c_1)^2/2 + (\gamma - 1)H'_C (1 - u_a/c_1) \right] = \phi_{SV} \quad (79)$$

or, since ablation velocity, particularly in this case, must be small compared with the sound speed in the vapor, $u_a/c_1 \ll 1$ and

$$\dot{m} \cong \phi_{SV} / [H_V + c_1^2/2 + (\gamma - 1)H'_C] \quad (80)$$

The remaining unknowns are then obtained by solving Eq. (69) for u_a , Eq. (70) for ρ_1 , Eq. (73) for P_1 , Eq. (71) for P_0 , and Eq. (74) for ρ_0 . The value of P_1 obtained by this procedure is denoted by P_T , or "P-test".

Case 2. Now assume, in contrast to Case 1, that the relative velocity of the interface and the vapor at the interface is less than the sound speed.

Then the interface remains within the range of influence of the external vapor, and the pressure P_V at the interface may be found as follows. Denote the pressure in the zone adjacent to the interface by P_K , the pressure in the next zone by P_{K+1} , and the widths of the zones by Δ_K , Δ_{K+1} . Then

$$P_V = P_K \quad \text{if} \quad P_K < P_{K+1} \quad (81)$$

$$P_V = P_K + \Delta_K \frac{P_K - P_{K-1}}{\Delta_K + \Delta_{K+1}} \quad \text{if} \quad P_K > P_{K+1} \quad (82)$$

and the true interface pressure is taken to be

$$P_1 = \max(P_T, P_V) \quad (83)$$

If $P_1 = P_T$, i. e., if $P_T > P_V$, the Case 1 calculation already performed is confirmed. Otherwise, it is dropped and the Case 2 calculation is substituted as follows. Equation (79) may be rewritten, using Eqs. (70) and (73) as

$$\frac{1}{2} \left[\frac{(\gamma - 1)H'_C}{P_1} - \frac{1}{\rho_o} \right]^2 \dot{m}^3 + \left[H_V + (\gamma - 1)H'_C \frac{P_1}{\rho_o} \right] \dot{m} = \varphi_{SV} \quad (84)$$

which is a cubic of the form

$$A\dot{m} + B\dot{m}^3 = \varphi_{SV}$$

Let

$$a = A^2 / \varphi_{SV}^2$$

$$b = \varphi_{SV} / 2B$$

$$S_A = b(\sqrt{1 + 4Aa/27B} + 1)$$

$$S_B = b(\sqrt{1 + 4Aa/27B} - 1)$$

The only real root, in physically valid cases, is then

$$\dot{m} = S_A^{1/3} - S_B^{1/3} \quad (85)$$

If $B/Aa = B\phi_{SV}^2/A^3$ is small, specifically less than 0.01, then S_A and S_B are nearly equal and the form

$$\dot{m} = \frac{\phi_{SV}}{A} \left(1 - \frac{B\phi_{SV}^2}{A^3} \right) \quad (86)$$

is used.

The procedure is as follows: Given P_1 , evaluate ρ_1 by Eq. (73) and provisionally assign the value ρ_s to ρ_o . Then evaluate $\dot{m}$ by Eq. (85) or (86), u_a by Eq. (69), c_1 by Eq. (70), and P_o by Eq. (71). If $\rho_1 \leq \rho_o$ or equivalently $P_1 \leq (\gamma - 1)H'_C \rho_o$, the calculation is then complete. If however, $P_1 > (\gamma - 1)H'_C \rho_o$, first try re-evaluating ρ_o from Eq. (74) to determine if the solid has been shocked to a sufficiently high density to pass the test. If this is insufficient, the Case 2 calculation is dropped and the Case 3 calculation is substituted.

Case 3. This is the constant density case; the solution is given by setting $P_o = P_1$, solving Eq. (74) for ρ_o , and setting $\rho_1 = \rho_o$. Since by Eq. (71) $c_1 = u_a$, Eq. (72) reduces to

$$\dot{m} = \frac{\phi_{SV}}{H_V} \quad (87)$$

which is essentially equivalent to

$$\dot{m} = \frac{\dot{E}}{H_V + H_C} \quad (88)$$

since conductive steady state is quickly achieved under these conditions.

Finally, u_a is determined by Eq. (69).

The HECTIC code at the present time employs a still simpler procedure in which ρ_o is identified with ρ_s under all conditions so that Eq. (74) is not used at all. The procedure described above merely indicates refinements which can be readily made without modifying the vapor state equation or introducing a complete solid state equation into the formulation.

2.3. CONDUCTION

The basic equation for the description of heat flow in the solid is

$$\rho_o C_V \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial s^2} + q(s, t) \quad (89)$$

where $q(s, t)$ represents the net source of heat at a fixed position s . It is convenient to transform this equation to a moving coordinate x such that

$$s = x + \frac{\dot{m}}{\rho_o} t \quad (90)$$

i. e., x represents the depth in the solid relative to the moving solid-vapor interface. The transformed equation is then

$$\rho_o C_V \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial x^2} + \dot{m} C_V \frac{\partial \theta}{\partial x} + q, \quad x \geq 0 \quad (91)$$

The additional term $\dot{m} C_V \partial \theta / \partial x$, which is negative, represents an effective reduction of the heating rate at a point x as this point moves down the temperature gradient. The term q is defined by

$$q = \dot{Q}(x, t) - \phi_{SV} \delta(x) \quad (92)$$

where $\dot{Q} = -(\partial \dot{E} / \partial x)$ is the local heating rate due to the external source and the second term accounts for the energy removal by vaporization at the interface, which is to be computed.

The physical model is that of an initially cold solid, which is heated by the incident flux until the surface temperature reaches H_C / C_V , at which time vaporization begins. On the assumption that at a time t the depth of

the conductive front $\sqrt{\alpha t}$ (where $\alpha = k/C_V \rho_0$ is the thermal diffusivity) is large compared with the characteristic depth of the solid in which the source $\dot{E}$ is deposited, the temperature is given by the general formula (Ref. 2) (cf. Eq. (24) in Section 1):

$$\theta(x, t) = (\pi k C_V \rho_0)^{-1/2} \int_0^t \frac{\dot{E}(0, t')}{\sqrt{t - t'}} e^{-x^2/4\alpha(t - t')} dt' \quad (93)$$

If, as is usually the case, the deposition depth can be neglected by the time the surface begins to vaporize, then this time t_c can be determined from Eq. (93):

$$\theta(0, t_c) = H_C / C_V = (\pi k C_V \rho_0)^{-1/2} \int_0^{t_c} \frac{\dot{E}(0, t')}{\sqrt{t_c - t'}} dt' \quad (94)$$

At time t_c the temperature distribution near the surface, given by Eq. (93), may be expanded in powers of x :

$$\theta(x, t_c) = \frac{H_C}{C_V} \left[1 - \frac{C_V \dot{E}(0, t_c)}{k H_C} x + O(x^2) \right] \quad (95)$$

which implies that the conductive flux at the surface

$$\varphi_c = -k \frac{\partial \theta}{\partial x} \Big|_0 \quad (96)$$

is equal to the source flux $\dot{E}(0, t_c)$. This is equivalent to stating that there is (for $t \leq t_c$) no surface singularity to make the energy flux discontinuous. It is also the case that the distribution of temperature defined by Eq. (93) is roughly exponential in x , and that this general shape holds at later times as well. The approximation

$$\theta(x, t) = \frac{H_C}{C_V} e^{-x/z(t)}, \quad t \geq t_c, \quad x \geq 0 \quad (97)$$

where, according to Eq. (95),

$$z(t_c) = \frac{kH_C}{C_V \dot{E}(0, t_c)} \quad (98)$$

is therefore not unreasonable, particularly in view of the fact that the detailed spatial distribution of temperature in the solid is not of interest.

The specification of the function $z(t)$ may be made by substituting Eq. (97) into the two first-derivative terms of Eq. (91) and integrating over x from -0 to ∞ ;

$$\rho_o H_C \frac{dz}{dt} = [\varphi_c(\infty) - \varphi_c(-0)] - \dot{m}H_C + \dot{E} - \varphi_{SV} \quad (99)$$

Since the conductive flux vanishes at infinity, and also at -0 , which is beyond the interface, the result is

$$\frac{dz}{dt} = \frac{1}{\rho_o H_C} [\dot{E}(0, t) - \dot{m}H] \quad (100)$$

where H , the total specific energy for heating and vaporization, is given by

$$\dot{m}H = \varphi_{SV} + \dot{m}H_C \cong \dot{m} [H_C + H_V + c_1^2/2 + (\gamma - 1)H'_C] \quad (101)$$

(which follows from Eq. (79) with $u_a/c_1 \ll 1$). The differential equation (100), with initial condition (98) therefore describes the advance of the conductive front in a straightforward manner, and provides a simple approximation to the true solution of the heat conduction equation. The explicit difference representation of Eq. (100) is solved at the conclusion of each cycle, following the vaporization procedure described above. The conductive flux, Eq. (96), is then calculated as

$$\varphi_c = \frac{kH_C}{C_V z(t)} \quad (102)$$

and the quantity φ_{SV} , defined by Eq. (77), is then updated.

2.4. APPENDIX: GLOSSARY AND USAGE OF HECTIC VARIABLES

Tables I and II list those variable names in common storage which are currently in use, and their relative locations, definitions, and defined values, if any. All units are in the cgs system, except for temperature, which has units of electron volts. A "specific" quantity always means "per unit mass," i. e., "per gram." Variable names followed by an asterisk are input quantities.

Various quantities associated with boiling are stored in the SOLID array. For each value of the radial cell index I , there may be up to 20 such quantities. Since the total array size is 400, a maximum of 20 "boiling" cells is permitted. With the assumption that $J = 20(I - 1) + 1$, the quantities SOLID ($J+N$) are defined in Table II for various values of N .

Table III is a cross-referencing of all the variable names and the subroutines which use common storage. As "X" in the table indicates that the variable listed on that row is used at least once by the subroutine listed in that column.

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES
USED IN HECTIC

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
PRØB	1	Problem identification number
CYCLE	2	Cycle number
DT	3	Time step Δt^n
PRINTS*	4	Cycle frequency for short prints
PRINTL*	5	Cycle frequency for long prints
DUMPT 7*	6	Cycle frequency for tape dumps
CSTØP*	7	Maximum allowed cycle number
PI	8	3.1415927
SCYCLE *	10	Start cycle number; if positive will search dump tape; if zero will generate mesh and start from time zero
SPRØB *	11	Problem identification number; used to check against PRØB read from restart dump tape
ETH	13	Total energy in system
FFA *	14	Maximum allowed increase in Δt per cycle (2.)
FFB *	15	Minimum allowed Δt (10^{-10} sec)
XMAX	18	Largest value of the radial coordinate
DNN	23	Used in EDIT to calculate the energy check number ECK
DMIN *	24	Maximum allowed value of ECK
DTNA	26	Time step on previous cycle Δt^{n-1}
NC	30	Integer value of cycle number
NPC	31	Number of cycles between short prints
IMAX	33	Number of zones in the radial direction
IMAXA	34	IMAX + 1
JMAX	35	Number of zones in the axial direction

Table I

**STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES
USED IN HECTIC (Continued)**

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
JMAXA	36	JMAX + 1
KMAX	37	(IMAX) (JMAX) + 1
KMAXA	38	KMAX + 1
I1	47	Active grid counter in the radial direction + 2
I2	48	Active grid counter in the axial direction + 2
N1 *	51	Input to SETUP; number of Δx_1 's or Δy_1 's
N2 *	52	Input to SETUP; number of Δx_2 's or Δy_2 's
N3 *	53	Input to SETUP; number of Δx_3 's or Δy_3 's
N4 *	54	Input to SETUP; number of Δx_4 's or Δy_4 's
N7	57	Dump tape number
NRM	62	Maximum permitted number of radiation cycles per hydrocycle; currently inoperative (bypassed when SN < 0)
TRAD	63	Radiation time step (currently not used)
SN *	65	Switch in PH1 to cause backward integration in time to correct the integration of internal energy (this occurs when SN = 0 and UT > 0) (-1.)
ECK	76	Energy check criterion. At the short-print cycle frequency, the relative error between ETH and the sum over cells of internal and kinetic energy is formed and stored in WSA. The difference between WSA and its value at the last short print cycle, divided by NPC, is the quantity ECK

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES
USED IN HECTIC (Continued)

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
T	84	Total time to cycle N
SI	90	Error flag. Its value indicates the sub-routine in which the error occurred
HVB *	100	Heat of vaporization (specific)
HCb *	101	Heat required to bring solid to boiling point (specific)
SVS *	103	Specific volume of solid
ATØM *	104	Atomic weight of material
CV *	105	Specific heat of solid
GV *	106	γ of vapor at vaporization temperature
ANN *	110	Exponent for laser pulse function
EZERØ *	111	Total laser pulse energy per unit area
PW *	112	Pulse width at half-maximum for laser source
CAPS *	113	Laser absorption coefficient in solid material
HNU *	114	Laser photon energy (ev)
COE *	115	Coefficient used in calculation of laser absorption coeff. at temperature below 2 ev.
SCR	116	Incident laser flux; derivative of the laser pulse function
ISR *	117	Index of largest radial zone irradiated by source
SCDR	118	Duration of source
AHN	119	$8.62 \times 10^{10} (\text{ATØM} * \text{HNU})^2$
DTH	120	Shortest cell transit time in the mesh, i. e. the minimum value of $\Delta x/u$ or $\Delta y/v$

Table I

**STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES
USED IN HECTIC (Continued)**

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
IH	121	I value of cell determining DTH
JH	122	J value of cell determining DTH
DTC	123	Δt determined by Courant stability condition
IC	124	I value of cell determining DTC
JC	125	J value of cell determining DTC
RFT *	126	Reflectivity of target surface to laser radiation
CDUT *	127	Conductivity of target material
HCP *	128	Energy of gas at zero temperature - ($H_c + H_v$)
HH	129	Enthalpy of gas at the boiling point
CØ	130	Sound speed in gas at the boiling point
J5*	135	J value of vapor zones adjacent to the solid-vapor interface
SVMAX *	138	Maximum specific volume allowed at free surface; no mass flows to the outer cells if the specific volume exceeds SVMAX (10^{14})
FRCDTC*	139	Fraction of DTC used to determine Δt (0.5)
VAPE	140	Total internal and kinetic energy in vapor
RADE	141	Total reflected source energy; this energy is lost from the system
CNDE	142	Total energy conducted to interior of target
SCRE	143	Total incident energy from source
IV	144	I value of cell which determined DTVF
JV	145	J value of cell which determined DTVF

Table I

**STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES
USED IN HECTIC (Continued)**

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
IU	146	I value of cell which determined DTUF
JU	147	J value of cell which determined DTUF
DTVf	148	Axial free surface velocity time control
DTUF	149	Radial free surface velocity time control
EII *	150	Constant used to compute laser absorption coefficient
X(I)	152	Radial coordinate, measured to outer boundary of cell
FLEFT (I)	205	Radial momentum flux across left boundary in PH2
UL(I)	205	Weighted velocity on left boundary of cell in PH1
YAMC (I)	305	Axial momentum flux across left boundary in PH2
GAMC (I)	405	Mass flux across left boundary in PH2
PL (I)	405	Pressure on left side of cell in PH1
PR (I)	405	Temporary storage in INPUT and EDIT
SIGC (I)	505	Total specific energy flux across left boundary in PH2
THETA (I)	605	Cell temperature
Y (I)	1806	Axial coordinate, measured to upper boundary of cell
AIX (I)	1907	Specific internal energy of cell
AMX (I)	3109	Mass in cell
DX (I)	4315	Radial cell width
DY (I)	4367	Axial cell width
P (I)	4472	Cell pressure
PIDTS	5674	Working storage in PH1 and PH2

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES
USED IN HECTIC (Continued)

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
PRR	5676	Average of cell pressure and pressure in zone on the right
RC	5933	X coordinate of cell center
RHØ (I)	5935	Cell density
RR	7136	X coordinate of center of cell on the right
SIG	7137	Working storage in CDT
TAU (I)	7190	Area of ring I: $\pi(x_{i+1}^2 - x_i^2)$
TAUDTS	7242	TAU (I) * DT in PH1
U (I)	7244	X-component of cell velocity
URR	8445	Weighted average of cell velocity U(I) and cell on right
UT	8446	Recycle variable in PH1 (-1, 0, or +1)
UU	8447	New Δt for recycling in PH1
UVMAX	8450	(Max. U or V)/(Min. Δx or Δy) in CDT
V (I)	8451	Y- component of cell velocity
VABOVE	9651	Velocity V in cell above
VBLØ	9652	Velocity V in cell below
VEL	9653	Tag in PH1 to note pass number
W2 (I)	9660	Laser radiation flux arriving at solid-vapor interface
WS	9761	Working storage
WSA	9762	Working storage
WSB	9763	Working storage
I	9774	Radial index
IWSA *	9779	Generator input: last card if = +1
IWSB *	9780	Generator input: x, Δx data if 0; y, Δy data if 1

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

<u>Variable name</u>	<u>Loc</u>	<u>Definition</u>
J	9832	Axial index
K	9836	Cell index, a composite of I and J
KP	9838	K + IMAX
L	9841	Running index in certain loops
M	9842	Running index in certain loops
MZ	9848	Number of words in the Z array (150)
N	9849	Temporary storage for zone index
NK	9850	Working storage
NK1	9852	Working storage
NR	9854	Number of radiation cycles per hydro- cycle (currently inoperative)
SOLID (I)	9905	See Table II
TEMP (I)	10305	Temporary storage
FIQUT (I)	10317	Source energy flux leaving cell
CAP (I)	11517	Used for both K_{Laser} and $\bar{Z}$
KFIT (I)	12717	Array for packed flags
ISEND, ISL	13917	Indicator for last cycle
IGOTØ	13918	Indicator in EDIT for type of print out
HEAD (I)	13919	Storage for problem identification heading

Table II

LAYOUT OF VARIABLES STORED IN SOLID

<u>N</u>	<u>Definition</u>
1	z , an effective conduction length for calculating the conductive heat loss at the surface
2	ϕ_{SV} , the net heating rate at the surface
3	E_C , the total heat loss into the interior
4	ϕ_S , the incident laser energy delivered per unit area up to time t
5	Not used
6	$\dot{m}$, the mass ablation rate
7	m , the mass ablated per unit area
8	$\phi_{S, surf}$, the incident laser energy delivered to the surface per unit area up to time t
9	Not used
10	P_v , the vapor pressure at the interface
11	P_{test} (see discussion of boiling)
12	P_o , the pressure on the solid side of the interface
13	I , the impulse per unit area, found by integrating P_o
14	Mass ablated on this cycle
15	v_1 , the velocity of injection of vaporized matter
16	Not used
17	Not used
18	Not used
19	Not used
20	Not used

Table III
CROSS REFERENCE OF HECTIC VARIABLES

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PHI	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
A, AREA		4309														
AHN		119														
AID		1965														
AIX	1200	1907		x	x	x	x		x				x			
ALCØ		109														
AM		3107											x			
AMD		3108														
AMDM		21														
AMK	15	220														
AMX	1200	3109		x	x	x	x		x				x			
AMXM		22														
ANN		110					x						x			
ATOM		104											x			
BBOUND		74														
BETA		108														
BIG		4310														
BOUNCE		4311														
CABLN		82														
CAP	1200	11517		x	x		x						x			
CAPS		113														
CB		102											x			
CDUT		127											x			
CNDE		142			x								x			
CØ		130											x			
CØE		115											x			
CSTØP		7			x											
CV		105														
CVIS		27											x			

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	LAG	DLOW	SETUP	SPRNT	ES	ESK
CYCLE		2		x	x	x							x	x		
DDVK		4313														
DDXN		4312														
DKE		605														
DMIN		24			x											
DNN		23		x	x											
DT		3		x	x	x	x	x	x				x			
DTC		123		x	x	x							x			
DTH		120		x	x	x							x			
DTNA		26				x		x					x			
DTRAD		70											x			
DUMPT 7		6			x											
DVK		4314														
DX	52	4315		x	x	x			x				x			
DXN		66														
DY	100	4367		x	x	x	x		x				x			
E		4467														
ECK		76														
ETH		13		x	x		x		x				x			
EZERØ		111					x						x			
FD		4468											x			
FEF		25														
FFA		14														
FFB		15				x										
F10OUT	1200	10317		x	x											
FLEFT	200	205					x			x			x			
FS		4469														
FX		4470														

Table III
CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PHI	PH2	FLAG	DJLOW	SETUP	SPRINT	CS	ESK
G	50	9855														
GAM, SCYCLE		10		x												
GAMC	10C	405														
GAMD, SPRØB		11		x												
GAMX		12														
GMADR		88														
GMAX		85														
GMAXR		89														
GV		106						x								
HCB		101						x								
HCP		128						x								
HEAD	12	13919		x												
HH		129						x								
HNU		114														
HVB		100						x								
I		9774		x				x								
IC		124			x											
IH		121			x											
II		9775														
IMAX		33														
IMAXA		34														
IN		9776		x				x								
IR		9777														
ISL, ISEND		13917														
ISR		117														
IWS		9778														
IWSA		9779														
IWSB		9780														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	IN PUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
IWSC		9781														
IW1	50	9782														
EXMAX		42														
I2	150	1			x								x			
I1		47			x					x						
I2		48			x						x					
I3		49														
I4		50														
J		9832		x	x	x	x	x	x				x			
JC		125			x	x										
JH		122			x	x										
JMAX		35			x	x				x						
JMAXA		36		x	x	x							x			
JN		9833														
JP		9834														
JR		9835														
J1		131														
J2		132														
J3		133														
J4		134														
J5		135								x						
J6		136			x		x	x				x				
K		9836			x											
KDT		41														
KFIT	1200	12717		x	x	x	x	x	x	x			x			
KMAX		37			x											
KMAXA		38		x	x											
KN		9837														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRING	ES	ESK
KP		9838								x						
KR		9839														
KRM		9840														
L		9841		x	x			x		x			x			
LP, IGOTØ		13918			x					x						
M		9842			x								x			
MA		9843														
MB		9844														
MC		9845														
MD		9846														
ME		9847														
MZ		9848		x	x											
N		9849							x							
NC		30			x								x			
ND		40														
NIMAX		45														
NIMAX		46														
NK		9850														
NKMAX		9851			x									x		
NK1		9852			x											
NMAX		39														
NØ		9853														
NØD		943														
NØPR		44														
NPC		31			x											
NPR		28														
NPRI		29														
NR		9854		x						x						

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	D'LOW	SETUP	SPRINT	ES	ESK
NRC		32														
NRM		62							x				x			
N1		51														
N10		60														
N11		61														
N2		52											x			
N3		53											x			
N4		54											x			
N5		55											x			
N6		56														
N7, NTAPE		57		x												
N8		58														
N9		59														
OUT		4471														
P	1200	4472		x	x	x		x	x	x			x			
PABOVE		5672														
PBLØ		5673							x							
PIDTS		5674							x							
PIDY		8							x							
PK	15	235														
PL	100	405							x							
PPABOV		5675														
PR	100	405			x											
PRINTL		5			x											
PRINTS		4			x											
PRØB		1			x											
PRR		5676		x					x							
PUL	225	5677														

Table III
CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PHI	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
PW		112											x			
QDT		5932														
QK	15	250														
Q000FL		7138											x			
RADE		141			x											
RADEB		69														
RADER		67														
RADET		68														
RC		5933							x							
REZ		5934														
REZFCT		71														
RFT		126											x			
RHØ	1200	5935		x	x	x	x			x			x			
RL		7135														
RR		7136							x							
RSTOP		72														
SBOUND		77														
SCDR		118					x						x			
SCR		116			x		x						x			
SCRE		143			x		x						x			
SHELL		73														
SIG		7137				x										
SIGC	100	100								x						
SN		65							x							
SOLID	400	9905		x	x		x	x	x	x			x			
SUMFE		107														
SVS		103						x								
SWITCH		7139											x			x

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
S1		90		x	x	x			x					x		
S10		99														
S2		91														
S3		92														
S4		93														
S5		94														
S6		95														
S7		96														
S8		97														
S9		98														
T		84			x	x							x			
TAB	15	205														
TABLM	50	7140														
TAU	52	7190		x	x		x	x	x	x			x			
TAUDTS		7242														
TAUDTX		7243														
TEMP	12	10305			x	x		x					x			
THETA	1200	605		x	x		x			x			x			
TMDZ		16														
TMXZ		17														
TMZ		9														
T0ZONE		75								x						
TRAD		63							x							
TXMAX		19														
TYMAX		20														
U	1200	7244		x	x				x	x				x		
UK		8444														
UL	200	205							x							

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
UR	200	205														
URR		8445														
UT		8446														
UTEF		8449														
UU		8447														
UUU		8448														
UVMAX		8450														
V	1200	8451														
VABOVE		9651														
VAPE		140														
VBLØ		9652														
VEL		9653														
VISC		83														
VK		9654														
VT		9655														
VTEF		9656														
VV		9657														
VVABOV		9658														
VVBLØ		9659														
WPS		9760														
WS		9761														
WSA		9762														
WSB		9763														
WSC		9764														
WSGD		86														
WSGX		87														
W2	50	9660														
W3	50	9710														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
X	53	152		x	x		x		x				x			
XL		9765														
XLF		9766														
XMAX		18			x								x			
XN		9767														
XNRG		64														
XR		9768														
XX	54	151			x											
X1		78			x											
X2		79			x											
Y	100	1806		x	x								x			
YAMC	100	305								x						
YL		9769														
YLW		9770														
YN		9771														
YU		9772														
YY	101	1805														
Y1		80			x											
Y2		81			x											
Z	150	1		x	x								x			
ZMAX		9773				x										
IV		144			x											
JV		145			x											
IU		146			x											
JU		147			x											
DTVF		148			x											
DTUF		149			x											

2.5. APPENDIX: LISTING OF HECTIC

```

01  FOR MAIN, MAIN/FJ
C
C  HECTIC PROGRAM MODIFIED 7/30/66
C
C*****
C*****
C  MAIN FOR INTER CODE
C  NOTE --- 1 MATERIAL (X) ONLY
C
C  CALL INPUT
C
C  CALL EDIT
C
C  CALCULATES TIME STEP AND PRESSURES
10  CALL CDY
C  SOURCE ROUTINE
C  CALL SCRC
C  CALL BOIL
C  VELOCITY AND ENERGY CHANGE DUE TO WORK TERMS ONLY
C
20  CALL PH1
C
C  VELOCITY AND ENERGY CHANGES DUE TO MASS TRANSPORT
C  CALL PH2
C  CALL EDIT
C  GO TO 10
C  END

```

```

01  FOR CARDS, CARDS/FJ
    SUBROUTINE CARDS
    DIMENSION TABLE(1),CARD(7),LABEL(1),CAHD(18)
    COMMON      TABLE
    EQUIVALENCE(TABLE(1),LABEL(1))
    WRITE (6,10)
1   READ(5,11) IEND,LOC,NUMWPC,(CARD(I),I=1,7),CAHD(17),CAHD(18)
    IF(IEND.EQ.9) GO TO 15
    WRITE(6,12) CAHD(17),CAHD(18),IEND,LOC,NUMWPC,(CARD(I),I=1,NUMWPC)
    IF(IEND.EQ.1.AND.LOC.EQ.0) GO TO 3
    IF(IAUS(NUMWPC-4).GT.3) GO TO 20
    DO 4 I=1,NUMWPC
        J=LOC+I-1
        IF(IEND-2)2,5,2
5    LABEL(J)=IFIX(CAHD(I))
        GO TO 4
2    TABLE(J)=CARD(I)
4    CONTINUE
    IF(IEND-1)1,3,1
3    RETURN
15  READ(5,16) (CAHD(I),I=1,16)
    WRITE(6,17) (CAHD(I),I=1,16)
    GO TO 1
20  WRITE(6,21)
    CALL EXIT

C      FORMATS
10  FORMAT(20H1HECTIC  INPUT CARDS///)
11  FORMAT(I1,I5,I1,UP7E9.4,2A5)
12  FORMAT(1H 2A5,I4,I7,I3,1P7E14.6)
16  FORMAT(16A5)
17  FORMAT(1X,16A5)
21  FORMAT(20X,24H THE ABOVE CARD IN ERROR)
    END

```

CARD0010

CARD0030

CARD0050

CARD0070

CARD0100

CARD0110

CARD0120

CARD0130

CARD0140

CARD0150

CARD0160

CARD0170

CARD0180

CARD0190

CARD0230

AFWL-TR-66-108, Vol II

W1 FOR INPUT, INPUT/FJ
SUBROUTINE INPUT

THRU0020

C
C
C

D I M E N S I O N

DIMENSION

1U(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOU(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4UX(52), X(53), XX(54), UY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), WK(15), Z(150), LZ(150),
6TAU(52), PL(200), PR(200), UL(200), UR(200),
7LEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)

COMMON	Z	XX	UR	PR	THETA	YY
COMMON	AID	AIX	AM	AMD	AMX	ARIA
COMMON	BIG	BOUNCE	DDXN	DDVK	DVK	DIJ
COMMON	UY	E	FD	FS	FX	OUT
COMMON	P	PAHOVE	PBLO	PIDTS	PPAHOV	PRR
COMMON	PUL	QDT	RC	REZ	RHO	RL
COMMON	RR, SIG	GUOFL	SWITCH	TABLM, TAU		
COMMON	TAUDTS	TAUDTX	U	UK	URR	UT
COMMON	UU	UUU	UTEF	UVMAX	V	VAHOVE
COMMON	VBLO	VEL	VK	VT	VTEF	VV
COMMON	VVABOV	VVBLO	W2	W3	WPS	WS
COMMON	WSA	WSH	WSC	XL	XLF	XN
COMMON	XR	YL	YLW	YN	YU	ZMAX
COMMON	I	II	IN	IR	IWS	IWSA
COMMON	IWSB	IWSC	IWI	J	JN	JP
COMMON	JR	K	KN	KP	KR	KRM
COMMON	L	M	MA	MB	MC	MD
COMMON	ME	MZ	N	NK	NKMAX	NK1
COMMON	NO	NR	G	SOLID	TEMP	
COMMON	FIOU	CAP	KFIT	ISEND	IGOTO	HEAD

C
C
C

DEQUIVALENCE	(Z(12), PROB),	(Z(2), CYCLE),	(Z(3), DT),
1(Z(4), PRINTS),	(Z(5), PRINTL),	(Z(6), DUMPT7),	(Z(7), CSTOP),
2(Z(8), PIDY),	(Z(9), TMZ),	(Z(10), SCYCLE),	(Z(11), SPROB),
3(Z(12), GAMX),	(Z(13), ETH),	(Z(14), FFA),	(Z(15), FFB),
4(Z(16), TMDZ),	(Z(17), TMXZ),	(Z(18), XMAX),	(Z(19), TXMAX),
5(Z(20), TYMAX),	(Z(21), AMDM),	(Z(22), AMXM),	(Z(23), DNN),
6(Z(24), UMIN),	(Z(25), FEF),	(Z(26), DTNA),	(Z(27), CVIS),
7(Z(28), NPK),	(Z(29), NPRI),	(Z(30), NC),	(Z(31), NPC),
8(Z(32), NRC),	(Z(33), IMAX),	(Z(34), IMAXA),	(Z(35), JMAX),
9(Z(36), JMAXA),	(Z(37), KMAX),	(Z(38), KMAXA),	(Z(39), NMAX),
DEQUIVALENCE	(Z(40), ND),	(Z(41), KDT),	(Z(42), IXMAX),
1(Z(43), NOU),	(Z(44), NOPR),	(Z(45), NIMAX),	(Z(46), NJMAX),
2(Z(47), I1),	(Z(48), I2),	(Z(49), I3),	(Z(50), I4),
3(Z(51), N1),	(Z(52), N2),	(Z(53), N3),	(Z(54), N4),
4(Z(55), N5),	(Z(56), N6),	(Z(57), N7),	(Z(58), N8),
5(Z(59), N9),	(Z(60), N10),	(Z(61), N11),	(Z(62), NRM),
6(Z(63), TRAD),	(Z(64), XNRG),	(Z(65), SN),	(Z(66), DXN),
7(Z(67), RADER),	(Z(68), RADER),	(Z(69), RADEH),	(Z(70), DTRAD),
8(Z(71), REZFCT),	(Z(72), RSTOP),	(Z(73), SHELL),	(Z(74), BBOUND),
9(Z(75), TOZONE),	(Z(76), ECK),	(Z(77), SBOUND),	(Z(78), X1),
DEQUIVALENCE	(Z(79), X2),	(Z(80), Y1),	(Z(81), Y2),
1(Z(82), CABLN),	(Z(83), VISC),	(Z(84), T),	(Z(85), GMAX),
2(Z(86), WSGD),	(Z(87), WSGX),	(Z(88), GMADR),	(Z(89), GMAXR),
3(Z(90), S1),	(Z(91), S2),	(Z(92), S3),	(Z(93), S4),
4(Z(94), S5),	(Z(95), S6),	(Z(96), S7),	(Z(97), S8),
5(Z(98), S9),	(Z(99), S10),		

C

DEQUIVALENCE (Z(100), HVU), (Z(101), HCH), (Z(102), CH),

48

60 S1=0.0
RETURN

C
C ERROR

9902 S1=3.1005
60 TO 9999

9903 S1=3.1006
60 TO 9999

9904 S1=3.1024
60 TO 9999

9905 S1=3.0050
9999 CALL EDIT

C
C
C FORMATS

8004 FORMAT(12A6)

8005 FORMAT(1H1,12A6)

END

INPU2200

INPU2210

INPU2250

INPU2270

INPU2290

INPU2390

INPU2470

INPU2480

INPU2530

WI FOR EDIT, EDIT/FJ
SUBROUTINE EDIT

EDIT0010

C
C
C

U I M L N S I O N

DIMENSION

1U(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4UX(52), X(53), XX(54), DY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PR(200), UL(200), UR(200),
7FLEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)

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C

C O M M O N

EDIT0990

COMMON	Z	XX	UR	PR	THETA	YY
COMMON	AID	AIX	AM	AMD	AMX	A
COMMON	BIG	BOUNCE	DDXN	DDVK	DVK	DX
COMMON	DY	E	FD	FS	FX	OUT
COMMON	P	PABOVE	PBLO	PIDTS	PPAIOV	PRR
COMMON	PUL	QDT	RC	REZ	RHO	RL
COMMON	RR	SIG	W000FL	SWITCH	TABLM	TAU
COMMON	TAUDTS	TAUDTX	U	UK	URR	UT
COMMON	UU	UUU	UTEF	UVMAX	V	VABOVE
COMMON	VBLO	VEL	VK	VT	VTEF	VV
COMMON	VVABOV	VVBLO	W2	W3	WPS	WS
COMMON	WSA	WSB	WSC	XL	XLF	XN
COMMON	XR	YL	YLW	YN	YU	ZMAX
COMMON	I	II	IN	IR	IWS	IWSA
COMMON	IWSB	IWSC	IW1	J	JN	JP
COMMON	JR	K	KN	KP	KR	KRM
COMMON	L	M	MA	MB	MC	MD
COMMON	ME	MZ	N	NK	NKMAX	NK1
COMMON	NO	NR	G	SOLID	TEMP	
COMMON	FIOUT	CAP	KFIT	ISEND	IGOTO	HEAD

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EDIT0920

E Q U I V A L E N C E

OEQUIVALENCE	(Z(12),PROB),	(Z(2),CYCLE),	(Z(3),DT),
1(Z(4),PRINTS),	(Z(5),PRINTL),	(Z(6),DUMPT7),	(Z(7),CSTOP),
2(Z(8),PIDY),	(Z(9),TMZ),	(Z(10),SCYCLE),	(Z(11),SPROB),
3(Z(12),GAMX),	(Z(13),ETH),	(Z(14),FFA),	(Z(15),FFB),
4(Z(16),TMDZ),	(Z(17),TMXZ),	(Z(18),XMAX),	(Z(19),TXMAX),
5(Z(20),TYMAX),	(Z(21),AMDM),	(Z(22),AMXM),	(Z(23),DNN),
6(Z(24),UMIN),	(Z(25),FEF),	(Z(26),DTNA),	(Z(27),CVIS),
7(Z(28),NPR),	(Z(29),NPRI),	(Z(30),NC),	(Z(31),NPC),
8(Z(32),NRC),	(Z(33),IMAX),	(Z(34),IMAXA),	(Z(35),JMAX),
9(Z(36),JMAXA),	(Z(37),KMAX),	(Z(38),KMAXA),	(Z(39),NMAX),
OEQUIVALENCE	(Z(40),ND),	(Z(41),KD1),	(Z(42),IXMAX),
1(Z(43),NOO),	(Z(44),NOPR),	(Z(45),NIMAX),	(Z(46),NJMAX),
2(Z(47),I1),	(Z(48),I2),	(Z(49),I3),	(Z(50),I4),
3(Z(51),N1),	(Z(52),N2),	(Z(53),N3),	(Z(54),N4),
4(Z(55),N5),	(Z(56),N6),	(Z(57),N7),	(Z(58),N8),
5(Z(59),N9),	(Z(60),N10),	(Z(61),N11),	(Z(62),NRM),
6(Z(63),TRAD),	(Z(64),XNRG),	(Z(65),SN),	(Z(66),DXN),
7(Z(67),RADER),	(Z(68),RADER1),	(Z(69),RADER),	(Z(70),DTRAD),
8(Z(71),REZFCT),	(Z(72),RSTOP),	(Z(73),SHELL),	(Z(74),HBOUND),
9(Z(75),TOZONE),	(Z(76),ECK),	(Z(77),SBOUND),	(Z(78),X1),
OEQUIVALENCE	(Z(79),X2),	(Z(80),Y1),	(Z(81),Y2),
1(Z(82),CABL),	(Z(83),SC),	(Z(84),T),	(Z(85),GMAX),

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      2(Z(80),WSGD),      (Z(87),WSGA),      (Z(88),GMAOR),      (Z(89),GMAXR),
      3(Z(90),S1),        (Z(91),S2),        (Z(92),S3),        (Z(93),S4),
      4(Z(94),S5),        (Z(95),S6),        (Z(96),S7),        (Z(97),S8),
      5(Z(98),S9),        (Z(99),S10)

C
      EQUIVALENCE      (Z(100),HMH),      (Z(101),HCH),      (Z(102),CH),
      1(Z(103),SVS),    (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
      2(Z(107),SUMFE),  (Z(108),BETA),    (Z(109),ALCO),    (Z(110),AHN),
      3(Z(111),EZERO),  (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
      3(Z(115),COE),    (Z(116),SCH),    (Z(117),ISR),    (Z(118),SCDR),
      4(Z(119),AHN),    (Z(120),DTH),    (Z(121),IH),      (Z(122),JH),
      5(Z(123),DTC),    (Z(124),IC),     (Z(125),JC),      (Z(126),RFT),
      X(Z(127),CDUT),   (Z(128),HCP),    (Z(129),HH),      (Z(130),CO),
      6(Z(131),J1),     (Z(132),J2),     (Z(133),J3),      (Z(134),J4),
      7(Z(135),J5),     (Z(136),J6),     (Z(138),SYMXX),
      8(Z(139),FRCDT.)
      EQUIVALENCE      (Z(140),VAPE),      (Z(141),RADE),      (Z(142),CNDE),
      1(Z(143),SCRE),   (Z(144),IV),     (Z(145),JV),      (Z(146),IU),
      2(Z(147),JU),     (Z(148),DTVF),   (Z(149),DTUF),    (Z(150),E1)

C
C
      EQUIVALENCE      (XX(2),X(1)),      (UR,UL,FLEET),      (UR(100),YAMC),
      1(PR(100),S16C),  (PR,PL,GAMC),     (DKE,THETA),      (UR,TAR),
      2(UR(16),AMK),    (UR(31),PK),      (UR(46),QK),      (YY(2),Y(1))

C
C
C
C
      ISEND = 1, FIRST CYCLE
      ISEND = 2, INTERMEDIATE CYCLES
      ISEND = 3, LAST CYCLE

C
C
C
C
C
C
      E D I T
      1600=1
      GO TO(6000,101,101),ISEND
      101 IF(S1.GT.0.) GO TO 110
      108 IF(CYCLE-CSTOP)115,109,115
      109 S1=4.0108
      110 ISEND=3
C
      ALL PRINTS PLUS WRITE ON BINARY TAPE
      GO TO 6000
      115 IF(AMOD(CYCLE,PRINTS))118,117,118
C
      SHORT PRINTS ONLY
      117 1600=2
      GO TO 6000
      118 IF(AMOD(CYCLE,PRINTL))120,119,120
C
      LONG PRINTS ONLY
      119 1600=3
      GO TO 5000
      120 IF(AMOD(CYCLE,DUMPT7))126,121,126
      121 IF(1600.EQ.1) GO TO 6000
      1600=1
      GO TO 1
      125 IF(ISEND.EQ.3) CALL SPRINT
      126 IF(ABS(ACK).GT.DMIN) GO TO 9901
      140 RETURN

C
C
C**** SUBROUTINE WTAPE *****
C
      DUMP ON TAPE N7
C
      IF DUMPT7 IS NEGATIVE SUPPRESS ANY WRITING ON TAPE 7
C
      1 IF(ISEND.EQ.1.AND.N7.EQ.10) GO TO 126
      IF(DUMPT7)30,3,3
      3 WS=555.0

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EDIT1000

EDIT1030

EDIT1100

EDIT1110

EDIT1120

EDIT1500

EDIT1510

EDIT1520

EDIT1530

EDIT1540

EDIT1550

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      WRITE(N7) WS,CYCLL,PROB
      WRITE(N7) (Z(I),I=1,MZ)
      WRITE(N7) (U(I),V(I),AMX(I),AIX(I),P(I),THETA(I),
1  RHO(I),FIOUT(I),CAP(I),KFIT(I),I=1,KMAX)
      WRITE(N7) X(0),(X(I),TAU(I),I=1,IMAX)
      WRITE(N7) (Y(I),I=0,JMAX)
      WRITE(N7) (W2(I),I=1,50)
      WRITE(N7) (SOLID(I),I=1,400)
      WS=666.0
      WRITE(N7) WS,WS,WS
      WRITE(6,8120)NC
      30 GO TO 125
C**** END OF WTape SUBROUTINE *****E
C
C
C**** SUBROUTINE S P *****E
6000 NK=12
6010 DO 6012 I=1,18
6012 PR(I)=0.0
      DO 6028 K=2,KMAX
      WSB=(U(K)**2+V(K)**2)/2.0
6019 IF(AMX(K))9902,6028,6020
6020 I=NKI
6026 WS=AMX(K)
      PR(1)= PR(1)+AIX(K)*WS
      PR(2)= PR(2)+WSB*WS
      PR(3)= PR(2)+PR(1)
6028 CONTINUE
      WSA=(ETH-PR(3))/ETH
      ECK =(WSA-DNN)/FLOAT(NPC)
      DNN=WSA
      NPC=0
      WRITE(6,8116)PROB,NC,T,DT ,DTH,DTC,Z(148),Z(149),IH,JH,IC,JC,
1  IZ(144),IZ(145),IZ(146),IZ(147)
      WRITE(6,6902) PR(1),PR(2),PR(3),VAPE,RADE,CNDE,SCRE,ETH,ECK
      PR(1)=0.
      PR(2)=0.
      PR(3)=0.
      PR(4)=0.0
      WRITE(6,6904)
      DO 6040 I=1,15K
      J=(I-1)*20+1
      TEMP(1)=SOLID(J+12)/ SCR
      TEMP(2)=SOLID(J+13)/ SOLID(J+4)
      TEMP(3)=SOLID(J+6) / SCR
      TEMP(4)=SOLID(J+7) / SOLID(J+4)
      IF( SCR.NE.0.) GO TO 6030
      TEMP(1)=0.
      TEMP(3)=0.
6030 CONTINUE
      PR(1) = PR(1) + TAU(1)*SOLID(J+6)
      PR(2) = PR(2) + TAU(1)*SOLID(J+7)
      PR(3) = PR(3) + TAU(1)*SOLID(J+12)
      PR(4) = PR(4) + TAU(1)*SOLID(J+13)
      PR(5) = PR(5) + TAU(1)*W2(1)
      PR(6) = PR(6) + TAU(1)*SOLID(J+8)
      PR(7) = PR(7) + TAU(1)*SOLID(J+2)
      PR(8) = PR(8) + TAU(1)*TEMP(1)
      PR(9) = PR(9) + TAU(1)*TEMP(2)
      PR(10)= PR(10) + TAU(1)*TEMP(3)
      PR(11)= PR(11) + TAU(1)*TEMP(4)
      WRITE(6,6906)I,SOLID(J+6),SOLID(J+7),SOLID(J+12),SOLID(J+13),W2(1)
1  ,SOLID(J+8),SOLID(J+2),TEMP(1),TEMP(2),TEMP(3),TEMP(4)
6040 CONTINUE
      WRITE(6,6908) (PR(I),I=1,11)

```

EDIT1730

EDIT1750

EDIT1770

EDIT1780

EDIT1790

EDIT1800

EDIT1820

EDIT1950

EDIT1960

EDIT2020

EDIT1750

EDIT2090

EDIT2160

EDIT2230

EDIT2340

EDIT2350

EDIT1730

AFWL-TR-66-108, Vol II

```

C**** END OF S P SUBROUTINE *****EDIT2920
C                                          EDIT2930
C                                          EDIT2940
C**** SUBROUTINE PLOT *****EDIT2950
1000 CONTINUE
  WRITE(6,8116)PROB,NC,T,DT ,DTH,DTC,Z(148),Z(149),IH,JH,IC,JC,
  11Z(144),1Z(145),1Z(146),1Z(147)
  JMAX=JMAX
  WRITE (6,8307)X1,X2,XMAX,Y1,Y2,Y(JMAX)
  M=1
  1F(JMAX-52)1034,1036,1036
  1034 M=1ABS(51-JMAX)/2
  1036 DO 1040 I=1,M
    WRITE (6,8308)
  1040 CONTINUE
  1044 J=JMAX
  1100 K=(J-1)*IMAX+1
  1105 DO 1180 I=1,IMAX
    K=K+1
  1126 PR(I)=IH
  1130 1F(J-J5-1)1136,1132,1136
  1132 1F(I-I1-1)1140,1134,1134
  1134 1F(I-I2-1)1144,1144,1136
  1136 1F(I-I1-1)1140,1138,1140
  1138 1F(J-J5)1140,1140,1144
  1140 1F(I-I2-1)1150,1142,1150
  1142 1F(J-J5)1150,1150,1144
  1144 PR(I)=2H
  GO TO 1180
C    TEST FOR X PARTICLE
1150 1F(AMX(K))9903,1166,1160
1160 PR(I)=2H X
  GO TO 1180
1166 PR(I)=2H
1180 CONTINUE
1200 1F(MOD(J,5))1210,1204,1210
1204 1F(DY(J)-DY(J-1))1206,1208,1206
1206 WRITE (6,8211)DY(J),J,(PR(I),I=1,IMAX)
  GO TO 1224
1208 WRITE (6,8201)J,(PR(I),I=1,IMAX)
  GO TO 1224
1210 1F(DY(J)-DY(J-1))1212,1214,1212
1212 WRITE (6,8222)DY(J),(PR(I),I=1,IMAX)
  GO TO 1224
1214 WRITE (6,8202)(PR(I),I=1,IMAX)
1224 J=J-1
1226 1F(J)1230,1230,1100
1230 PR(I)=2H -
  WRITE (6,8201)J,(PR(I),I=1,IMAX)
  WRITE (6,8302)(I,I=0,IMAX,5)
1240 GO TO(5060,118,9906),IGOTO
C**** END OF PLOT SUBROUTINE *****EDIT3600
C                                          EDIT3610
C                                          EDIT3620
C**** SUBROUTINE L P *****EDIT3630
5000 CONTINUE
  WRITE(6,8116)PROB,NC,T,DT ,DTH,DTC,Z(148),Z(149),IH,JH,IC,JC,
  11Z(144),1Z(145),1Z(146),1Z(147)
5004 DO 5050 I=1,IMAX
  LPP=1
  J=JMAX
  K=KMAX+I
  DO 5046 L=1,JMAX
  J=J-1
  K=K-IMAX

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AFWL-TR-66-108, Vol II

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      YTAB=Y(J51-Y(J)
5012 IF (AMX(K))9904,5046,5014
5014 GO TO(5016,5018),LPP
5016 LPP=2
      WRITE(6,8135) I,X(I),DX(I)
5018 WRITE(6,8108) J,U(K),V(K),P(K),THETA(K),AMX(K),
      IAI(K),RHQ(K),FIOUT(K),CAP(K),YTAB
5046 CONTINUE
5050 CONTINUE
5051 GO TO(1,9905,120),IGOTO
C**** END OF L P SUBROUTINE *****
C
C
C      ERROR
9901 S1=4.0120
      GO TO 9999
9902 S1=4.6019
      GO TO 9999
9903 S1=4.1150
      GO TO 9999
9904 S1=4.5012
      GO TO 9999
9905 S1=4.5051
      GO TO 9999
9906 S1=4.1240
9999 CALL SPRINT
C
C      FORMATS
6902 FORMAT(//6X7HINT ENG7X,7HIN ENG,7X,7HINT+KIN,7X,7HIVP ENG,7X,7HRA
      10 ENG,7X,7HEND ENG,7X,7HSCR ENG / 3X,1P7E14.7 //34X,7HTHE ENG,7X,
      27HREL ERR /31X1P2E14.7 //)
6904 FORMAT(5H 12X6HMDOT/A4X3HM/A7X6HIDOT/A4X3H1/A7X7HESDOT/A3X
      2 4HE5/A6X7HEBDOT/A3X8H(I/E)DOT2X3H1/E7X7HM/E DOT3X3HM/E /)
6906 FORMAT(13,1P11E10.3)
6908 FORMAT(//1X14HSUM TIMES AREA/3X1P11E10.3)
8108 FORMAT(13,1P11E10.3)
8116 FORMAT( 7H1 PROB5X,5HCYCLE5X,4HTIME6X,2HDT8X,3HDT7X,
      1 3HOTC7X,4HDTVFGX,4HDTUF6X,2HIM2X,2HJM2X,2HIC2X,2HJC2X,2HIV2X,2HJV
      2 2X,2HIU2X,2HJU2X / F7.1,5X,15,3X,1P6E10.4,814 )
8120 FORMAT(1H0//21H TAPE 7 DUMP ON CYCLE15////)
8127 FORMAT(13,4(1P2E12.6,15))
8128 FORMAT(3H0 2(1P2E12.6,5X))
8135 FORMAT(1H //3H I=13,6X,6HX(1) =F12.3,6X,7HDX(1) =F12.3/ 3H J 3X
      11HU9X,1HV9X,1HP9X,5HTHETA5X,4HMASS6X,3HAI7X,3HRH07X,4HFLUX6X,3HCA
      2P7X,1HY /)
8201 FORMAT(110,2H 154A2)
9040 FORMAT(1H / 616)
8202 FORMAT(10X,2H 154A2)
8211 FORMAT(F7.1,13,2H 154A2)
8222 FORMAT(F7.1,3X,2H 154A2)
8302 FORMAT(112,10I10)
83070FORMAT(5H X1 =1PE12.6,3X,4HX2 =E12.6,3X,6HMAX =E12.6,6X,4HY1 =E12
      1.6,3X,4HY2 =E12.6,3X,6HYMAX =E12.6)
8308 FORMAT(1H /)
      END

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EDIT3830
 EDIT3840
 EDIT3860
 EDIT3870
 EDIT3880
 EDIT3890

EDIT4100
 EDIT4110

EDIT4220
 EDIT4300

EDIT4360
 EDIT4370
 EDIT4380
 EDIT4390
 EDIT4400
 EDIT4410
 EDIT4420
 EDIT4430
 EDIT4440
 EDIT4450

AFWL-TR-66-108, Vol II

WI FOR COT, COT/1J
SUBROUTINE COT

C
C
C

D I M E N S I O N

DIMENSION

10(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), F1OUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IWI(50), W2(50), W3(50), TAILM(50),
4DX(52), X(53), XX(54), DY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PR(200), UL(200), UR(200),
7LEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)

COMMON Z, XX, UR, PR, THE TA, YY
COMMON AID, AIX, AM, AMI, AMX, ARI A
COMMON BIG, BOUNCE, DDXH, DDVK, DVK, DX
COMMON DY, E, ED, ES, FX, OUT
COMMON P, PABOVL, PBLO, PIDTS, PPAOV, PRR
COMMON PUL, QDT, RC, REZ, RHO, RL
COMMON RR, SIG, GOODFL, SWITCH, TAILM, TAU
COMMON TAUDTS, TAUDTX, U, UK, URR, UT
COMMON UU, UUU, UTEF, UVMAX, V, VAROVL
COMMON VBLO, VEL, VK, VT, VTEF, VV
COMMON VVABOV, VVBLO, W2, W3, WPS, WS
COMMON WSA, WSH, WSC, XL, XLF, XN
COMMON XR, YL, YLW, YN, YU, ZMAX
COMMON I, II, IN, IR, IWS, IWSA
COMMON IWSH, IWSC, IWI, J, JN, JP
COMMON JR, K, KN, KP, KR, KRM
COMMON L, M, MA, MB, MC, MD
COMMON ME, MZ, N, NK, NKMAX, NK1
COMMON NO, NR, G, SOLID, TEMP
COMMON F1OUT, CAP, KFIT, ISEND, IGOTO, HEAD

C
C
C
C

E Q U I V A L E N C E

OEQUIVALENCE (Z, IZ, PROB), (Z(2), CYCLE), (Z(3), DT),
1(Z(4), PRINTS), (Z(5), PRINTL), (Z(6), DUMPT7), (Z(7), CSTOP),
2(Z(8), PIUY), (Z(9), TMZ), (Z(10), SCYCLE), (Z(11), SPROB),
3(Z(12), GAMX), (Z(13), LTH), (Z(14), FFA), (Z(15), FFB),
4(Z(16), TMU2), (Z(17), TMX2), (Z(18), XMAX), (Z(19), TXMAX),
5(Z(20), TYMAX), (Z(21), AMDM), (Z(22), AMXM), (Z(23), DNN),
6(Z(24), DMIN), (Z(25), FEF), (Z(26), DTNA), (Z(27), CV15),
7(Z(28), NPR), (Z(29), NPR1), (Z(30), NC), (Z(31), NPC),
8(Z(32), HRC), (Z(33), IMAX), (Z(34), IMAXA), (Z(35), JMAX),
9(Z(36), JMAXA), (Z(37), KMAX), (Z(38), KMAXA), (Z(39), NMAX),
OEQUIVALENCE (Z(40), ND), (Z(41), KDT), (Z(42), IXMAX),
1(Z(43), NOD), (Z(44), NOPR), (Z(45), NIMAX), (Z(46), NJMAX),
2(Z(47), I1), (Z(48), I2), (Z(49), I3), (Z(50), I4),
3(Z(51), N1), (Z(52), N2), (Z(53), N3), (Z(54), N4),
4(Z(55), N5), (Z(56), N6), (Z(57), N7), (Z(58), N8),
5(Z(59), N9), (Z(60), N10), (Z(61), N11), (Z(62), NRM),
6(Z(63), TRAD), (Z(64), XNRG), (Z(65), SN), (Z(66), DXN),
7(Z(67), RADEK), (Z(68), RADET), (Z(69), RAUER), (Z(70), DTRAD),
8(Z(71), REZFCT), (Z(72), RSTOP), (Z(73), SHELL), (Z(74), BUOUND),
9(Z(75), TOZONE), (Z(76), ECK), (Z(77), SBOUND), (Z(78), X1),
OEQUIVALENCE (Z(79), X2), (Z(80), Y1), (Z(81), Y2),
1(Z(82), CABLN), (Z(83), VISC), (Z(84), T), (Z(85), GMAX),
2(Z(86), WSGD), (Z(87), WSGX), (Z(88), GMADR), (Z(89), GMAXR),
3(Z(90), S1), (Z(91), S2), (Z(92), S3), (Z(93), S4),
4(Z(94), S5), (Z(95), S6), (Z(96), S7), (Z(97), S8),
5(Z(98), S9), (Z(99), S10)

C

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01EQUIVALENCE (Z(100),HVB), (Z(101),HCB), (Z(102),CB),
02 (Z(103),SVS), (Z(104),ATOM), (Z(105),CV), (Z(106),GV),
03 (Z(107),SUMFE), (Z(108),BETA), (Z(109),ALCO), (Z(110),ANH),
04 (Z(111),ELERO), (Z(112),PW), (Z(113),CAPS), (Z(114),HNU),
05 (Z(115),COL), (Z(116),SCR), (Z(117),ISR), (Z(118),SCOR),
06 (Z(119),AHN), (Z(120),DTH), (Z(121),IH), (Z(122),JH),
07 (Z(123),DTC), (Z(124),IC), (Z(125),JC), (Z(126),KFI),
08 (Z(127),COUT), (Z(128),HCP), (Z(129),HH), (Z(130),CO),
09 (Z(131),J1), (Z(132),J2), (Z(133),J3), (Z(134),J4),
10 (Z(135),J5), (Z(136),J6), (Z(138),SVMAX),
11 (Z(139),FXCUTC)
12EQUIVALENCE (Z(140),VAPL), (Z(141),RADE), (Z(142),CNDE),
13 (Z(143),SICR), (Z(144),IV), (Z(145),JV), (Z(146),IU),
14 (Z(147),JU), (Z(148),DTVF), (Z(149),DTUF), (Z(150),E11)
15
16EQUIVALENCE (XX(2),X(1)), (UR,UL,FLLFT), (UR(100),YAMC),
17 (PR(100),SIGC), (PR,PL,GAMC), (UKE,THETA), (UR,TAB),
18 (UR(16),AMK), (UR(31),PK), (UR(46),QK), (YY(2),Y(1))
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AFWL-TR-66-108, Vol II

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      IV=I
      JV=J
3270 IF(THETA(K).EQ.0.) GO TO 3280
      TEMP(3)=DX(I)/ABS(THETA(K))*0.25
      IF(TEMP(3).GT.DTUF) GO TO 3280
      DTUF=TEMP(3)
      IU=I
      JU=J
3280 CONTINUE
      DTNA=DT
      DTN=2(139)/ABS(TEMP(1))
      DTC=1./SQRT(ABS(UVMAX))
      DT=AMINI(AMINI(AMINI(AMINI(DTNA*FFA,DTC),DTN),DTVF),DTUF)
3029 IF(DT.LT.FFB) GO TO 9902
3290 IF(T.LT.0.) GO TO 9903
3300 T=T+DT
      NC=NC+1
      CYCLE=NC
      NPC=NPC+1
      RETURN
C      NEGATIVE MASS
9901 S1=5.3004
      GO TO 9999
9902 S1=5.3029
      GO TO 9999
9903 S1=5.3290
9999 CALL EDIT
      END

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AFWL-TR-66-108, Vol II

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C  FOR SCRC, SCRC/FJ
C  SUBROUTINE SCRC
C  D I M E N S I O N
C
C  DIMENSION
1U(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4DX(52), X(53), XX(54), UY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), OK(15), Z(150), IZ(150),
6TAU(52), PL(200), PR(200), UL(200), UR(200),
7LEFT(100), YAMC(100), SIGC(100), GAMC(100),
8B(50), SOLID(400), TEMP(12), HEAD(12)
COMMON Z, XX, UR, PR, THETA, YY
COMMON AID, AIX, AM, AMU, AMX, AREA
COMMON UIG, BOUNCE, DDYN, DDVK, DVK, DX
COMMON UY, E, FD, FS, FX, OUT
COMMON P, PABOVE, PBLO, PIDTS, PPAHOV, PRR
COMMON PUL, QDT, RC, REZ, RHO, RL
COMMON RR, SIG, GUOFL, SWITCH, TABLM, TAU
COMMON TAUITS, TAUITS, U, UK, URR, UT
COMMON UU, UUU, UTEF, UVMAX, V, VABOVE
COMMON VBLO, VEL, VK, VT, VTEF, VV
COMMON VVABOV, VVBLO, W2, W3, WPS, WS
COMMON WSA, WSB, WSC, XL, XLF, XN
COMMON XR, YL, YLW, YN, YU, ZMAX
COMMON I, II, IN, IR, IWS, IWSA
COMMON IWSB, IWSC, IW1, J, JN, JP
COMMON JK, K, KN, KP, KR, KRM
COMMON L, M, MA, MB, MC, MD
COMMON ME, MZ, N, NK, NKMAX, NK1
COMMON NO, NR, G, SOLID, TEMP
COMMON FIOUT, CAP, KFIT, ISEND, IGOTO, HEAD
C
C  E Q U I V A L E N C E
C
C  DEQUIVALENCE (Z(12),PROB), (Z(2),CYCLE), (Z(3),UT),
1(Z(4),PRINTS), (Z(5),PRINTL), (Z(6),DUMPT7), (Z(7),CSTOP),
2(Z(8),PIDY), (Z(9),TMZ), (Z(10),SCYCLE), (Z(11),SPROB),
3(Z(12),GAMX), (Z(13),ETH), (Z(14),FFA), (Z(15),FFB),
4(Z(16),TMUZ), (Z(17),TMXZ), (Z(18),XMAX), (Z(19),TXMAX),
5(Z(20),TYMAX), (Z(21),AMDM), (Z(22),AMXM), (Z(23),DNN),
6(Z(24),DMIN), (Z(25),FEF), (Z(26),DTNA), (Z(27),CVIS),
7(Z(28),NPR), (Z(29),NPRI), (Z(30),NC), (Z(31),NPC),
8(Z(32),NRC), (Z(33),IMAX), (Z(34),IMAXA), (Z(35),JMAX),
9(Z(36),JMAXA), (Z(37),KMAX), (Z(38),KMAXA), (Z(39),NMAX),
DEQUIVALENCE (Z(40),ND), (Z(41),KDT), (Z(42),IXMAX),
1(Z(43),NOD), (Z(44),NOPR), (Z(45),NIMAX), (Z(46),NJMAX),
2(Z(47),I1), (Z(48),I2), (Z(49),I3), (Z(50),I4),
3(Z(51),N1), (Z(52),N2), (Z(53),N3), (Z(54),N4),
4(Z(55),N5), (Z(56),N6), (Z(57),N7), (Z(58),N8),
5(Z(59),N9), (Z(60),N10), (Z(61),N11), (Z(62),NRM),
6(Z(63),TRAD), (Z(64),XNRG), (Z(65),SN), (Z(66),DXN),
7(Z(67),RADEX), (Z(68),RADET), (Z(69),RADEB), (Z(70),OTRAD),
8(Z(71),REZFACT), (Z(72),RSTOP), (Z(73),SHELL), (Z(74),BBOUND),
9(Z(75),TOZONE), (Z(76),ECK), (Z(77),SBOUND), (Z(78),X1),
DEQUIVALENCE (Z(79),X2), (Z(80),Y1), (Z(81),Y2),
1(Z(82),CABL), (Z(83),VISC), (Z(84),T), (Z(85),GMAX),
2(Z(86),WSGD), (Z(87),WSGX), (Z(88),GMADR), (Z(89),GMAXR),
3(Z(90),S1), (Z(91),S2), (Z(92),S3), (Z(93),S4),
4(Z(94),S5), (Z(95),S6), (Z(96),S7), (Z(97),S8),
5(Z(98),S9), (Z(99),S10)
C
C  DEQUIVALENCE (Z(100),HVB), (Z(101),HCB), (Z(102),CH),

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1(Z(103),SVS), (Z(104),ATOM), (Z(105),CV), (Z(106),GV),
2(Z(107),SUMFL), (Z(108),BETA), (Z(109),ALCO), (Z(110),ANN),
3(Z(111),LEZRO), (Z(112),PW), (Z(113),CAPS), (Z(114),HNU),
4(Z(115),COL), (Z(116),SCR), (Z(117),ISR), (Z(118),SCDR),
5(Z(119),AHN), (Z(120),DTI), (Z(121),IH), (Z(122),JH),
6(Z(123),UTC), (Z(124),IC), (Z(125),JC), (Z(126),RFT),
7(Z(127),CDUT), (Z(128),HCP), (Z(129),HH), (Z(130),CO),
8(Z(131),J1), (Z(132),J2), (Z(133),J3), (Z(134),J4),
9(Z(135),J5), (Z(136),J6), (Z(137),J7), (Z(138),SVMAX),
10(Z(139),FRCDTC)
DEQUIVALENCE (Z(140),VAPL), (Z(141),RADL), (Z(142),CNDE),
1(Z(143),SCRE), (Z(144),IV), (Z(145),JV), (Z(146),IU),
2(Z(147),JU), (Z(148),DTVF), (Z(149),DTUF), (Z(150),EII)

C
DEQUIVALENCE (XX(2),X(1)), (UR,UL,FLFT), (UP(100),YAMC), 0 D0750
1(PH(100),SIGC), (PR,PL,GAMC), (DUKE,THETA), (UR,TAB), 0 D0760
2(UR(16),AMK), (UR(31),PK), (UR(46),QK), (YY(2),Y(1)) 0 D0770
C 0 D0740
C 0 D0780
C 0 D0790
C 0 D0800
C 0 D0810
C 0 D0950
C 0 D1020

W2(I) W2(I) FLUX INTO SOLID
Z(115) COE ABSORPTION COEF. (CM**2/GM)
Z(116) SCR INITIAL SOURCE (JERK/CM**2-SH)
Z(117) ISR NO. OF ZONES WITH SOURCE IN I DIRECTION
Z(118) SOURCE DURATION
FIFT1=LEZRO
IF( NC.EQ.1)
1FIFT=0.5*EZERO*(2.*(T-DT)/SCDR)**(ANN+1.)
IF(T.LT.0.5*SCDR) GO TO 1
IF(T.GT.0.5*SCDR) GO TO 2
FIFT1=EZERO*(1.-.5*(2.*(1.-T/SCDR))**(ANN+1.))
GO TO 2
1 FIFT1=0.5*EZERO*(2.*T/SCDR)**(ANN+1.)
2 SCR=ABS(FIFT1-FIFT)/DT
FIFT=FIFT1
SCRE = FIFT* PIDY*X(ISR)**2
IF((T.GE.SCDR).AND.((T-DT).LE.SCDR)) SCR =0.
I4P=J5+1
DO 200 I=1,ISR
IS=(I-1)*20+1
SOLID(I5+4)=FIFT
UFIS=0.
FIIN = SCR
W2(I)=0.
DO 100 J=2,I4P
K=(J-1)*IMAX+I+1
N=K-1MAX
IF(J.EQ.I4P) GO TO 20
IF(JMK(KFIT(K),2).NE.1) GO TO 100
IF(JMK(KFIT(N),2).NE.1) GO TO 50
IF( J.EQ.2) FIOUT(N)=FIIN
IF(SCDR.EQ.0.) FIOUT(K)=0.
20 FIIN=FIOUT(N)
IF(J.EQ.I4P) GO TO 40
50 SY=1./RHO(K)
CALL ESK(THETA(K),SV,N,CAP(K))
ROSC=-RHO(K)*DY(J)*CAP(K)
IF(ROSC.NE.0.) GO TO 65
FIOUT(K)=FIIN
DFI=0.
GO TO 70

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AFWL-TR-66-108, Vol II

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65 CONTINUE
   F1OUT(K)=F1IN*EXP(ROSC)
   DF1=F1IN-F1OUT(K)
   GO TO 70
60 #2(I)=F1IN
   DF1=0.
70 DFIS=DFIS+DF1 *DT*TAU(I)
   AIX(K) =AIX(K) +DF1*TAU(I)/AMX(K)*DT
100 CONTINUE
   ETH=ETH +DFIS
200 CONTINUE
   RETURN
   END
```

BI FOR BOIL, BOIL/FJ
SUBROUTINE BOIL

C D I M E N S I O N
C

DIMENSION

10(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFI(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4DX(52), X(53), XX(54), DY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PR(200), UL(200), UR(200),
7FLEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)
COMMON Z, XX, UR, PR, THETA, YY
COMMON AID, AIX, AM, AMD, AMX, AREA
COMMON BIG, BOUNCE, DNN, DDVK, DVK, DX
COMMON DY, E, FD, FS, FX, OUT
COMMON P, PABOVE, PILO, PIDTS, PPAOV, PRR
COMMON PUL, QDT, RC, REZ, RHO, RL
COMMON HR, SIG, QUOOF, SWITCH, TABLM, TAU
COMMON TAUITS, TAUITS, U, UK, URR, UT
COMMON UU, UUU, UTEF, UVMAX, V, VABOVE
COMMON VBLO, VEL, VK, VT, VTEF, VV
COMMON VVABOV, VVBLO, W2, W3, WPS, WS
COMMON WSA, WSB, WSC, XL, XLF, XN
COMMON XR, YL, YLW, YN, YU, ZMAX
COMMON I, II, IN, IR, IWS, IWSA
COMMON IWSB, IWSC, IW1, J, JN, JP
COMMON JR, K, KN, KP, KR, KRM
COMMON L, M, MA, MB, MC, MD
COMMON ME, MZ, N, NK, NKMAX, NK1
COMMON NO, NR, G, SOLID, TEMP
COMMON FIOUT, CAP, KFI, ISEND, IGOTO, HEAD

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E Q U I V A L E N C E

DEQUIVALENCE (Z(12),PROB), (Z(2),CYCLE), (Z(3),DT),
1(Z(4),PRINTS), (Z(5),PRINTL), (Z(6),DUMPT7), (Z(7),CSTOP),
2(Z(8),PIUY), (Z(9),TMZ), (Z(10),SCYCLE), (Z(11),SPROB),
3(Z(12),GAMX), (Z(13),ETH), (Z(14),FFA), (Z(15),FFH),
4(Z(16),TMUZ), (Z(17),TMXZ), (Z(18),XMAX), (Z(19),TXMAX),
5(Z(20),TYMAX), (Z(21),AMD), (Z(22),AMXM), (Z(23),DNN),
6(Z(24),UMIN), (Z(25),FEF), (Z(26),DTNA), (Z(27),CVIS),
7(Z(28),NPR), (Z(29),NPRI), (Z(30),NC), (Z(31),NPC),
8(Z(32),NRC), (Z(33),IMAX), (Z(34),IMAXA), (Z(35),JMAX),
9(Z(36),JMAXA), (Z(37),KMAX), (Z(38),KMAXA), (Z(39),NMAX),
DEQUIVALENCE (Z(40),ND), (Z(41),KDT), (Z(42),IXMAX),
1(Z(43),NOD), (Z(44),NOPR), (Z(45),NIMAX), (Z(46),NJMAX),
2(Z(47),I1), (Z(48),I2), (Z(49),I3), (Z(50),I4),
3(Z(51),N1), (Z(52),N2), (Z(53),N3), (Z(54),N4),
4(Z(55),N5), (Z(56),N6), (Z(57),N7), (Z(58),N8),
5(Z(59),N9), (Z(60),N10), (Z(61),N11), (Z(62),NRM),
6(Z(63),IRAD), (Z(64),XNRG), (Z(65),SN), (Z(66),DXN),
7(Z(67),RADER), (Z(68),RADET), (Z(69),RADEB), (Z(70),DTRAD),
8(Z(71),REZFCT), (Z(72),RSTOP), (Z(73),SHELL), (Z(74),BBOUND),
9(Z(75),TOZONE), (Z(76),ECK), (Z(77),SBOUND), (Z(78),X1),
DEQUIVALENCE (Z(79),X2), (Z(80),Y1), (Z(81),Y2),
1(Z(82),CAULN), (Z(83),VISC), (Z(84),T), (Z(85),GMAX),
2(Z(86),WSGD), (Z(87),WSGX), (Z(88),GMADR), (Z(89),GMAXR),
3(Z(90),S1), (Z(91),S2), (Z(92),S3), (Z(93),S4),
4(Z(94),S5), (Z(95),S6), (Z(96),S7), (Z(97),S8),
5(Z(98),S9), (Z(99),S10)

C

DEQUIVALENCE (Z(100),HVB), (Z(101),HCH), (Z(102),CB),

1(Z(103),SVS),	(Z(104),ATOM),	(Z(105),CV),	(Z(106),GV),
2(Z(107),SUMFL),	(Z(108),BETA),	(Z(109),ALCO),	(Z(110),ANN),
3(Z(111),EZERO),	(Z(112),PW),	(Z(113),CAPS),	(Z(114),HNU),
4(Z(115),COE),	(Z(116),SCR),	(Z(117),ISR),	(Z(118),SCOR),
5(Z(119),AHN),	(Z(120),DTH),	(Z(121),IH),	(Z(122),JH),
6(Z(123),DTC),	(Z(124),IC),	(Z(125),JC),	(Z(126),RFT),
7(Z(127),CDUT),	(Z(128),HCP),	(Z(129),HH),	(Z(130),CO),
8(Z(131),J1),	(Z(132),J2),	(Z(133),J3),	(Z(134),J4),
9(Z(135),J5),	(Z(136),J6),		(Z(138),SVMAX),
10(Z(139),FRCDTC)			
DEQUIVALENCE	(Z(140),VAPE),	(Z(141),RADE),	(Z(142),CNDE),
1(Z(143),SCRE),	(Z(144),IV),	(Z(145),JV),	(Z(146),IU),
2(Z(147),JU),	(Z(148),DTVF),	(Z(149),DTUF),	(Z(150),E11),
DEQUIVALENCE	(XX(2),X(1)),	(UR,UL,FLEFT),	(UR(100),YAMC),
1(PR(100),SIGC),	(PR,PL,GAMC),	(DKE,THETA),	(UR,TAB),
2(UR(16),AMK),	(UR(31),PK),	(UR(46),QK),	(YY(2),Y(1))

C
C
C
C
C

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CONTINUOUS BOILING VERSION
CNDE=0.
DO 1000 1=1,ISR
J=J5
10 K=(J5-1)*IMAX+1+1
J=(1-1)*20+1
C SOLID(J+2)=PH1 SUB(SV) SUP(N+1/2)
TEMP(1)=CDUT*HCB/(SOLID(J+1)*CV)
IF(CDUT.EQ.0.) TEMP(1)=HCB*W2(1)/HH
SOLID(J+2)=W2(1)-TEMP(1)
IF(SOLID(J+2).GT.0.) GO TO 20
SOLID(J+2)=0.
SOLID(J+6)=0.
SOLID(J+12)=P(K)
SOLID(J+11)=0.
SOLID(J+14)=0.
SOLID(J+15)=0.
GO TO 450
20 CONTINUE
P TEST
C SOLID(J+11)=SOLID(J+2)*CO/(GV*(HH-HCB))
200 L=K-IMAX
SOLID(J+10)=P(K)
IF(JMR(KFIT(L),2).NE.1) GO TO 210
IF(P(L).GE.P(K)) GO TO 210
SOLID(J+10)=(3.*P(L)-P(K))/2.
210 IF(SOLID(J+11).LT.SOLID(J+10)) GO TO 300
M DOT
C SOLID(J+6)=SOLID(J+11)*GV/CO
C VELOCITY V1
SOLID(J+15)=-CO
SOLID(J+12)=SOLID(J+11)+SOLID(J+6)*ABS(SOLID(J+15))
GO TO 450
300 IF(SOLID(J+10).GE.(GV-1.)*HCP/SVS) GO TO 400
AA=HVB+(GV-1.)*HCP-SOLID(J+10)*SVS
BB=.5*((GV-1.)*HCP/SOLID(J+10)-SVS)**2
TBB=2.*BB
AAP=(AA/SOLID(J+2))**2
IF(BB.GT.1.E-2*AA*AAP) GO TO 340
SOLID(J+6)=SOLID(J+2)/AA*(1.-BB/(AA*AAP))
GO TO 360
340 BBP=.5*SOLID(J+2)/BB
SBA=SQRT(1.+AA*AAP/(6.75*BB))
SAA=(SBA+1.)*BBP

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$$SAA = (SBA + 1.) * HWP$$

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SUBB = (SBA - 1.) * HWP
IF (SUBB.LT.0.) GO TO 350
SOLID(J+6) = SAA** .33333 - SUBB** .33333
GO TO 360
350 SUBB = -SUBB
SOLID(J+6) = SAA** .33333 + SUBB** .33333
360 CONTINUE
SOLID(J+15) = -SQRT(TBB) * SOLID(J+6)
SOLID(J+12) = SOLID(J+10) + SOLID(J+6) * ABS(SOLID(J+15))
GO TO 450
400 SOLID(J+15) = 0.
SOLID(J+6) = W2(I) / (HVB + HCB)
SOLID(J+12) = SOLID(J+10)
450 SOLID(J+14) = SOLID(J+6) * TAU(I) * DT
IF (SOLID(J+7).LE.0.) GO TO 460
SOLID(J+3) = SOLID(J+3) - HCB * SOLID(J+1) / SVS
GO TO 465
460 SOLID(J+3) = SOLID(J+3) + W2(I) * DT
SOLID(J+1) = SOLID(J+1) + W2(I) * DT * SVS / HCB
GO TO 470
465 CONTINUE
C SOLID(J+1) = Z(N+1)
WMDOT = (W2(I) - SOLID(J+6) * HH) * SVS * DT / HCB
IF (WMDOT.LT.0.) WMDOT = 0.
SOLID(J+1) = SOLID(J+1) + WMDOT
TEMP(1) = CDUT / (CV * SOLID(J+6))
IF (SOLID(J+1).GE.TEMP(1)) SOLID(J+1) = TEMP(1)
SOLID(J+3) = SOLID(J+3) + HCB * SOLID(J+1) / SVS
470 CONTINUE
SOLID(J+7) = SOLID(J+7) + SOLID(J+6) * DT
SOLID(J+8) = SOLID(J+8) + W2(I) * DT
SOLID(J+13) = SOLID(J+13) + SOLID(J+12) * DT
VAPE = SOLID(J+2) * TAU(I) * DT + VAPE + HCB * SOLID(J+14)
CNDE = SOLID(J+3) * TAU(I) + CNDE
500 CONTINUE
1000 CONTINUE
8001 RETURN
END

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AFWL-TR-66-108, Vol II

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WI  FOR PH1, PH1/FJ
C    SUBROUTINE PH1
C      DIMENSION
C      1U(1200), V(1200), AMX(1200), AIX(1200), P(1200),
C      2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFIT(1200),
C      3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
C      4UX(52), X(53), XX(54), DY(100), Y(100), YY(101), PH1 0080
C      5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150), PH1 0090
C      6TAU(52), PL(200), PR(200), UL(200), UR(200), PH1 0100
C      7LEFT(100), YAMC(100), SIGC(100), GAMC(100), PH1 0110
C      8G(50), SOLID(400), TEMP(12), HEAD(12)
C      COMMON Z, XX, UR, PR, THETA, YY, PH1 0130
C      COMMON AID, AIX, AM, AMD, AMX, AREA, PH1 0140
C      COMMON BIG, BOUNCE, DDXN, DDVK, DVK, UX, PH1 0150
C      COMMON DY, E, FD, FS, FX, OUT, PH1 0160
C      COMMON P, PAHOVE, PBLO, PIDTS, PPAHOV, PRR, PH1 0170
C      COMMON PUL, QDT, RC, REZ, RHO, RL, PH1 0180
C      COMMON RR, SIG, G000FL, SWITCH, TABLM, TAU, PH1 0190
C      COMMON TAUOTS, TAUOTX, U, UK, URR, UT, PH1 0200
C      COMMON UU, UUU, UTEF, UVMAX, V, VAROVE, PH1 0210
C      COMMON VBLO, VEL, VK, VT, VTEF, VV, PH1 0220
C      COMMON VVABOV, VVBLO, W2, W3, WPS, WS, PH1 0230
C      COMMON WSA, WSB, WSC, XL, XLF, XN, PH1 0240
C      COMMON XR, YL, YLW, YN, YU, ZMAX, PH1 0250
C      COMMON I, II, IN, IR, IWS, IWSA, PH1 0260
C      COMMON IWSB, IWSC, IW1, J, JN, JP, PH1 0270
C      COMMON JR, K, KN, KP, KR, KRM, PH1 0280
C      COMMON L, M, MA, MB, MC, MD, PH1 0290
C      COMMON ME, MZ, N, NK, NKMAX, NK1, PH1 0300
C      COMMON NO, NR, G, SOLID, TEMP, PH1 0310
C      COMMON FIOUT, CAP, KFIT, ISEND, IGOTO, HEAD, PH1 0410
C      PH1 0420
C      EQUIVALENCE
C      1(Z(4), PRINTS), (Z(5), PRINTL), (Z(6), DUMPT7), (Z(7), CSTOP),
C      2(Z(8), PIDY), (Z(9), TMZ), (Z(10), SCYCLE), (Z(11), SPROB),
C      3(Z(12), GAMX), (Z(13), ETH), (Z(14), FFA), (Z(15), FFB),
C      4(Z(16), TMOZ), (Z(17), TMXZ), (Z(18), XMAX), (Z(19), TXMAX),
C      5(Z(20), TYMAX), (Z(21), AMDM), (Z(22), AMXM), (Z(23), DNN),
C      6(Z(24), DMIN), (Z(25), FEF), (Z(26), DTNA), (Z(27), CVIS),
C      7(Z(28), NPR), (Z(29), NPR1), (Z(30), NC), (Z(31), NPC),
C      8(Z(32), NRC), (Z(33), IMAX), (Z(34), IMAXA), (Z(35), JMAX),
C      9(Z(36), JMAXA), (Z(37), KMAX), (Z(38), KMAXA), (Z(39), NMAX),
C      10(Z(40), ND), (Z(41), KDT), (Z(42), IXMAX),
C      11(Z(43), NOU), (Z(44), NOPR), (Z(45), NIMAX), (Z(46), NJMAX),
C      12(Z(47), I1), (Z(48), I2), (Z(49), I3), (Z(50), I4),
C      13(Z(51), N1), (Z(52), N2), (Z(53), N3), (Z(54), N4),
C      14(Z(55), N5), (Z(56), N6), (Z(57), N7), (Z(58), N8),
C      15(Z(59), N9), (Z(60), N10), (Z(61), N11), (Z(62), NRM),
C      16(Z(63), TRAD), (Z(64), XNRG), (Z(65), SN), (Z(66), DXN),
C      17(Z(67), RADEH), (Z(68), RADET), (Z(69), RADEB), (Z(70), DTRAD),
C      18(Z(71), REZFCT), (Z(72), RSTOP), (Z(73), SHELL), (Z(74), BBOUND),
C      19(Z(75), TOZONE), (Z(76), ECK), (Z(77), SBOUND), (Z(78), X1),
C      20(Z(79), X2), (Z(80), Y1), (Z(81), Y2),
C      21(Z(82), CABLN), (Z(83), VISC), (Z(84), T), (Z(85), GMAX),
C      22(Z(86), WSGU), (Z(87), WSGX), (Z(88), GMADR), (Z(89), GMAXR),
C      23(Z(90), S1), (Z(91), S2), (Z(92), S3), (Z(93), S4),
C      24(Z(94), S5), (Z(95), S6), (Z(96), S7), (Z(97), S8),
C      25(Z(98), S9), (Z(99), S10)
C      EQUIVALENCE (Z(100), HVB), (Z(101), HCB), (Z(102), CB),

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1(Z(103),SV5),	(Z(104),ATOM),	(Z(105),CV),	(Z(106),GV),	
2(Z(107),SUMFE),	(Z(108),HETA),	(Z(109),ALCO),	(Z(110),ANH),	
3(Z(111),EZEHO),	(Z(112),PW),	(Z(113),CAPS),	(Z(114),HNU),	
3(Z(115),COE),	(Z(116),SCR),	(Z(117),ISR),	(Z(118),SCUR),	
4(Z(119),AHN),	(Z(120),UTH),	(Z(121),IH),	(Z(122),JH),	
5(Z(123),UTC),	(Z(124),IC),	(Z(125),JC),	(Z(126),RFT),	
X(Z(127),CUUT),	(Z(128),HCP),	(Z(129),HH),	(Z(130),CO),	
6(Z(131),J1),	(Z(132),J2),	(Z(133),J3),	(Z(134),J4),	
7(Z(135),J5),	(Z(136),J6),		(Z(138),SVMAX),	
8(Z(139),FRCUTC)				
OEQUIVALLNCE	(Z(140),VAPE),	(Z(141),RADE),	(Z(142),CNOE),	
1(Z(143),SCHR),	(Z(144),IV),	(Z(145),JV),	(Z(146),IU),	
2(Z(147),JU),	(Z(148),DTVF),	(Z(149),DTUF),	(Z(150),E11)	

C	OEQUIVALENCE	(XX(2),X(1)),	(UR,UL,FLEFT),	(UR(100),YAMC),	PH1 0710
	1(PH(100),SIGC),	(PK,PL,GAMC),	(DKE,THETA),	(UR,TAB),	PH1 0720
	2(UR(16),AMK),	(UR(31),PK),	(UR(46),QK),	(YY(2),Y(1))	PH1 0730
C					PH1 0740
C					PH1 0750
C					PH1 0760
C					PH1 0770
C					PH1 0780
C					PH1 0920
C					PH1 1060
C					PH1 1070
C					PH1 1080

C O M M O N

VELOCITIES AND INTERNAL ENERGY FOR PHASE ONE

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      UC=1.0E+15
      UT=0.0
      8000 CEL=1.0
      3301 KC=DX(1)/2.0
      RH=(X(1)+X(2))/2.0
      3304 DO 3360 I=1,IMAX
      TAUDTS=TAU(I)*DT
C
C   DETERMINE LIMITS ON J LOOP
      CALL DJLOW(JLOW,JHIGH)
C
      K=I+1+(JLOW-1)*IMAX
      DO 3348 J=JLOW,JHIGH
      T1=0.
      KB=K-IMAX
      N=K+IMAX
      PIDTS=1.0/(PIDY*DT*DY(J))
C   DOES CELL CONTAIN ACTIVE MASS
      10 IF(JMR(KFIT(K),2))9901,3340,20
C   DETERMINE LOCATION IN GRID FORM I,J(I.E.KFLAG)
      20 KFLAG=JMR(KFIT(K),1)
C   COMPUTATION OF PRESSURE AND VELOCITY AT RIGHT INTERFACE
      AND ASSOCIATED ENERGY CHANGES.
C
      GO TO(80,80,80,60,80,80,80,80,60,60,80,40,80,40,40,80),KFLAG
C   RIGHT TRANSMITTING INTERFACE AND ASSOCIATED TOTAL ENERGY CHANGE
      40 PRR=PL(J)
      URN=U(K)*KC
      ETH=ETH-(PRR*U(K)*KC)/PIDTS
      GO TO 110
C   REFLECTION AT RIGHT BOUNDARY.
      60 PRR=P(K)
      URN=0.0
      GO TO 110
C   NORMAL RIGHT INTERFACE COMPUTATION
      80 IF(JMR(KFIT(K+1),2))9902,107,106
      106 PRR=(P(K)+P(K+1))/2.0
      URN=(U(K)*KC+U(K+1)*KC)/2.0
      GO TO 110
      107 URN=U(K)*KC
  
```

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      PHR=0.0
C     COMPUTATION OF PRESSURE AND VELOCITY AT TOP INTERFACE
C     OF CELL AND ASSOCIATED ENERGY CHANGE.
110 GO TO(160,160,140,160,160,160,120,140,140,160,160,160,120,120,160,
      160),KFLAG
C     TRANSMITTING CONDITION AT TOP CELL INTERFACE AND ASSOCIATED
C     ENERGY LOSS
120 PABOVE=PBLO
      VABOVE=V(K)
      ETH=ETH-(PABOVE*V(K)*TAUDTS)/2.0
      GO TO 200
C     REFLECTION AT TOP INTERFACE OF CELL
140 JB=(I-1)*20+1
      IF(1.6T.15R) GO TO 150
      IF(SOLID(JB+2).EQ.0.) GO TO 150
      PT=AMAX1(SOLID(JB+1),AMAX1((3.*P(K)-P(KH))/2.0,P(K)) )
      IF(JMR(KFIT(KB)/2).EQ.0) PT=SOLID(JB+1)
145 PABOVE=PT
      T1= PT      *(V(K)- SOLID(JB+15))/2.0
      VABOVE= V(K)
      ETH=ETH- PT      *SOLID(JB+15)*TAUDTS/ 2.0
      GO TO 200
150 PABOVE=P(K)
      VABOVE=0.0
      GO TO 200
C     NORMAL CALCULATION AT TOP INTERFACE
160 IF(JMR(KFIT(N),2))9903,186,185
185 PABOVE=(P(K)+P(N))/2.0
      VABOVE=(V(K)+V(N))/2.0
      GO TO 200
186 PABOVE=0.0
      VABOVE=V(K)
C     DETERMINE IF THERE ARE BOUNDARY CONDITIONS
C     AT THE LEFT AND BOTTOM INTERFACES.
200 GO TO(3328,220,3328,3328,320,340,3328,220,3328,320,220,3328,220,
      13328,340,220),KFLAG
C     REFLECTION AT LEFT INTERFACE OF CELL
220 PL(J)=P(K)
      UL(J)=0.0
C     DETERMINE BOUNDARY CONDITIONS AT BOTTOM INTERFACE
      GO TO(3328,3328,3328,3328,320,340,3328,3328,3328,320,320,
      13328,3328,3328,340,340),KFLAG
C     REFLECTION AT BOTTOM INTERFACE
320 PBLO=P(K)
      VBLO=0.0
      GO TO 3328
C     TRANSMITTIVE AT BOTTOM INTERFACE
340 PBLO=PABOVE
      VBLO=V(K)
      ETH=ETH+(PABOVE*V(K)*TAUDTS)/2.0
C     VEL=1, FIRST PASS
3328 IF(VEL)9904,3327,3326
3326 CONTINUE
      V(K)=V(K)+(PBLO-PABOVE)/AMX(K)*TAUDTS
      IF(ABS(V(K)).LT.1.E1) V(K)=0.
      PH1 1800
3329 U(K)=U(K)+(PL(J)-PHR)/AMX(K)*RC/PIDTS*2.0
      IF(ABS(U(K)).LT.1.E1) U(K)=0.
      PH1 1830
3327 AIP=P(K)*((TAUDTS/2.0)*(VBLO-VABOVE)
      1 +(1.0/PIDTS)*(UL(J)-U(K)))
      PH1 1860
      PH1 1870
C     T1 IS ZERO EXCEPT AT J=WS
      AIP=AIP+TAUDTS *T1
      WSX=AIX(K)+AIP/AMX(K)
      PH1 1900
1000 IF(WSX)1011,1001,1001
1001 AIX(K)=WSX
      GO TO 3342

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1011	UT=1.0	PH1	1930
	*SA=2.0*AIK(KI/3.0*UT/(AIK(K)-WSX)	PH1	1940
1013	IF(WSA-UU)1014,1001,1001	PH1	1950
1014	UU=WSA	PH1	1960
	GO TO 1001	PH1	1970
3340	PRH=0.0	PH1	1980
	PABOVE=0.0	PH1	1990
	UHR=U(K+1)*HR	PH1	2000
	VABOVE=V(N)	PH1	2010
3342	VBLO=VABOVE	PH1	2020
	PL(J)=PRH	PH1	2030
	UL(J)=UHR	PH1	2040
	K=N	PH1	2050
3348	PBLO=PABOVE	PH1	2060
3355	KC=RH	PH1	2070
	HR=(X(1+1)+X(1+2))/2.0	PH1	2080
3360	CONTINUE	PH1	2090
3361	IF(VEL)9905,7040,3363		
3363	VEL=0.0	PH1	2110
	GO TO 3301	PH1	2120
C	ERROR	PH1	2130
9901	S1=8.0010		
	GO TO 9999		
9902	S1=8.0080		
	GO TO 9999		
9903	S1=8.0160		
	GO TO 9999		
9904	S1=8.3328		
	GO TO 9999		
9905	S1=8.3361		
9999	CALL EUIT		
C	NOTE, IF SN=0, CODE WILL INTEGRATE		
C	BACKWARDS TO CORRECT THE INTEGRATION OF		
C	INTERNAL ENERG, IF SN NOT 0, NEGATIVE		
C	ENERGIES ARE LEFT ALONE.		
7040	IF(SN)7030,7031,7030		
7031	IF(UT)7020,7030,7010		
7010	UT=-1.		
	UT=-UT	PH1	2270
	GO TO 8000	PH1	2280
7020	UT=0.		
	UT=UU	PH1	2300
	NR1=UT/TRAD+1.		
	NR=MIND(NRM,NR1)		
	WS=NR		
	TRAD=UT/WS	PH1	2330
	UTNA=UT	PH1	2340
	GO TO 8000	PH1	2350
7030	RETURN		
	END		

01 FOR PH2, PH2/FJ
SUBROUTINE PH2

PH2 0010

C
C
C

D I M E N S I O N

DIMENSION

10(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), F1OUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4UX(52), X(53), XX(54), DY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PR(200), UL(200), UR(200),
7LEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)
COMMON Z, XX, UR, PR, THETA, YY
COMMON AID, AIX, AM, AMU, AMX, AREA
COMMON BIG, BOUNCE, DDXN, DDVK, DVK, DX
COMMON UY, E, FD, FS, FX, OUT
COMMON P, PABOVE, PULO, PIOTS, PPAOV, PRR
COMMON PUL, QDT, RC, REZ, RHO, RL
COMMON KR, SIG, QUOOFL, SWITCH, TABLM, TAU
COMMON TAUOTS, TAUOTX, U, UK, URR, UT
COMMON UU, UUU, UTEF, UVMAX, V, VABOVE
COMMON VBLO, VEL, VK, VT, VTEF, VV
COMMON VVAOV, VVBLO, W2, W3, WPS, WS
COMMON WSA, WSB, WSC, XL, XLF, XN
COMMON XR, YL, YLW, YN, YU, ZMAX
COMMON I, II, IN, IR, IWS, IWSA
COMMON IWSU, IWSC, IW1, J, JN, JP
COMMON JK, K, KN, KP, KR, KRM
COMMON L, M, MA, MB, MC, MD
COMMON ME, NZ, N, NK, NKMAX, NK1
COMMON NO, NR, G, SOLID, TEMP
COMMON F1OUT, CAP, KFIT, ISEND, IGOTO, HEAD

C
C
C
C

E Q U I V A L E N C E

0EQUIVALENCE (Z, IZ, PROB), (Z(2), CYCLE), (Z(3), DT),
1(Z(4), PRINTS), (Z(5), PRINTL), (Z(6), DUMPT7), (Z(7), CSTOP),
2(Z(8), PIUY), (Z(9), TMZ), (Z(10), SCYCLE), (Z(11), SPROB),
3(Z(12), GAMX), (Z(13), ETH), (Z(14), FFA), (Z(15), FFB),
4(Z(16), TMDZ), (Z(17), TMXZ), (Z(18), XMAX), (Z(19), TXMAX),
5(Z(20), TYMAX), (Z(21), AMDH), (Z(22), AMXM), (Z(23), DNN),
6(Z(24), DMIN), (Z(25), FEF), (Z(26), DTNA), (Z(27), CVIS),
7(Z(28), NPR), (Z(29), NPR1), (Z(30), NC), (Z(31), NPC),
8(Z(32), NRC), (Z(33), IMAX), (Z(34), IMAXA), (Z(35), JMAX),
9(Z(36), JMAXA), (Z(37), KMAX), (Z(38), XMAXA), (Z(39), NMAX),
0EQUIVALENCE (Z(40), ND), (Z(41), KDT), (Z(42), IXMAX),
1(Z(43), NOD), (Z(44), NOPR), (Z(45), NIMAX), (Z(46), NJMAX),
2(Z(47), I1), (Z(48), I2), (Z(49), I3), (Z(50), I4),
3(Z(51), N1), (Z(52), N2), (Z(53), N3), (Z(54), N4),
4(Z(55), N5), (Z(56), N6), (Z(57), N7), (Z(58), N8),
5(Z(59), N9), (Z(60), N10), (Z(61), N11), (Z(62), NRM),
6(Z(63), TRAD), (Z(64), XNRG), (Z(65), SN), (Z(66), DXN),
7(Z(67), RADER), (Z(68), RADET), (Z(69), RADEB), (Z(70), DTRAD),
8(Z(71), REZFCT), (Z(72), RSTOP), (Z(73), SHELL), (Z(74), DBOUND),
9(Z(75), TOZONE), (Z(76), ECK), (Z(77), SBOUND), (Z(78), X1),
0EQUIVALENCE (Z(79), X2), (Z(80), Y1), (Z(81), Y2),
1(Z(82), CABLN), (Z(83), VISC), (Z(84), T), (Z(85), GMAX),
2(Z(86), WSGD), (Z(87), WSGX), (Z(88), GMADR), (Z(89), GMAXR),
3(Z(90), S1), (Z(91), S2), (Z(92), S3), (Z(93), S4),
4(Z(94), S5), (Z(95), S6), (Z(96), S7), (Z(97), S8),
5(Z(98), S9), (Z(99), S10)

C

PH2 0740
PH2 0760
PH2 0900
PH2 0980
PH2 0990
PH2 1010

PH2 1060
PH2 1070
PH2 1080
PH2 1090
PH2 1100
PH2 1110
PH2 1120

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      AMMV=0.0
      DELEB=0.0
      GO TO 99
85  AMMY=(AMX(K)*V(K)*DT)/DY(J)
      IF (AMMY+AMX(K)) 97,100,100
97  AMMY=-AMX(K)
100 AMMV=2.0*AMMY+V(K)
      AMMY=0.0
      AMMU=0.0
      DELEB=0.0
      GO TO 99
C   TRANSMITTIVE AT BOTTOM INTERFACE
82  IF (V(K).EQ.0.) GO TO 84
      AMMU=AMMY+U(K)
      AMMV =AMMY+V(K)
      DELEB =AIX(K)+ (U(K)**2 +V(K)**2)/2.
      ETH =ETH + AMMY*DELEB
C   TEST BOUNDARY CONDITION AT LEFT CELL INTERFACE
99  GO TO (301,105,301,301,301,301,301,105,301,301,105,
      301,105,301,301,105),KFLAG
C   REFLECT AT LEFT INTERFACE OF CELL
105 IF (U(K))108,107,107
107 FLEFT(J)=0
      GO TO 767
108 GAMC(J)=(AMX(K)*X(I)*2.0*U(K))/(TAU(I)*PIDS)
      IF (GAMC(J)+AMX(K)) 765,766,766
765 GAMC(J)=-AMX(K)
766 FLEFT(J)=2.0*GAMC(J)*U(K)
767 GAMC(J)=0.0
      YAMC(J)=0.0
      SIGC(J)=0.0
C   TOP INTERFACE OF CELL COMPUTATION
301 GO TO (304,304,302,304,304,304,304,303,302,302,304,
      1304,304,303,303,304,304),KFLAG
C   REFLECT AT TOP CELL INTERFACE
302 IF ((I.GT.ISH) .OR. (SOLID(I5+2).EQ.0.)) GO TO 3302
      AMPY=-SOLID(I5+14)
      IF (AMPY.EQ.0.) GO TO 501
      GO TO 503
3302 IF (V(K)) 305,305,300
305 AMVT=0.0
      GO TO 501
306 AMPY=(AMX(K)*V(K)*DT)/DY(J)
      IF (AMPY+AMX(K)) 307,308,308
307 AMPY=-AMX(K)
308 AMVT=2.0*AMPY+V(K)
501 AMPY=0.0
      AMUT=0.0
      DELET=0.0
      GO TO 503
C   TRANSMIT AT TOP CELL INTERFACE
303 IF (V(K))504,504,508
504 AMPY=0.0
      AMUT=0.0
      AMVT=0.0
      DELET=0.0
      GO TO 503
508 IF (AMX(K))504,504,98
98  AMPY=(AMX(K)*V(K)*DT)/DY(J)
      GO TO 503
C   NO BOUNDARY CONDITIONS AT TOP INTERFACE
304 IF ((AMX(L).NE.0.) .AND. (JMK(KFIT(L),2).EQ.0)
      1 .AND. (J.EQ.J5-1)) GO TO 214
      IF (JMR(KFIT(L),2).EQ.0 ) GO TO 703
214 IF (JMK(KFIT(K ),2).NE.0) GO TO 209

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DLTZ=UY(J+1)
DLZ=FIOUT(K)
FMT=.5
VFR=P(K)
IF((J.LT.J5-1).OR.(1.GT.ISH).OR.(AMX(K).NE.0.)) GO TO 216
VFR=(GV+1.)*(-CO)/(GV-1.)
P(K)=VFR
GO TO 2166
216 IF(AUS(V(L)).GT.ABS(P(K))) VFR=V(L)
IF((AMX(K).NE.0.).AND.(AUS(V(K)).GT.ABS(P(K)))) VFR=V(K)
P(K)=VFR
2166 VABOVE=V(L)+(VFR-V(L))*DY(J+1)/(DY(J+1)+2.*FIOUT(K))
FIOUT(K)=ABS(VFR)*DT+FIOUT(K)
IF(FIOUT(K).GE.DY(J)-1.E-7) P(K)=P(K)
IF((FIOUT(K).GE.DY(J)-1.E-7).AND.(JMR(KFIT(K+1),2).LT.0.))
2 THETA(K+1)=THETA(K)
IF(FIOUT(K).GE.DY(J)) FIOUT(K)=FIOUT(K)-DY(J)
FMT=(FIOUT(K)/(DLTZ+DLZ))*4*(1.-(DLZ/FIOUT(K))*4)*FMT
IF(FMT.GT.1.) FMT=1.
AMPY=-AMX(L)*FMT
VFI=VABOVE**2+U(L)**2-AMX(K)/(AMX(K)-AMPY)*((V(K)-VABOVE)**2
2 +(U(K)-U(L))**2)
GO TO 503
215 IF(JMR(KFIT(K),2).EQ.0) GO TO 504
208 VABOVE=V(K)
GO TO 212
209 VABOVE=V(L)+(V(K)-V(L))*DY(J+1)/(DY(J+1)+DY(J))
212 CONTINUE
IF(VABOVE)701,703,700
700 IF(AMX(K))703,703,704
703 AMPY=0
AMUT=0
AMVT=0
DELET=0
GO TO 503
704 KC=L
KD=K
JJ=J
IF(((RHO(L).GT.RHO(K)).AND.(VABOVE.LT.0.)).OR.
2 ((RHO(L).LT.RHO(K)).AND.(VABOVE.GE.0.)))
3 GO TO 6140
AMPY=TAU(I)*RHO(KD)*VABOVE*DT
IF(V(KD)*V(KC).LT.0.) AMPY=0.
GO TO 6150
6140 AMPY=TAU(I)/3.*(RHO(L)*V(L)+RHO(K)*V(K)
1+VABOVE*SQRT(RHO(K)*RHO(L)))*DT
IF(AMPY+VABOVE.LT.0.) AMPY=0.
6150 AVW=.5*(1.+RHO(KC)/RHO(KD))
VABOVE=AVW*V(KD)+(1.-AVW)*V(KC)
GO TO 503
701 IF(AMX(L))703,703,705
705 KC=K
KD=L
JJ=J+1
IF(((RHO(L).GT.RHO(K)).AND.(VABOVE.LT.0.)).OR.
2 ((RHO(L).LT.RHO(K)).AND.(VABOVE.GE.0.)))
3 GO TO 6140
AMPY=TAU(I)*RHO(KD)*VABOVE*DT
IF(V(KD)*V(KC).LT.0.) AMPY=0.
GO TO 6150
C RIGHT INTERFACE OF CELL CALCULATION
503 GO TO(405,405,405,706,405,405,405,405,706,706,
1405,707,405,707,707,405),KFLAG
C REFLECT AT RIGHT CELL INTERFACE
706 IF(U(K))708,708,710

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PH2 1510

PH2 1520

PH2 1540

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708 AMJR=0.0
GO TO 709
710 AMMP=(AMX(K)*X(I)*2.0*U(K))/(TAU(I)*PIDTS)
IF (AMMP-AMX(K)) 712,712,711
711 AMMP=AMX(K)
712 AMUR=2.0*AMMP*U(K)
709 AMMP=0.0
AMVR=0.0
DELER=0.0
GO TO 716
C TRANSMIT AT RIGHT CELL INTERFACE
707 IF (U(K)) 713,713,714
713 AMMP=0.0
AMUR=0.0
AMVR=0.0
DELER=0.0
GO TO 716
714 IF (AMX(K)) 713,713,715
715 AMMP=(2.0*AMX(K)*X(I)*U(K))/(TAU(I)*PIDTS)
GO TO 716
405 IF (JMR(KFIT(K+1),2)) 411,411,409
409 IF (AMX(K)) 410,410,407
410 URR=U(K+1)
GO TO 408
411 IF (JMR(KFIT(K),2).EQ.1) GO TO 406
405 URR=0.0
GO TO 408
406 CONTINUE
DLTZ= DX(I+1)
DLZ= CAP(K+1)
LFR=THETA(K+1)
IF (ABS(U(K)).GT.ABS(THETA(K+1))) UFR=U(K)
IF (J.EQ.J5) UFR=2.*CU/(GV-1.)
IF ((AMX(K+1).NE.0.).AND.(ABS(U(K+1)).GT.ABS(THETA(K+1))))
2 UFR=U(K+1)
THETA(K+1)=UFR
URR=U(K)+(UFR -U(K))*DX(I)/(DX(I)+CAP(K+1))
CAP(K+1)= ABS(UFR)*DT+CAP(K+1)
IF (CAP(K+1).GE.DX(I+1)-1.E-7) THETA(K+2)=THETA(K+1)
IF ((CAP(K+1).GE.DX(I+1)-1.E-7).AND.(JMR(KFIT(KB+1),2).EQ.0))
2 P(KB+1)=P(K+1)
IF (CAP(K+1).GT.DX(I+1)) CAP(K+2)=CAP(K+1)-DX(I+1)
FMT=(CAP(K+1)/(DLTZ+DLZ))**4*(1.-(DLZ/CAP(K+1))**4)
FMT=.5*FMT
IF (FMT.GT.1.) FMT=1.
AMMP=AMX(K)*FMT
UFI=URR**2+V(K)**2-AMX(K+1)/(AMX(K+1)+AMMP)*((U(K+1)-URR)**2
2 +(V(K+1)-V(K))**2)
GO TO 716
407 URR=U(K)+(U(K+1)-U(K))*DX(I+1)/(DX(I)+DX(I+1))
408 CONTINUE
C NO BOUNDARY CONDITIONS AT RIGHT INTERFACE
IF (URR) 718,719,717
717 IF (AMX(K)) 719,719,720
720 KC=K+1
KD=K
GO TO 730
6100 CONTINUE
XB=X(I)-DX(I)/2.
XBP=X(I+1)-DX(I+1)/2.
AMMP=((RHO(K)*XB *U(K)+RHO(K+1)*XBP *U(K+1))
1 +URR*X(I)*SQRT(RHO(K)*RHO(K+1)))*2./PIDTS*.33333*DY(J)
IF (AMMP*URR.LT.0.) AMMP=0.
6110 AUW=.5*(1.+RHO(KC)/RHO(KD))
IF (AUW.GT.1.) AUW=1.

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PH2 1600
PH2 1610
PH2 1620

PH2 1640
PH2 1650

PH2 1700

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      URR=AUR*U(KD)+(1.-AUR)*U(KC)
      IF (U(K).NE.0.) GO TO 716
      URR=0.
719  AMMP=0.0
      AMUR=0.0
      AMVR=0.0
      UELER=0.0
      GO TO 716
718  IF (AMX(K+1)) 719,719,721
721  KC=K
      KD=K+1
730  IF (((RHO(K).GT.RHO(K+1)).AND. (URR.GT.0.)) .OR.
2    ((RHO(K).LT.RHO(K+1)).AND. (URR.LT.0.)))
3    TEST=DONNER
      AMMP=RHO(KD)*X(I)*URR*2./PIDTS*DY(J)
      IF (U(KD)*U(KC).LT.0.) AMMP=0.
      GO TO 6110
716  CONTINUE
      IF (JMR(KFIT(K ),2).EQ.0) GO TO 7260
      IF (J.EQ.J5) GO TO 7160
      IF (JMR(KFIT(L),2).EQ.0) GO TO 7160
      VPLUS=V(LP)+(V(L)-V(LP))*DY(J+2)/(DY(J+2)+DY(J+1))
      IF (VPLUS) 7020,7010,7010
7010  KC=LP
      KD=L
      JJ=J+1
      GO TO 7030
7020  KC=L
      KD=LP
      JJ=J+2
7030  IF ((( RHO(LP).GT.RHO(L)).AND.(VPLUS.LE.0.)) .OR.
2    (( RHO(LP).LT.RHO(L)).AND.(VPLUS.GE.0.)))
3    GO TO 7040
      AMMPY=TAU(I )*RHO(KD)*VPLUS*DT
      IF (V(KD)*V(KC).LT.0.) AMMPY=0.
      GO TO 7050
7040  CONTINUE
      AMMPY=TAU(I)/3.*(RHO(LP)*V(LP)+RHO(L)*V(L)
1    +VPLUS*SQRT(RHO(L)*RHO(LP)))*DT
      IF (AMMPY*VPLUS.LT.0.) AMMPY=0.
7050  CONTINUE
      IF (JMR(KFIT(LP),2).EQ.0) AMMPY=0.
      IF ( (J.EQ.J5-1).AND.(I.LE.ISR) ) AMMPY =-SOLID(15+14 )
      IF ( (J.EQ.J5-1).AND.(I.GT.ISR) ) AMMPY =0.
      UPS=U(L)+(U(L+1)-U(L))*DX(I)/(DX(I)+DX(I+1))
      IF (UPS) 7070,7065,7065
7065  KD=L
      KC=L+1
      GO TO 7080
7070  KC=L
      KD=L+1
7080  IF (((RHO(L).GT.RHO(L+1)).AND. (UPS.GT.0.)) .OR.
2    ((RHO(L).LT.RHO(L+1)).AND.(UPS.LT.0.)))
3    TEST=DONER
      AMMMP = RHO(KD)*X(I)*UPS*2./ PIDTS*DY(J)
      IF (U(KD)*U(KC).LT.0.) AMMMP=0.
      GO TO 7095
7090  CONTINUE
      XB=X(I)-DX(I)/2.
      XBP=X(I+1)-DX(I+1)/2.
      AMMMP= (RHO(L)*XB*U(L)+RHO(L+1)*XBP*U(L+1)
1    +UPS*X(I)*SQRT(RHO(L)*RHO(L+1)))*2./PIDTS*.33333*DY(J+1)
      IF (AMMMP*UPS.LT.0.) AMMMP=0.
7095  CONTINUE
      IF (JMR(KFIT(L+1),2).EQ.1) GO TO 7060

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      IF (AMX(L+1).EQ.0.)      UFR = 1.5*U(L)
      IF (ABS(THETA(L+1)).LT.ABS(U(L)))      UFR= U(L)
      ULTZ=UX(I+1)
      ULZ=CAP(L+1)
      CAPLP=CAP(L+1)+ABS(UFR)*DT
      FMT=(CAPLP/(ULTZ+ULZ))*4*(1.-(ULZ/CAPLP))*4)
      FMT=.5+FMT
      AMMMP=AMX(L)*(AMIN1(FMT,1.))
7060 CONTINUE
      IF ((GAMC(J+1)-AMMPY+AMX(L)*.5).GE.(AMMMP-AMPY)) GO TO 7160
      WSA =(GAMC(J+1)-AMMPY+AMX(L)*.5)/(AMMMP-AMPY)
      AMPY=AMPY+WSA
7160 CONTINUE
      IF (JMR(KFIT(K+1),2).EQ.0) GO TO 7260
      AMMPY=AMPY
      IF ((J.EQ.J5) .AND. (I.LE.ISR)) AMMPY=-SOLID(IS+14)
      IF ((J.EQ.J5) .AND. (I.GT.ISR)) AMMPY=0.
      IF (GAMC(J)-AMMPY+AMX(K)*.5.GT.AMMP-AMMY) GO TO 7260
      AMMP = GAMC(J)-AMMPY+AMMY+AMX(K)*.5
      IF (AMMP.LT.0.) AMMP = 0.
7260 CONTINUE
      FLO=F IOUT(K)-(DY(J)-1.E-7)
309 IF (AMPY)8834,8831,8833
8833 IF (JHIGH-J)9901,318,8835
8835 IF (JMR(KFIT(K),2).EQ.1) GO TO 8837
      KM=K-IMAX
      IF (JMR(KFIT(KM),2).EQ.0) GO TO 8838
      IF (FLO.LT.0.) GO TO 8837
      CALL MFST(KFIT(K),2)
      GO TO 318
8837 IF (TAU(I )+DY(J )/ AMPY .LT.Z(138) ) GO TO 318
8838 AMPY=0.0
      GO TO 8831
8834 IF (J-JLOW)9902,325,8839
8839 KP=K+IMAX
      IF (J.EQ.JHIGH) GO TO 8840
      IF (JMR(KFIT(K),2).EQ.1) GO TO 8840
      IF (JMR(KFIT(KP),2).EQ.0) GO TO 8841
      IF (FLO.LT.0.) GO TO 8840
      CALL MFST(KFIT(K),2)
      GO TO 325
8840 IF (TAU(I )+DY(J+1)/(-AMPY).LT.Z(138) ) GO TO 325
8841 AMPY=0.0
      GO TO 8831
318 UELM=GAMC(J)+AMMY-AMPY
322 IF (J-JHIGH)324,323,324
323 WS=U(K)**2+V(K)**2
      ETH=ETH-AMPY*(AIX(K)+WS/2.0)
      IF (AMPY/(TAU(I)+DY(J))-TOZONE)324,324,6900
6900 REZ=1.0
324 GO TO (6901,6901,326,6901,6901,6901,6901,326,326,
16901,6901,6901,6901,6901,6901,6901),KFLAG
6901 AMUT=AMPY*U(K)
      AMVT=AMPY*V(K)
      GO TO 326
325 CONTINUE
8831 GO TO(6902,6902,6903,6902,6902,6902,6902,6903,6903,
16902,6902,6902,6902,6902,6902,6902),KFLAG
6902 AMUT=AMPY*U(L)
      AMVT =AMPY*VABOVE
      IF (ABS(AMVT).GT.ABS(AMX(L)*V(L))) AMVT=SIGN((AMX(L)*V(L)),AMVT)
6903 UELM=GAMC(J)-AMPY+AMMY
326 IF (AMPY)327,328,328
327 DELET=AIX(L)+(U(L)**2+V(L)**2)/2.0
      IF ( (I.GT.ISR) .OR. (J.LT.J5) ) GO TO 3327

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PH2 3390

PH2 3440
PH2 3450PH2 3490
PH2 3500
PH2 3510PH2 3530
PH2 3540
PH2 3550
PH2 3560PH2 3580
PH2 3590
PH2 3600PH2 3640
PH2 3650

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DELET=HVB+HCB+SOLID(15+15)**2/2.
AMUT=0.
AMVT=AMPY+SOLID(15+15)
ETH=ETH-AMPY*(HVB+HCB+SOLID(15+15)**2/2.)
GO TO 333
3327 CONTINUE
AMAS=RHO(K)/RHO(L)
AMW= 0.63 + 0.233*AMAS
IF(AMAS.GE..3)
  I AMW=.25+1.5*AMAS
  IF(AMW.GE.1.) AMW=1.
  DEKTT=AIX(K)+(U(L)**2+V(K)**2) /2.
  DELET=AMW*DELET+(1.-AMW)*DEKTT
  IF(JMR(KFIT(K),2).NE.1) DELET=HVB+HCB-HCP +VFI/2.
  GO TO 333
328 IF(AMMY)329,330,330
329 DELET=DELEB
GO TO 333
330 IF(GAMC(J))331,332,332
331 DELET=SIGC(J)
GO TO 333
332 DELET=AIX(K)+(U(K)**2+V(K)**2)/2.0
333 SIGMU=LEFT(J)+AMMU-AMUT
SIGMV=YAMC(J)+AMMV-AMVT
DELEK=GAMC(J)*SIGC(J)+AMMY*DELEB-AMPY*DELET
FLO=CAP(K+1)-(DX(I+1)-I.E-7)
509 IF(AMMP)8843,518,8844
8844 IF(I.EQ.IMAX) GO TO 518
IF(JMR(KFIT(K),2).NE.1) GO TO 8847
IF(JMR(KFIT(K+1),2).EQ.1) GO TO 8846
IF(FLO.LT.0.) GO TO 8846
CALL MFST(KFIT(K+1),2)
GO TO 518
8846 GO TO 518
8847 AMMP=0.0
GO TO 518
8843 IF(I.EQ.II+1) GO TO 512
IF(JMR(KFIT(K+1),2).NE.1) GO TO 8850
IF(JMR(KFIT(K),2).EQ.1) GO TO 8849
IF(FLO.LT.0.) GO TO 8849
CALL MFST(KFIT(K),2)
GO TO 512
8849 IF( TAU(I+1)*DY(J )/(-AMMP).LT.Z(138) ) GO TO 512
8850 AMMP=0.0
GO TO 518
512 DELM=DELM-AMMP+AMX(K)
513 CONTINUE
514 CONTINUE
8828 AMUR=AMMP*U(K+I)
AMVR=AMMP*V(K+I)
GO TO 525
518 DELM=DELM-AMMP+AMX(K)
521 CONTINUE
522 GO TO (524,524,524,524,524,524,524,524,524,
I524,524,523,524,523,523,524),KFLAG
523 WS=U(K)**2+V(K)**2
ETH=ETH-AMMP*(AIX(K)+WS/2.0)
524 AMUR = AMMP*U(K)
IF(ABS(AMUR).GT.ABS(AMX(K)*U(K))) AMUR=SIGN((AMX(K)*U(K)),AMUR)
AMVR=AMMP*V(K)
525 SIGMU=SIGMU-AMUR
SIGMV=SIGMV-AMVR
526 TIC=0.0
531 IF(AMMP)532,533,534
532 DELEK= AIX(K+1)+(U(K+1)**2+V(K+1)**2)/2.

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PH2 3660
 PH2 3670
 PH2 3680
 PH2 3690
 PH2 3700
 PH2 3710
 PH2 3720
 PH2 3730
 PH2 3740
 PH2 3750
 PH2 3760

 PH2 3770

 PH2 3810
 PH2 3820

 PH2 3860
 PH2 3870
 PH2 3880
 PH2 3890
 PH2 3900
 PH2 3910
 PH2 3920
 PH2 3930
 PH2 3940
 PH2 3950

 PH2 3970
 PH2 3980

 PH2 4020
 PH2 4030
 PH2 4040
 PH2 4050

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GO TO 535
533 DELEK=0.
GO TO 535
534 DELEK= AIX(K)+(U(K)**2+V(K)**2) /2.
      AMAS = RHO(K+1)/RHO(K)
      AMW = 0.63+0.233*AMAS
      IF (AMAS.GE..3)
1 AMW=.25+1.5*AMAS
      IF (AMW.GE.1.) AMW=1.
      DEKTT=AIX(K+1)+(U(K+1)**2+V(K )**2)/2.
      DELEK=AMW*DELEK+(1.-AMW)*DEKTT
      IF (JMR(KFIT(K+1),2).NE.1) DELEK=HVB+HCB-HCP+UF1/2.
535 DELEK= DELEK-AMMP*DELEK
      WS= AIX(K)+(U(K)**2+V(K)**2)/2.
538 ETH=ETH+FSR+FSB
540 ENK=AMX(K)*WS+DELEK+FSB+FSR
541 U(K)=(SIGMU+AMX(K)*U(K))/DELM
601 V(K)=(SIGMV+AMX(K)*V(K))/DELM
603 WS=U(K)**2+V(K)**2
542 AIX(K)=ENK/DELM-WS/2.0
543 AMX(K)=DELM
      RHO(K)=AMX(K)/(DY(J)*TAU(1))
      IF (AMX(K).GT.0.) GO TO 544
      AIX(K)=0.
      U(K)=0.0
      V(K)=0.0
      P(K)=0.0
      RHO(K)=0.
544 GAMC(J)=AMMP
      FLEFT(J)=AMUH
      YAMC(J)=AMVR
      SIGC(J)=DELEK
545 AMMY=AMPY
      AMMU=AMUT
      AMMV=AMVT
      DELEB=DELET
702 CONTINUE
      GO TO (546,546,549,546,546,546,546,549,549,546,546,
1546,546,546,546,546),KFLAG
546 K=K+IMAX
      LL=K-1MAX
549 CONTINUE
547 CONTINUE
6801 CONTINUE
6802 GO TO 548
9901 S1=9.8833
      GO TO 9999
9902 S1=9.8834
9999 CALL ED1T
548 SUM=0.0
      UO 650 I=1,IMAX
      UO 650 J=1,JMAX
      K=(J-1)*IMAX+1+1
      IF ((JMR(KFIT(K),2).EQ.2).AND.(AMX(K).GT.0.)) GO TO 610
      GO TO 645
610 L=K+1MAX
      CALL MFST(KFIT(K),1)
645 SV=1./RHO(K)
      IF (JMR(KFIT(K),2).NE.0)
1CALL ES(SV,AIX(K),THETA(K),P(K),CAP(K),GG)
650 CONTINUE
8001 RETURN
      END

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PH2 4300
PH2 4310
PH2 4400
PH2 4410
PH2 4420

PH2 4450
PH2 4460
PH2 4470

PH2 4480
PH2 4490
PH2 4500
PH2 4510
PH2 4520
PH2 4530
PH2 4540
PH2 4550

PH2 4560

PH2 4640
PH2 4720
PH2 4730

PH2 4970

PH2 5260
PH2 5270

```

01  FOR FLAG, FLAG/FJ
    SUBROUTINE FLAG(KFLAG, JLOW, JHIGH)
        DIMENSION
10(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4DX(52), X(53), XX(54), OY(100), Y(100), YY(101),
5TAU(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PH(200), UL(200), UR(200),
7FLEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)
COMMON Z, XX, UR, PR, THETA, YY
COMMON AID, AIX, AM, AMD, AMX, AREA
COMMON BIG, BOUNCE, DDXN, DDVK, DVK, DX
COMMON OY, E, FO, FS, FX, OUT
COMMON P, PABOVE, PBLO, PIDTS, PPAHOV, PRR
COMMON PUL, QUT, RC, REZ, RHO, RL
COMMON HR, SIG, QOOFL, SWITCH, TABLM, TAU
COMMON TAUUTS, TAUUTX, U, UK, URR, UT
COMMON UU, UUU, UTEF, UVMAX, V, VAROVE
COMMON VBLO, VEL, VK, VT, VTEF, VV
COMMON VVABOV, VVBLO, W2, W3, WPS, WS
COMMON WSA, WSB, WSC, XL, XLF, XN
COMMON XR, YL, YLW, YN, YU, ZMAX
COMMON I, II, IN, IR, IWS, IWSA
COMMON IWSB, IWSC, IW1, J, JN, JP
COMMON JR, K, KN, KP, KR, KRM
COMMON L, M, MA, MB, MC, MD
COMMON ME, MZ, N, NK, NKMAX, NK1
COMMON NO, NR, G, SOLID, TEMP
COMMON FIOUT, CAP, KFIT, ISEND, IGOTO, HEAD

C
C
C
E Q U I V A L E N C E

0EQUIVALENCE (Z(12),PROB), (Z(2),CYCLE), (Z(3),DT),
1(Z(4),PRINTS), (Z(5),PRINTL), (Z(6),DUMPT7), (Z(7),CSTOP),
2(Z(8),PIUY), (Z(9),TMZ), (Z(10),SCYCLE), (Z(11),SPROB),
3(Z(12),GAMX), (Z(13),ETH), (Z(14),FFA), (Z(15),FFB),
4(Z(16),TMDZ), (Z(17),TMXZ), (Z(18),XMAX), (Z(19),YXMAX),
5(Z(20),TYMAX), (Z(21),AMD), (Z(22),AMXM), (Z(23),DNN),
6(Z(24),DMIN), (Z(25),FEF), (Z(26),DTNA), (Z(27),CVIS),
7(Z(28),NPR), (Z(29),NPRI), (Z(30),NC), (Z(31),NPC),
8(Z(32),NRC), (Z(33),IMAX), (Z(34),IMAXA), (Z(35),JMAX),
9(Z(36),JMAXA), (Z(37),KMAX), (Z(38),KMAXA), (Z(39),NMAX),
0EQUIVALENCE (Z(40),ND), (Z(41),KDT), (Z(42),IXMAX),
1(Z(43),NOD), (Z(44),NOPR), (Z(45),NIMAX), (Z(46),NJMAX),
2(Z(47),I1), (Z(48),I2), (Z(49),I3), (Z(50),I4),
3(Z(51),N1), (Z(52),N2), (Z(53),N3), (Z(54),N4),
4(Z(55),N5), (Z(56),N6), (Z(57),N7), (Z(58),N8),
5(Z(59),N9), (Z(60),N10), (Z(61),N11), (Z(62),NRM),
6(Z(63),TRAD), (Z(64),XNRG), (Z(65),SN), (Z(66),DXN),
7(Z(67),RADER), (Z(68),RADET), (Z(69),RAUEB), (Z(70),DTRAD),
8(Z(71),REZFCT), (Z(72),RSTOP), (Z(73),SHELL), (Z(74),BBOUND),
9(Z(75),TOZONE), (Z(76),ECK), (Z(77),SBOUND), (Z(78),X1),
0EQUIVALENCE (Z(79),X2), (Z(80),Y1), (Z(81),Y2),
1(Z(82),CABL), (Z(83),VISC), (Z(84),T), (Z(85),GMAX),
2(Z(86),WSGD), (Z(87),WSGX), (Z(88),GMADR), (Z(89),GMAXR),
3(Z(90),S1), (Z(91),S2), (Z(92),S3), (Z(93),S4),
4(Z(94),S5), (Z(95),S6), (Z(96),S7), (Z(97),S8),
5(Z(98),S9), (Z(99),S10)

C
0EQUIVALENCE (Z(100),HVB), (Z(101),HCB), (Z(102),CB),
1(Z(103),SVS), (Z(104),ATOM), (Z(105),CV), (Z(106),GV),
2(Z(107),SUMFL), (Z(108),BETA), (Z(109),ALCO), (Z(110),ANN),

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3(Z(111),EZERO),	(Z(112),PW),	(Z(113),CAPS),	(Z(114),HNU),
3(Z(115),COE),	(Z(116),SCR),	(Z(117),ISH),	(Z(118),SCUR),
4(Z(119),AHN),	(Z(120),DTH),	(Z(121),IH),	(Z(122),JH),
5(Z(123),DTC),	(Z(124),IC),	(Z(125),JC),	(Z(126),RFT),
X(Z(127),CDUT),	(Z(128),HCP),	(Z(129),HH),	(Z(130),CO),
6(Z(131),J1),	(Z(132),J2),	(Z(133),J3),	(Z(134),J4),
7(Z(135),J5),	(Z(136),J6),		(Z(138),SVMAX),
8(Z(139),FRCUTC)			
OEQUIVALENCE	(Z(140),VAPE),	(Z(141),HADE),	(Z(142),CNDE),
1(Z(143),SCRE),	(Z(144),IV),	(Z(145),JV),	(Z(146),IU),
2(Z(147),JU),	(Z(148),DTVF),	(Z(149),DTUF),	(Z(150),E11)

C

OEQUIVALENCE	(XX(2),X(1)),	(UR,UL,FLEFT),	(UR(100),YAMC),
1(PRI(100),S1GC),	(PK,PL,GAMC),	(DKE,THETA),	(UR,TAU),
2(UR(16),AMK),	(UR(31),PK),	(UR(46),OK),	(YY(2),Y(1))

C
C
C
C

C O M M O N

TEST RIGHT BOUNDARY.
IF(1.EQ.I1+1) GO TO 20
IF(1.EQ.I2) GO TO 40
C TEST LEFT BOUNDARY.
IF(1.EQ.IMAX) GO TO 60
IF(1.LT.I2) GO TO 40
KFLAG=1
IF(J.EQ.JLOW)KFLAG=5
IF(J.EQ.JHIGH)KFLAG=7
RETURN
20 KFLAG=2
IF(J.EQ.JLOW)KFLAG=11
IF(J.EQ.JHIGH)KFLAG=8
RETURN
40 KFLAG=1
IF(J.EQ.JLOW)KFLAG=5
IF(J.EQ.JHIGH)KFLAG=3
IF((1.EQ.I2).AND.(I2.EQ.IMAX)) GO TO 70
RETURN
60 KFLAG=12
IF(J.EQ.JHIGH)KFLAG=14
65 IF(J.EQ.JLOW)KFLAG=10
RETURN
70 KFLAG=12
IF(J.EQ.JHIGH) KFLAG=9
GO TO 65
END

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01 FOR DJLOW, DJLOW/FJ
SUBROUTINE DJLOW(JLOW, JHIGH)
C U I M L N S I O N
C

DIMENSION
1J(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TABLM(50),
4UX(52), X(53), XX(54), DY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PK(200), UL(200), UR(200),
7FLEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)

COMMON	Z	XX	UR	PR	THETA	YY
COMMON	AID	AIX	AM	AMD	AMX	AREA
COMMON	BIG	BOUNCE	DDXN	DDVK	DVK	UX
COMMON	DY	E	FD	FS	FX	OUT
COMMON	P	PABOVE	PBLO	PIOTS	PPAHOV	PRR
COMMON	PUL	QUT	RC	REZ	RHO	RL
COMMON	RR, SIG	000FL, SWITCH	TABLM, TAU			
COMMON	TAUDTS	TAUDTX	U	UK	URR	UT
COMMON	UU	UUU	UTEF	UVMAX	V	VAHOVE
COMMON	VBLO	VEL	VK	VT	VTEF	VV
COMMON	VVABOV	VVBLO	W2	W3	WPS	WS
COMMON	WSA	WSB	WSC	XL	XLF	XN
COMMON	XR	YL	YLW	YN	YU	ZMAX
COMMON	I	II	IN	IR	IWS	IWSA
COMMON	IWSB	IWSC	IW1	J	JN	JP
COMMON	JR	K	KN	KP	KR	KRM
COMMON	L	M	MA	MB	MC	MD
COMMON	ME	MZ	N	NK	NKMAX	NK1
COMMON	NO	NR	G	SOLID	TEMP	
COMMON	FIOUT	CAP	KFIT	ISEND	IGOTO	HEAD

C
C
C
C

E Q U I V A L E N C E

0EQUIVALENCE	(Z(12), PROB),	(Z(2), CYCLE),	(Z(3), DT),
1(Z(4), PRINTS),	(Z(5), PRINTL),	(Z(6), DUMPT7),	(Z(7), CSTOP),
2(Z(8), PIUY),	(Z(9), TMZ),	(Z(10), SCYCLE),	(Z(11), SPROB),
3(Z(12), GAMX),	(Z(13), ETH),	(Z(14), FFA),	(Z(15), FFB),
4(Z(16), TMDZ),	(Z(17), TMXZ),	(Z(18), XMAX),	(Z(19), TXMAX),
5(Z(20), TYMAX),	(Z(21), AMDH),	(Z(22), AMXM),	(Z(23), DNN),
6(Z(24), DMIN),	(Z(25), FEF),	(Z(26), DTNA),	(Z(27), CVIS),
7(Z(28), NPR),	(Z(29), NPRI),	(Z(30), NC),	(Z(31), NPC),
8(Z(32), NHC),	(Z(33), IMAX),	(Z(34), IMAXA),	(Z(35), JMAX),
9(Z(36), JMAXA),	(Z(37), KMAX),	(Z(38), KMAXA),	(Z(39), NMAX),
0EQUIVALENCE	(Z(40), ND),	(Z(41), KDT),	(Z(42), IXMAX),
1(Z(43), NOD),	(Z(44), NOPR),	(Z(45), NIMAX),	(Z(46), NJMAX),
2(Z(47), I1),	(Z(48), I2),	(Z(49), I3),	(Z(50), I4),
3(Z(51), N1),	(Z(52), N2),	(Z(53), N3),	(Z(54), N4),
4(Z(55), N5),	(Z(56), N6),	(Z(57), N7),	(Z(58), N8),
5(Z(59), N9),	(Z(60), N10),	(Z(61), N11),	(Z(62), NRM),
6(Z(63), THAD),	(Z(64), XNRG),	(Z(65), SN),	(Z(66), DXN),
7(Z(67), RADER),	(Z(68), RADET),	(Z(69), RADEB),	(Z(70), DTRAD),
8(Z(71), RELZFT),	(Z(72), RSTOP),	(Z(73), SHELL),	(Z(74), RBOUND),
9(Z(75), TOZONE),	(Z(76), ECK),	(Z(77), SBOUND),	(Z(78), X1),
0EQUIVALENCE	(Z(79), X2),	(Z(80), Y1),	(Z(81), Y2),
1(Z(82), CAULN),	(Z(83), VISC),	(Z(84), T),	(Z(85), GMAX),
2(Z(86), WSGD),	(Z(87), WSGX),	(Z(88), GMADR),	(Z(89), GMAXR),
3(Z(90), S1),	(Z(91), S2),	(Z(92), S3),	(Z(93), S4),
4(Z(94), S5),	(Z(95), S6),	(Z(96), S7),	(Z(97), S8),
5(Z(98), S9),	(Z(99), S10)		

C 0EQUIVALENCE (Z(100), HVB), (Z(101), HCB), (Z(102), CB),

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OEQUIVALENCE (Z(100),HVB), (Z(101),HCB), (Z(102),CB),

1(Z(103),SVS), (Z(108),BETA), (Z(105),CV), (Z(106),GV),
 2(Z(107),SUME), (Z(116),SCH), (Z(109),ALCO), (Z(117),ISK),
 3(Z(115),COE), (Z(121),IH), (Z(118),SCOR), (Z(123),UTC),
 4(Z(120),UTH), (Z(125),JC), (Z(122),JH),
 5(Z(124),IC), (Z(132),J2), (Z(133),J3), (Z(134),J4),
 6(Z(131),J1), (Z(136),J6), (Z(135),J5), (Z(138),SVMAX),
 7(Z(135),J5),
 8(Z(139),FHCUTC)
 OEQUIVALENCE (Z(140),VAPE), (Z(141),RAUE), (Z(142),CNDE),
 1(Z(143),SCRE), (Z(144),IV), (Z(145),JV), (Z(146),IU),
 2(Z(147),JU), (Z(148),DTVF), (Z(149),DTUF), (Z(150),EII)

C
 OEQUIVALENCE (XX(2),X(1)), (UR(UL),FLEFT), (UR(100),YAMC),
 1(PH(100),SIGC), (PH(PL),GAMC), (UR(46),QK), (UR(TAB),
 2(UR(16),AMK), (UR(31),PK), (YY(2),Y(1))

C
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 C

C O M M O N

IF(I.LE.12) GO TO 20
 JLOW=1
 JHIGH=JMAX
 GO TO 100
 20 JLOW=1
 JHIGH=J5
 100 RETURN
 END

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01  FOR LINEX, LINEX/FJ
    SUBROUTINE LINEX(TAU, L, IHA, P, ZHAR, GG)
    COMMON Z(90)
    EQUIVALENCE (Z(90), S1)
C*****PLACE DATA STATEMENTS PRODUCED BY PROGRAM GLST HERE *****
    DATA TAUM, LM, TAUZ, ELZ, V1, VZ/
    1 5.000E+10, 1.583E+12, 5.000E-02, 1.583E+09, 7.980E+00, 1.126E+03/
    DATA TAUZ, ELZ, S, T, PHI/
    1 -1.301E+0, 4.2, 2.000E+0, 8.000E+0, 5.244E+9/
    DATA NN, MM, 11, 12, 13, 14, 15, 16, 17, 18/
    1 25, 25, 1, 1, 1, 1, 1, 1, 0, 0/
    DIMENSION ZB(25,25), EILN(25,25)
    EQUIVALENCE (ZB, ZB1), (EILN, EILN1)
    COMMON/EST/ZB 1(54)
    DATA ZB 1/
    1 2.200E-10, 3.912E-10, 6.957E-10, 1.237E-09, 2.200E-09, 3.912E-09,
    2 6.957E-09, 1.237E-08, 2.200E-08, 3.912E-08, 6.957E-08, 1.237E-07,
    3 2.200E-07, 3.911E-07, 6.955E-07, 1.235E-06, 2.197E-06, 3.904E-06,
    4 6.930E-06, 1.229E-05, 2.173E-05, 3.828E-05, 6.694E-05, 1.156E-04,
    5 1.957E-04, 3.911E-08, 6.956E-08, 1.237E-07, 2.200E-07, 3.911E-07,
    6 6.955E-07, 1.237E-06, 2.198E-06, 3.907E-06, 6.941E-06, 1.232E-05,
    7 2.184E-05, 3.863E-05, 6.803E-05, 1.189E-04, 2.054E-04, 3.475E-04,
    8 5.694E-04, 9.132E-04, 1.382E-03, 1.984E-03, 2.722E-03, 3.553E-03,
    9 4.455E-03, 5.399E-03, 2.001E-06, 3.563E-06, 6.333E-06, 1.125E-05/
    COMMON/EST/ZB 2(54)
    DATA ZB 2/
    1 1.997E-05, 3.542E-05, 6.265E-05, 1.104E-04, 1.932E-04, 3.342E-04,
    2 3.669E-04, 9.331E-04, 1.499E-03, 2.279E-03, 3.284E-03, 4.485E-03,
    3 5.898E-03, 7.394E-03, 8.953E-03, 1.054E-02, 1.217E-02, 1.375E-02,
    4 1.529E-02, 1.679E-02, 1.823E-02, 4.031E-05, 7.149E-05, 1.263E-04,
    5 2.223E-04, 3.879E-04, 6.677E-04, 1.124E-03, 1.847E-03, 2.903E-03,
    6 4.337E-03, 6.138E-03, 8.283E-03, 1.064E-02, 1.312E-02, 1.566E-02,
    7 1.820E-02, 2.075E-02, 2.318E-02, 2.552E-02, 2.776E-02, 2.989E-02,
    8 3.192E-02, 3.384E-02, 3.567E-02, 3.739E-02, 3.950E-04, 6.918E-04,
    9 1.189E-03, 1.996E-03, 3.264E-03, 5.096E-03, 7.557E-03, 1.060E-02/
    COMMON/EST/ZB 3(54)
    DATA ZB 3/
    1 1.416E-02, 1.801E-02, 2.200E-02, 2.601E-02, 2.995E-02, 3.382E-02,
    2 3.747E-02, 4.093E-02, 4.419E-02, 4.725E-02, 5.013E-02, 5.283E-02,
    3 5.535E-02, 5.772E-02, 5.994E-02, 6.203E-02, 6.399E-02, 6.214E-03,
    4 3.697E-03, 5.987E-03, 9.230E-03, 1.348E-02, 1.861E-02, 2.446E-02,
    5 3.061E-02, 3.685E-02, 4.298E-02, 4.887E-02, 5.446E-02, 5.981E-02,
    6 6.471E-02, 6.927E-02, 7.349E-02, 7.741E-02, 8.103E-02, 8.439E-02,
    7 8.751E-02, 9.041E-02, 9.310E-02, 9.561E-02, 9.795E-02, 1.001E-01,
    8 7.936E-03, 1.251E-02, 1.867E-02, 2.629E-02, 3.501E-02, 4.446E-02,
    9 5.399E-02, 6.331E-02, 7.220E-02, 8.052E-02, 8.823E-02, 9.533E-02/
    COMMON/EST/ZB 4(54)
    DATA ZB 4/
    1 1.018E-01, 1.079E-01, 1.134E-01, 1.184E-01, 1.230E-01, 1.272E-01,
    2 1.311E-01, 1.346E-01, 1.379E-01, 1.410E-01, 1.438E-01, 1.464E-01,
    3 1.489E-01, 2.062E-02, 3.056E-02, 4.261E-02, 5.613E-02, 7.047E-02,
    4 8.465E-02, 9.826E-02, 1.110E-01, 1.227E-01, 1.334E-01, 1.431E-01,
    5 1.518E-01, 1.597E-01, 1.668E-01, 1.733E-01, 1.792E-01, 1.845E-01,
    6 1.894E-01, 1.938E-01, 1.979E-01, 2.016E-01, 2.051E-01, 2.083E-01,
    7 2.112E-01, 2.140E-01, 4.294E-02, 6.053E-02, 8.040E-02, 1.013E-01,
    8 1.223E-01, 1.421E-01, 1.605E-01, 1.772E-01, 1.922E-01, 2.057E-01,
    9 2.177E-01, 2.284E-01, 2.380E-01, 2.465E-01, 2.542E-01, 2.612E-01/
    COMMON/EST/ZB 5(54)
    DATA ZB 5/
    1 2.674E-01, 2.731E-01, 2.783E-01, 2.830E-01, 2.873E-01, 2.913E-01,
    2 2.950E-01, 2.983E-01, 3.015E-01, 7.700E-02, 1.047E-01, 1.346E-01,
    3 1.647E-01, 1.936E-01, 2.207E-01, 2.450E-01, 2.667E-01, 2.859E-01,
    4 3.029E-01, 3.178E-01, 3.310E-01, 3.426E-01, 3.532E-01, 3.624E-01,
    5 3.708E-01, 3.782E-01, 3.850E-01, 3.911E-01, 3.966E-01, 4.016E-01,
    6 4.061E-01, 4.103E-01, 4.146E-01, 4.182E-01, 4.214E-01, 4.244E-01,

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7 2.078E-01, 2.497E-01, 2.891E-01, 3.250E-01, 3.570E-01, 3.850E-01,
 8 4.100E-01, 4.316E-01, 4.505E-01, 4.671E-01, 4.817E-01, 4.948E-01,
 9 5.054E-01, 5.145E-01, 5.226E-01, 5.299E-01, 5.368E-01, 5.427E-01/
 COMMON/EST/ZB 6(54)

DATA ZB 6/

1 5.481E-01, 5.530E-01, 5.575E-01, 5.616E-01, 5.654E-01, 1.863E-01,
 2 2.434E-01, 3.020E-01, 3.588E-01, 4.117E-01, 4.595E-01, 5.017E-01,
 3 5.345E-01, 5.624E-01, 5.855E-01, 6.052E-01, 6.218E-01, 6.370E-01,
 4 6.499E-01, 6.613E-01, 6.715E-01, 6.806E-01, 6.887E-01, 6.960E-01,
 5 7.026E-01, 7.087E-01, 7.142E-01, 7.192E-01, 7.239E-01, 7.281E-01,
 6 2.629E-01, 3.396E-01, 4.174E-01, 4.923E-01, 5.592E-01, 6.139E-01,
 7 6.593E-01, 6.960E-01, 7.272E-01, 7.534E-01, 7.758E-01, 7.950E-01,
 8 8.117E-01, 8.262E-01, 8.390E-01, 8.504E-01, 8.605E-01, 8.695E-01,
 9 8.777E-01, 8.851E-01, 8.918E-01, 8.979E-01, 9.035E-01, 9.087E-01/
 COMMON/EST/ZB 7(54)

DATA ZB 7/

1 9.135E-01, 3.533E-01, 4.511E-01, 5.555E-01, 6.501E-01, 7.268E-01,
 2 7.895E-01, 8.404E-01, 8.818E-01, 9.168E-01, 9.463E-01, 9.714E-01,
 3 9.929E-01, 1.012E 00, 1.020E 00, 1.042E 00, 1.055E 00, 1.066E 00,
 4 1.076E 00, 1.085E 00, 1.093E 00, 1.101E 00, 1.108E 00, 1.114E 00,
 5 1.120E 00, 1.125E 00, 4.540E-01, 5.919E-01, 7.244E-01, 8.329E-01,
 6 9.206E-01, 9.913E-01, 1.049E 00, 1.096E 00, 1.135E 00, 1.168E 00,
 7 1.196E 00, 1.220E 00, 1.241E 00, 1.259E 00, 1.275E 00, 1.289E 00,
 8 1.302E 00, 1.313E 00, 1.323E 00, 1.332E 00, 1.340E 00, 1.348E 00,
 9 1.355E 00, 1.361E 00, 1.367E 00, 6.232E-01, 7.683E-01, 9.209E-01/
 COMMON/EST/ZB 8(47)

DATA ZB 8/

1 1.045E 00, 1.144E 00, 1.224E 00, 1.289E 00, 1.341E 00, 1.386E 00,
 2 1.422E 00, 1.453E 00, 1.480E 00, 1.504E 00, 1.525E 00, 1.544E 00,
 3 1.560E 00, 1.575E 00, 1.588E 00, 1.600E 00, 1.611E 00, 1.619E 00,
 4 1.628E 00, 1.636E 00, 1.644E 00, 1.650E 00, 8.692E-01, 9.739E-01,
 5 1.149E 00, 1.290E 00, 1.402E 00, 1.492E 00, 1.569E 00, 1.633E 00,
 6 1.686E 00, 1.730E 00, 1.768E 00, 1.799E 00, 1.827E 00, 1.851E 00,
 7 1.872E 00, 1.890E 00, 1.907E 00, 1.922E 00, 1.935E 00, 1.947E 00,
 8 1.958E 00, 1.968E 00, 1.977E 00, 1.985E 00, 1.993E 00/
 COMMON/EST/ZB 9(29)

DATA ZB 9/

5 9.721E-1, 1.216E+0, 1.415E+0, 1.580E+0, 1.718E+0,
 6 1.829E+0, 1.918E+0, 1.991E+0, 2.051E+0, 2.100E+0, 2.143E+0,
 7 2.180E+0, 2.211E+0, 2.239E+0, 2.263E+0, 2.284E+0, 2.303E+0,
 8 2.320E+0, 2.335E+0, 2.348E+0, 2.361E+0, 2.372E+0, 2.382E+0,
 9 2.391E+0, 2.401E+0, 1.217E+0, 1.497E+0, 1.743E+0, 1.944E+0/
 COMMON/EST/ZB10(54)

DATA ZB10/

1 2.103E+0, 2.229E+0, 2.331E+0, 2.415E+0, 2.485E+0, 2.538E+0,
 2 2.584E+0, 2.623E+0, 2.656E+0, 2.685E+0, 2.711E+0, 2.733E+0,
 3 2.754E+0, 2.772E+0, 2.788E+0, 2.803E+0, 2.817E+0, 2.828E+0,
 4 2.839E+0, 2.850E+0, 2.859E+0, 1.505E+0, 1.854E+0, 2.143E+0,
 5 2.373E+0, 2.550E+0, 2.681E+0, 2.786E+0, 2.872E+0, 2.943E+0,
 6 3.003E+0, 3.054E+0, 3.097E+0, 3.135E+0, 3.168E+0, 3.197E+0,
 7 3.223E+0, 3.246E+0, 3.266E+0, 3.285E+0, 3.301E+0, 3.317E+0,
 8 3.331E+0, 3.343E+0, 3.355E+0, 3.366E+0, 1.870E+0, 2.276E+0,
 9 2.600E+0, 2.834E+0, 3.019E+0, 3.164E+0, 3.284E+0, 3.381E+0/
 COMMON/EST/ZB11(54)

DATA ZB11/

1 3.461E+0, 3.527E+0, 3.582E+0, 3.630E+0, 3.672E+0, 3.708E+0,
 2 3.739E+0, 3.788E+0, 3.793E+0, 3.815E+0, 3.836E+0, 3.854E+0,
 3 3.871E+0, 3.886E+0, 3.900E+0, 3.913E+0, 3.925E+0, 2.303E+0,
 4 2.746E+0, 3.082E+0, 3.344E+0, 3.548E+0, 3.706E+0, 3.834E+0,
 5 3.938E+0, 4.025E+0, 4.098E+0, 4.161E+0, 4.214E+0, 4.261E+0,
 6 4.301E+0, 4.337E+0, 4.369E+0, 4.397E+0, 4.422E+0, 4.445E+0,
 7 4.466E+0, 4.485E+0, 4.502E+0, 4.518E+0, 4.532E+0, 4.545E+0,
 8 2.780E+0, 3.256E+0, 3.627E+0, 3.909E+0, 4.130E+0, 4.307E+0,
 9 4.449E+0, 4.566E+0, 4.661E+0, 4.743E+0, 4.812E+0, 4.872E+0/
 COMMON/EST/ZB12(54)

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DATA ZH12/
1 4.924E+0, 4.969E+0, 5.009E+0, 5.045E+0, 5.076E+0, 5.105E+0,
2 5.130E+0, 5.153E+0, 5.174E+0, 5.194E+0, 5.211E+0, 5.228E+0,
3 5.243E+0, 5.307E+0, 5.328E+0, 4.230E+0, 4.544E+0, 4.789E+0,
4 4.986E+0, 5.145E+0, 5.274E+0, 5.383E+0, 5.474E+0, 5.536E+0,
5 5.582E+0, 5.623E+0, 5.659E+0, 5.692E+0, 5.721E+0, 5.748E+0,
6 5.772E+0, 5.794E+0, 5.814E+0, 5.833E+0, 5.850E+0, 5.866E+0,
7 5.880E+0, 5.894E+0, 5.901E+0, 4.474E+0, 4.921E+0, 5.267E+0,
8 5.526E+0, 5.658E+0, 5.767E+0, 5.859E+0, 5.939E+0, 6.007E+0,
9 6.067E+0, 6.119E+0, 6.166E+0, 6.207E+0, 6.244E+0, 6.277E+0/
COMMON/EST/ZH13( 9)
DATA ZH13/
1 6.306E+0, 6.334E+0, 6.358E+0, 6.381E+0, 6.402E+0, 6.419E+0,
2 6.437E+0, 6.453E+0, 6.468E+0/
COMMON/EST/E1LN 1(54)
DATA E1LN 1/
1-1.961E 01,-1.961E 01,-1.961E 01,-1.822E 01,-1.782E 01,-1.731E 01,
2-1.672E 01,-1.614E 01,-1.555E 01,-1.498E 01,-1.440E 01,-1.383E 01,
3-1.325E 01,-1.268E 01,-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,
4-9.802E 00,-9.229E 00,-8.659E 00,-8.093E 00,-7.534E 00,-6.987E 00,
5-6.461E 00,-1.499E 01,-1.440E 01,-1.383E 01,-1.325E 01,-1.268E 01,
6-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,-9.800E 00,-9.227E 00,
7-8.654E 00,-8.084E 00,-7.518E 00,-6.959E 00,-6.413E 00,-5.887E 00,
8-5.393E 00,-4.921E 00,-4.507E 00,-4.145E 00,-3.829E 00,-3.562E 00,
9-3.336E 00,-3.144E 00,-1.104E 01,-1.047E 01,-9.892E 00,-9.317E 00/
COMMON/EST/E1LN 2(54)
DATA E1LN 2/
1-8.743E 00,-8.171E 00,-7.600E 00,-7.034E 00,-6.474E 00,-5.926E 00,
2-5.398E 00,-4.899E 00,-4.425E 00,-4.006E 00,-3.641E 00,-3.329E 00,
3-3.055E 00,-2.829E 00,-2.638E 00,-2.475E 00,-2.331E 00,-2.209E 00,
4-2.103E 00,-2.009E 00,-1.927E 00,-1.841E 00,-1.746E 00,-1.689E 00,
5-6.334E 00,-5.777E 00,-5.234E 00,-4.713E 00,-4.216E 00,-3.764E 00,
6-3.363E 00,-3.016E 00,-2.716E 00,-2.466E 00,-2.256E 00,-2.079E 00,
7-1.929E 00,-1.797E 00,-1.687E 00,-1.591E 00,-1.506E 00,-1.432E 00,
8-1.367E 00,-1.308E 00,-1.256E 00,-1.209E 00,-1.159E 00,-1.119E 00,
9-4.657E 00,-4.139E 00,-3.647E 00,-3.202E 00,-2.808E 00,-2.469E 00/
COMMON/EST/E1LN 3(54)
DATA E1LN 3/
1-2.179E 00,-1.939E 00,-1.739E 00,-1.572E 00,-1.431E 00,-1.309E 00,
2-1.207E 00,-1.118E 00,-1.042E 00,-9.745E 01,-9.154E 01,-8.630E 01,
3-8.163E 01,-7.744E 01,-7.366E 01,-7.024E 01,-6.714E 01,-6.435E 00,
4-3.523E 00,-3.040E 00,-2.608E 00,-2.229E 00,-1.906E 00,-1.633E 00,
5-1.409E 00,-1.223E 00,-1.069E 00,-9.409E 01,-8.327E 01,-7.390E 01,
6-6.601E 01,-5.921E 01,-5.329E 01,-4.810E 01,-4.352E 01,-3.946E 01,
7-3.583E 01,-3.257E 01,-2.964E 01,-2.698E 01,-2.456E 01,-2.235E 01,
8-2.759E 00,-2.303E 00,-1.903E 00,-1.561E 00,-1.275E 00,-1.035E 00,
9-8.412E 01,-6.819E 01,-5.506E 01,-4.415E 01,-3.501E 01,-2.727E 01/
COMMON/EST/E1LN 4(54)
DATA E1LN 4/
1-2.067E 01,-1.484E 01,-9.905E 02,-5.591E 02,-1.794E 02, 1.568E 02,
2 4.563E 02, 7.246E 02, 9.660E 02, 1.184E 01, 1.383E 01, 1.564E 01,
3 1.729E 01,-1.804E 00,-1.411E 00,-1.078E 00,-8.024E 01,-5.749E 01,
4-3.915E 01,-2.424E 01,-1.206E 01,-2.026E 02, 6.316E 02, 1.332E 01,
5 1.925E 01, 2.432E 01, 2.870E 01, 3.250E 01, 3.583E 01, 3.876E 01,
6 4.136E 01, 4.368E 01, 4.576E 01, 4.764E 01, 4.934E 01, 5.088E 01,
7 5.229E 01, 5.358E 01,-1.070E 00,-7.269E 01,-4.430E 01,-2.121E 01,
8-2.386E 02, 1.265E 01, 2.481E 01, 3.471E 01, 4.286E 01, 4.962E 01,
9 5.529E 01, 6.010E 01, 6.420E 01, 6.774E 01, 7.082E 01, 7.351E 01/
COMMON/EST/E1LN 5(54)
DATA E1LN 5/
1 7.588E 01, 7.799E 01, 7.986E 01, 8.154E 01, 8.306E 01, 8.443E 01,
2 8.568E 01, 8.682E 01, 8.786E 01,-4.863E 01,-1.788E 01, 7.220E 02,
3 2.742E 01, 4.359E 01, 5.660E 01, 6.712E 01, 7.560E 01, 8.256E 01,
4 8.832E 01, 9.314E 01, 9.722E 01, 1.006E 00, 1.037E 00, 1.063E 00,
5 1.086E 00, 1.105E 00, 1.123E 00, 1.139E 00, 1.153E 00, 1.165E 00,

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6 1.177E 00, 1.187E 00, 1.197E 00, 1.206E 00, -6.935E -03, 2.768E -01,
 7 5.063E -01, 6.901E -01, 8.367E -01, 9.538E -01, 1.048E 00, 1.123E 00,
 8 1.186E 00, 1.238E 00, 1.280E 00, 1.317E 00, 1.347E 00, 1.374E 00,
 9 1.395E 00, 1.413E 00, 1.429E 00, 1.444E 00, 1.457E 00, 1.469E 00/

COMMON/EST/EILN 6(54)

DATA EILN 6/

1 1.479E 00, 1.488E 00, 1.497E 00, 1.505E 00, 1.512E 00, 3.972E -01,
 2 6.645E -01, 8.802E -01, 1.053E 00, 1.190E 00, 1.300E 00, 1.388E 00,
 3 1.453E 00, 1.506E 00, 1.550E 00, 1.587E 00, 1.617E 00, 1.644E 00,
 4 1.668E 00, 1.688E 00, 1.706E 00, 1.722E 00, 1.736E 00, 1.748E 00,
 5 1.760E 00, 1.770E 00, 1.779E 00, 1.788E 00, 1.796E 00, 1.803E 00,
 6 7.419E -01, 9.976E -01, 1.204E 00, 1.369E 00, 1.500E 00, 1.603E 00,
 7 1.684E 00, 1.748E 00, 1.801E 00, 1.845E 00, 1.882E 00, 1.913E 00,
 8 1.939E 00, 1.962E 00, 1.982E 00, 2.000E 00, 2.015E 00, 2.029E 00,
 9 2.042E 00, 2.053E 00, 2.063E 00, 2.072E 00, 2.080E 00, 2.088E 00/

COMMON/EST/EILN 7(54)

DATA EILN 7/

1 2.095E 00, 1.037E 00, 1.282E 00, 1.493E 00, 1.668E 00, 1.801E 00,
 2 1.904E 00, 1.985E 00, 2.048E 00, 2.100E 00, 2.143E 00, 2.179E 00,
 3 2.209E 00, 2.235E 00, 2.258E 00, 2.277E 00, 2.295E 00, 2.310E 00,
 4 2.323E 00, 2.337E 00, 2.346E 00, 2.356E 00, 2.365E 00, 2.373E 00,
 5 2.381E 00, 2.387E 00, 1.288E 00, 1.562E 00, 1.797E 00, 1.973E 00,
 6 2.106E 00, 2.207E 00, 2.286E 00, 2.349E 00, 2.400E 00, 2.442E 00,
 7 2.477E 00, 2.506E 00, 2.532E 00, 2.554E 00, 2.573E 00, 2.589E 00,
 8 2.604E 00, 2.617E 00, 2.629E 00, 2.640E 00, 2.649E 00, 2.658E 00,
 9 2.666E 00, 2.673E 00, 2.680E 00, 1.619E 00, 1.870E 00, 2.106E 00/

COMMON/EST/EILN 8(47)

DATA EILN 8/

1 2.281E 00, 2.412E 00, 2.512E 00, 2.589E 00, 2.650E 00, 2.700E 00,
 2 2.741E 00, 2.774E 00, 2.803E 00, 2.828E 00, 2.850E 00, 2.869E 00,
 3 2.886E 00, 2.901E 00, 2.914E 00, 2.926E 00, 2.936E 00, 2.944E 00,
 4 2.953E 00, 2.961E 00, 2.968E 00, 2.974E 00, 2.979E 00, 2.983E 00,
 5 2.419E 00, 2.591E 00, 2.718E 00, 2.815E 00, 2.895E 00, 2.958E 00,
 6 3.008E 00, 3.049E 00, 3.082E 00, 3.110E 00, 3.134E 00, 3.154E 00,
 7 3.172E 00, 3.188E 00, 3.202E 00, 3.214E 00, 3.225E 00, 3.234E 00,
 8 3.243E 00, 3.251E 00, 3.258E 00, 3.265E 00, 3.271E 00/

COMMON/EST/EILN 9(29)

DATA EILN 9/

5 2.180E+0, 2.501E+0, 2.732E+0, 2.906E+0, 3.038E+0,
 6 3.236E+0, 3.211E+0, 3.270E+0, 3.316E+0, 3.354E+0, 3.386E+0,
 7 3.412E+0, 3.435E+0, 3.455E+0, 3.472E+0, 3.487E+0, 3.500E+0,
 8 3.511E+0, 3.522E+0, 3.530E+0, 3.539E+0, 3.546E+0, 3.553E+0,
 9 3.559E+0, 3.565E+0, 2.504E+0, 2.820E+0, 3.061E+0, 3.232E+0/

COMMON/EST/EILN10(54)

DATA EILN10/

1 3.356E+0, 3.447E+0, 3.519E+0, 3.575E+0, 3.620E+0, 3.654E+0,
 2 3.683E+0, 3.707E+0, 3.728E+0, 3.746E+0, 3.762E+0, 3.775E+0,
 3 3.788E+0, 3.799E+0, 3.808E+0, 3.817E+0, 3.826E+0, 3.833E+0,
 4 3.839E+0, 3.846E+0, 3.851E+0, 2.829E+0, 3.157E+0, 3.385E+0,
 5 3.547E+0, 3.662E+0, 3.744E+0, 3.807E+0, 3.858E+0, 3.900E+0,
 6 3.935E+0, 3.965E+0, 3.989E+0, 4.011E+0, 4.029E+0, 4.045E+0,
 7 4.060E+0, 4.072E+0, 4.083E+0, 4.093E+0, 4.103E+0, 4.111E+0,
 8 4.118E+0, 4.125E+0, 4.131E+0, 4.137E+0, 3.171E+0, 3.482E+0,
 9 3.693E+0, 3.836E+0, 3.945E+0, 4.027E+0, 4.093E+0, 4.145E+0/

COMMON/EST/EILN11(54)

DATA EILN11/

1 4.188E+0, 4.222E+0, 4.251E+0, 4.275E+0, 4.296E+0, 4.315E+0,
 2 4.331E+0, 4.345E+0, 4.357E+0, 4.369E+0, 4.379E+0, 4.388E+0,
 3 4.396E+0, 4.403E+0, 4.410E+0, 4.417E+0, 4.422E+0, 3.500E+0,
 4 3.783E+0, 3.980E+0, 4.125E+0, 4.233E+0, 4.314E+0, 4.378E+0,
 5 4.429E+0, 4.471E+0, 4.506E+0, 4.535E+0, 4.560E+0, 4.581E+0,
 6 4.600E+0, 4.616E+0, 4.630E+0, 4.643E+0, 4.655E+0, 4.665E+0,
 7 4.674E+0, 4.682E+0, 4.690E+0, 4.697E+0, 4.703E+0, 4.709E+0,
 8 3.804E+0, 4.078E+0, 4.274E+0, 4.415E+0, 4.521E+0, 4.602E+0,
 9 4.667E+0, 4.718E+0, 4.759E+0, 4.794E+0, 4.823E+0, 4.848E+0/

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COMMON/EST/EILN12(54)
DATA EILN12/
1 4.870E+0, 4.888E+0, 4.905E+0, 4.919E+0, 4.932E+0, 4.943E+0,
2 4.953E+0, 4.962E+0, 4.971E+0, 4.978E+0, 4.985E+0, 4.992E+0,
3 4.997E+0, 4.106E+0, 4.375E+0, 4.567E+0, 4.709E+0, 4.814E+0,
4 4.895E+0, 4.959E+0, 5.010E+0, 5.052E+0, 5.086E+0, 5.109E+0,
5 5.127E+0, 5.143E+0, 5.158E+0, 5.171E+0, 5.183E+0, 5.194E+0,
6 5.204E+0, 5.214E+0, 5.222E+0, 5.230E+0, 5.238E+0, 5.245E+0,
7 5.251E+0, 5.257E+0, 4.411E+0, 4.678E+0, 4.869E+0, 5.007E+0,
8 5.105E+0, 5.157E+0, 5.202E+0, 5.242E+0, 5.277E+0, 5.308E+0,
9 5.335E+0, 5.359E+0, 5.380E+0, 5.399E+0, 5.416E+0, 5.432E+0/

COMMON/EST/EILN13( 9)
DATA EILN13/
1 5.446E+0, 5.458E+0, 5.470E+0, 5.481E+0, 5.490E+0, 5.499E+0,
2 5.507E+0, 5.515E+0, 5.522E+0/

IF(E.NE.0.) GO TO 5
THA = 1.E-3
ZBAR=0.
GO TO 950
5 CONTINUE
ALGT=ALOG10(TAU)
ALGE=ALOG10(L)
DLGT=ALGT-TAUZ
DLGE=ALGE-ELZ
AN=DLGT*5+1.
AM=DLGE*T+1.
IF (DLGT.LT.0.) AN=0.
IF (DLGE.LT.0.) AM=0.
N=IFIX(AN)
M=IFIX(AM)
IN=0
EO=E
IF(N.LE.0) GO TO 10
IF(N.GE.NN) GO TO 20
IF(M.LE.0) GO TO 800
IF(M.GE.MM) GO TO 400
8 CONTINUE
DNLT=AN-AINT(AN)
DMLE=AM-AINT(AM)
ZBAR=ZB(N,M)+(ZB(N+1,M)-ZB(N,M))*DNLT
1 +(ZB(N,M+1)-ZB(N,M))*DMLE
2 +(ZB(N+1,M+1)+ZB(N,M)-ZB(N+1,M)-ZB(N,M+1))
3 *(DNLT*DMLE)
ALIN=EILN(N,M)+(EILN(N+1,M)-EILN(N,M))*DNLT
1 +(EILN(N,M+1)-EILN(N,M))*DMLE
3 *(DNLT*DMLE)
2 +(EILN(N+1,M+1)+EILN(N,M)-EILN(N+1,M)-EILN(N,M+1))
THA=(EO/PHI-EXP(ALIN))/(1.5*(1.+ZBAR))
IF(IN.NE.0) GO TO (150,250,350,450,550,650,750,850),IN
GO TO 950
10 IF(M.LE.0) GO TO 100
IF(M.GE.MM) GO TO 300
GO TO 200
20 IF(M.LE.0) GO TO 700
IF(M.GE.MM) GO TO 500
GO TO 600
100 CONTINUE
IF(I1.EQ.1) GO TO 9901
150 CONTINUE
RETURN
200 CONTINUE
IF(I2.EQ.1) GO TO 9902
250 CONTINUE
RETURN
300 CONTINUE

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      IF(I3.EQ.1) GO TO 9903
350  CONTINUE
      RETURN
400  CONTINUE
      IF(I4.EQ.1) GO TO 9904
450  CONTINUE
      RETURN
500  CONTINUE
      IF(I5.EQ.1) GO TO 9905
550  CONTINUE
      RETURN
600  CONTINUE
      IF(I6.EQ.1) GO TO 9906
650  CONTINUE
      RETURN
700  CONTINUE
      IF(I7.EQ.1) GO TO 9907
      IN = 7
      M = 1
      N = NN
      EO=EZ
      GO TO 8
750  THAP = E * THA / EZ
      ZBAR = ZBAR * (THAP/THA)**.75 * SQRT(TAUM/TAU)*EXP(V1*(THAP-THA) /
      1 (THA*THAP*2.))
      AIN=V1*ZBAR
      GO TO 900
800  CONTINUE
      IF(I8.EQ.1) GO TO 9908
      IN = 8
      M = 1
      EO=EZ
      GO TO 8
850  THAP = E * THA / EZ
      ZBAR = ZBAR * (THAP/THA)**.75 * EXP(V1*( THAP - THA) /
      1(THA * THAP*2.))
      AIN=V1*ZBAR
900  CONTINUE
      THA=(E/PHI-AIN)/(1.5*(1.+ZBAR))
950  P=PHI*(1.+ZBAR )*THA/TAU
      RETURN
9901 S1=12.0100
      GO TO 9995
9902 S1=12.0200
      GO TO 9999
9903 S1=12.0300
      GO TO 9999
9904 S1=12.0400
      GO TO 9999
9905 S1=12.0500
      GO TO 9999
9906 S1=12.0600
      GO TO 9999
9907 S1=12.0700
      GO TO 9999
9908 S1=12.0800
9999 WRITE(6,1000)TAU,E,THA,P,ZBAR,GG,ALGT
1000 FORMAT(1H1,12X,6HTAU ,9X,6HE ,9X,6HTHA ,9X,6HP ,9X,6HZ
      1UAR ,9X,6HGG ,9X,6HALGT /7X,1P7E15.7)
      WRITE(6,1001)ALGE,DLGT,DLGE,AN,AM
1001 FORMAT(1H0,12X,6HALGE ,9X,6HDLGT ,9X,6HDLGE ,9X,6HAN ,9X,6HA
      1M /7X,1P5E15.7)
      WRITE(6,1002)N,M,NN,MM,S1
1002 FORMAT(1H0,12X,6HN ,9X,6HM ,9X,6HNN ,9X,6HMM ,9X,6HS
      11 /7X,19,3(6X,19),1P15.7)

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21  FOR ES, ES/FJ
    SUBROUTINE ES(TAU,E,THA,P,ZB,G)
    COMMON // Z
C      E  G  U  I  V  A  L  E  N  C  E
C
    OEQUIVALENCE      (Z(12),PROB),      (Z(2),CYCLE),      (Z(3),DT),
    1(Z(4),PRINTS),    (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
    2(Z(8),PIJY),      (Z(9),TMZ),      (Z(10),SCYCLE),   (Z(11),SPROB),
    3(Z(12),GAMX),     (Z(13),ETH),     (Z(14),FFA),      (Z(15),FFB),
    4(Z(16),TMDZ),     (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
    5(Z(20),TYMAX),    (Z(21),AMDM),    (Z(22),AMXM),     (Z(23),DNN),
    6(Z(24),DMIN),     (Z(25),FEF),     (Z(26),DTNA),     (Z(27),CVIS),
    7(Z(28),NPR),      (Z(29),NPRI),    (Z(30),NC),       (Z(31),NPC),
    8(Z(32),NRC),      (Z(33),IMAX),    (Z(34),IMAXA),    (Z(35),JMAX),
    9(Z(36),JMAXA),    (Z(37),KMAX),    (Z(38),KMAXA),    (Z(39),NMAX),
    OEQUIVALENCE      (Z(40),ND),      (Z(41),KDT),      (Z(42),IXMAX),
    1(Z(43),NOD),      (Z(44),NOPR),    (Z(45),NIMAX),    (Z(46),NJMAX),
    2(Z(47),I1),       (Z(48),I2),      (Z(49),I3),       (Z(50),I4),
    3(Z(51),N1),       (Z(52),N2),      (Z(53),N3),       (Z(54),N4),
    4(Z(55),N5),       (Z(56),N6),      (Z(57),N7),       (Z(58),N8),
    5(Z(59),N9),       (Z(60),N10),     (Z(61),N11),      (Z(62),NRM),
    6(Z(63),TRAD),     (Z(64),XNRG),    (Z(65),SN),       (Z(66),DXN),
    7(Z(67),RADEK),    (Z(68),RADET),   (Z(69),RADEB),    (Z(70),DTRAD),
    8(Z(71),REZFCT),   (Z(72),RSTOP),   (Z(73),SHELL),    (Z(74),BBOUND),
    9(Z(75),TOZONE),   (Z(76),ECK),     (Z(77),SBOUND),   (Z(78),X1),
    OEQUIVALENCE      (Z(79),X2),      (Z(80),Y1),      (Z(81),Y2),
    1(Z(82),CAULN),    (Z(83),VISC),    (Z(84),T),        (Z(85),GMAX),
    2(Z(86),WSGD),     (Z(87),WSGX),    (Z(88),GMADR),    (Z(89),GMAXR),
    3(Z(90),S1),       (Z(91),S2),      (Z(92),S3),       (Z(93),S4),
    4(Z(94),S5),       (Z(95),S6),      (Z(96),S7),       (Z(97),S8),
    5(Z(98),S9),       (Z(99),S10)

C
    OEQUIVALENCE      (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
    1(Z(103),SVS),     (Z(104),ATOM),   (Z(105),CV),      (Z(106),GV),
    2(Z(107),SUMFE),    (Z(108),BETA),   (Z(109),ALCO),    (Z(110),ANN),
    3(Z(111),EZERO),    (Z(112),PW),     (Z(113),CAPS),    (Z(114),HNU),
    4(Z(115),COE),      (Z(116),SCH),    (Z(117),ISK),     (Z(118),SCDR),
    5(Z(119),AHN),      (Z(120),OTH),    (Z(121),IH),      (Z(122),JH),
    6(Z(123),DTC),      (Z(124),IC),     (Z(125),JC),      (Z(126),RFT),
    7(Z(127),CDUT),     (Z(128),HCP),    (Z(129),HH),      (Z(130),CO),
    8(Z(131),J1),       (Z(132),J2),     (Z(133),J3),      (Z(134),J4),
    9(Z(135),J5),       (Z(136),J6),     (Z(137),J7),      (Z(138),SVMAX),
    10(Z(139),FRCDTC)
    OEQUIVALENCE      (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
    1(Z(143),SCRE),    (Z(144),IV),     (Z(145),JV),      (Z(146),IU),
    2(Z(147),JU),      (Z(148),DTVF),   (Z(149),DTUF),    (Z(150),E11)

    A= E-HVB-HCB+HCP
    TEMPA=S.E+6
    IF(A.LT.TEMPA) A=0.0
    CALL LIBEX(TAU,A,THA,P, ZB ,GG)
    RETURN
    END

```

DI FOR MFST, MFST/FJ
SUBROUTINE MFST(KFIT,N)
CALL PAC(KFIT,2,N)
RETURN
END

AFWL-TR-66-108, Vol II

01 FOR KFST, KFST/FJ
SUBROUTINE KFST(KFIT,N)
CALL PAC(KFIT,1,N)
RETURN
END

AFWL-TR-66-108, Vol II
SUBROUTINE KFST(KFIT,N)
CALL PAC(KFIT,1,N)
RETURN
END

```

91 FOR JMH,JMH/EJ
  FUNCTION JMH(K,I)
  CALL UNPACK(K,I,L)
  JMH=L
  RETURN
  END

```

```

      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
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      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011
      1011 1011 1011 1011 1011 1011 1011 1011 1011 1011

```

DI ASM PAC
 NBN .
 PAC* .
 L AO:*2,B11
 L B13:*1,B11
 AA,016 A1,1
 LSSL A1,1
 J S-1,B13
 S,015 AO:*0,B11
 J 4,B11
 S,014 AO:*0,B11
 J 4,B11
 S,013 AO:*0,B11
 J 4,B11
 S,012 AO:*0,B11
 J 4,B11
 S,011 AO:*0,B11
 J 4,B11
 S,010 AO:*0,B11
 J 4,B11
 END

01 ASM UNPACK
 NUPR .
 UNPACK .
 L U13,*1,U11
 AA,016 A1,1
 LSSL A1,1
 J S-1,U13
 L,015 A0,*0,U11
 J S+10
 L,014 A0,*0,U11
 J S+8
 L,013 A0,*0,U11
 J S+6
 L,012 A0,*0,U11
 J S+4
 L,011 A0,*0,U11
 J S+2
 L,010 A0,*0,U11
 S A0,*2,U11
 J 4,B11
 ENU

OEQUIVALENCE	(Z(100),HVB),	(Z(101),HCB),	(Z(102),CH),
1(Z(103),SVS),	(Z(104),ATOM),	(Z(105),CV),	(Z(106),GV),
2(Z(107),SUMFL),	(Z(108),HETA),	(Z(109),ALCO),	(Z(110),ANN),
3(Z(111),EZERO),	(Z(112),PW),	(Z(113),CAPS),	(Z(114),HNU),
4(Z(115),COE),	(Z(116),SCH),	(Z(117),ISR),	(Z(118),SCUR),
5(Z(119),AHN),	(Z(120),DTH),	(Z(121),IH),	(Z(122),JH),
6(Z(123),UTC),	(Z(124),IC),	(Z(125),JC),	(Z(126),RFT),
7(Z(127),CDUT),	(Z(128),HCP),	(Z(129),HH),	(Z(130),CU),
8(Z(139),FRCUTC)	(Z(132),J2),	(Z(133),J3),	(Z(134),J4),
OEQUIVALENCE	(Z(136),J6),		(Z(138),SVMAX),
1(Z(143),SCRE),	(Z(140),VAPE),	(Z(141),RADE),	(Z(142),CNDE),
2(Z(147),JU),	(Z(144),IV),	(Z(145),JV),	(Z(146),IU),
	(Z(148),DTVF),	(Z(149),DTUF),	(Z(150),EII),

OEQUIVALENCE	(XX(2),X(1)),	(UR,UL,FLEF),	(UR(100),YAMC),
1(PR(100),SIGC),	(PK,PL,GAMC),	(DKE,THETA),	(UR,TAH),
2(UR(16),AMK),	(UR(31),PK),	(UR(46),GK),	(YY(2),Y(1))

C U M M U N

WILL ONLY GENERATE (1) MATERIAL.
PACKAGES MUST BE RECTANGLES.

Z(14)	FFA	MAX INCREASE IN DT PER CYCLE
Z(15)	FFB	MIN POSSIBLE DT
Z(25)	FEF	ENERGY FLOW ALLOWABLE
Z(65)	SN	ONE ALLOWS NEG I
Z(74)	HBOUND	ZERO FOR RADIATION
Z(75)	TOZONE	DENSITY LIMIT AT FREE SURFACE
Z(77)	SBOUND	WT. FRACTION IN VEL. FOR MASS TRANS.
Z(104)	ATOM	ATOMIC NO.
Z(110)	ANN	EXP. FOR FN FUNCTION
Z(111)	EZERO	INITIAL SOURCE
Z(112)	PW	PULSE WIDTH AT HALF MAX
Z(113)	CAPS	KS ABSORPTION IN SOLID
Z(114)	HNU	LASER PHOTON ENERGY
Z(115)	COE	CK COEF FOR LOW TEMP
A(118)	SCUR	SOURCE DURATION
Z(119)	AHN	$8.62E10 / (ATOM * HNU) ** 2$
Z(126)	RFT	REFLECTIVITY
Z(127)	CDUT	CONDUCTIVITY
Z(138)		SPECIFIC DENSITY CUTOFF
Z(139)		PERCENT OF STABILITY FOR DT

PROB=SPROB

FFA=2.

FFB=1.E-10

FEF=6.

SN=-1.

HBOUND=0.

SBOUND=1.

SVMAX=1.E-14

FRCUTC=.5

CB=CV*(GV-1.)

AHN = $8.62E10 / (ATOM * HNU) ** 2$

KMAX=IMAX+JMAX+1

KMAXA=KMAX+1

JMAXA=JMAX+1

IMAXA=IMAX+1

PIDY=3.1415927

READ IN DY AND DX

I=0

J=0

SETU1090
SETU1100
SETU1110
SETU1120
SETU1230

SLTU0010

U I M E N S I O N

```

1U(1200),      V(1200),      AMX(1200),  AIX(1200),  P(1200),
2THETA(1200),  RHO(1200),    FICUT(1200), CAP(1200),  KFIT(1200),
3PUL(255), W1(50), W2(50), W3(50), TABLM(50),
4UX(52),      X(53),        XX(54),      UY(100),      YY(101),
5TAB(15),     AMK(15),       PK(15),       QK(15),       Z(150),      IZ(150),
6TAU(52),     PL(200),       PK(200),      UL(200),      UR(200),
7LEFT(100),   YAMC(100),     SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)

```

COMMON	Z	•XX	•UR	•PR	•THETA	•YY
COMMON	AID	•AIX	•AM	•AMD	•AMX	•AREA
COMMON	BIG	•BOUNCE	•DDXN	•DDVK	•DVK	•DX
COMMON	UY	•E	•FD	•FS	•FX	•OUT
COMMON	P	•PABOVE	•PBLO	•PIDT6	•PPAHOV	•PRR
COMMON	PUL	•QDT	•KC	•REZ	•RHO	•RL
COMMON	HR,SIG	•GUOOF	•L SWITCH	•TABLM	•TAU	
COMMON	TAUDTS	•TAUDTX	•U	•UK	•URK	•UT
COMMON	UU	•UUU	•UTEF	•UVMAX	•V	•VAHOVE
COMMON	VBLO	•VEL	•VK	•VT	•VTEF	•VV
COMMON	VVABOV	•VVBLO	•W2	•W3	•WPS	•WS
COMMON	WSA	•WSB	•WSC	•XL	•XLF	•XN
COMMON	XR	•YL	•YLW	•YN	•YU	•ZMAX
COMMON	I	•II	•IN	•IR	•IWS	•IWSA
COMMON	IWSB	•IWSC	•IW1	•J	•JN	•JP
COMMON	JK	•K	•KN	•KP	•KR	•KRM
COMMON	L	•M	•MA	•MB	•MC	•MD
COMMON	ME	•MZ	•N	•NK	•NKMAX	•NK1
COMMON	NO	•NR	•G	•SOLID	•TEMP	
COMMON	FIOUT	•CAP	•KFIT	•ISEND	•IGOTO	•HEAD

E Q U I V A L E N C E

DEEUIVALENCE	(Z(12),P'ROG),	(Z(2),CYCLE),	(Z(3),DT),
1(Z(4),PRINTS),	(Z(5),PRINTL),	(Z(6),DUMPT7),	(Z(7),CSTOP),
2(Z(8),PIDY),	(Z(9),TMZ),	(Z(10),SCYCLE),	(Z(11),SPROB),
3(Z(12),GAMX),	(Z(13),ETH),	(Z(14),FFA),	(Z(15),FFB),
4(Z(16),TMDZ),	(Z(17),TMXZ),	(Z(18),XMAX),	(Z(19),TXMAX),
5(Z(20),TYMAX),	(Z(21),AMOM),	(Z(22),AMXM),	(Z(23),DNN),
6(Z(24),DMIN),	(Z(25),FEF),	(Z(26),DTNA),	(Z(27),CVIS),
7(Z(28),NPH),	(Z(29),NPRI),	(Z(30),NC),	(Z(31),NPC),
8(Z(32),NHC),	(Z(33),IMAX),	(Z(34),IMAXA),	(Z(35),JMAX),
9(Z(36),JMAXA),	(Z(37),KMAX),	(Z(38),KMAXA),	(Z(39),NMAX),
DEEUIVALENCE	(Z(40),ND),	(Z(41),KDT),	(Z(42),IXMAX),
1(Z(43),NOD),	(Z(44),NOPR),	(Z(45),NIMAX),	(Z(46),NJMAX),
2(Z(47),I1),	(Z(48),I2),	(Z(49),I3),	(Z(50),I4),
3(Z(51),N1),	(Z(52),N2),	(Z(53),N3),	(Z(54),N4),
4(Z(55),N5),	(Z(56),N6),	(Z(57),N7),	(Z(58),N8),
5(Z(59),N9),	(Z(60),N10),	(Z(61),N11),	(Z(62),NRM),
6(Z(63),TRAD),	(Z(64),XNRG),	(Z(65),SN),	(Z(66),DXN),
7(Z(67),RADER),	(Z(68),RADET),	(Z(69),RADEB),	(Z(70),DTRAD),
8(Z(71),REZFFT),	(Z(72),RSTOP),	(Z(73),SHELL),	(Z(74),BBOUND),
9(Z(75),TOZONE),	(Z(76),ECK),	(Z(77),SBOUND),	(Z(78),X1),
DEEUIVALENCE	(Z(79),X2),	(Z(80),Y1),	(Z(81),Y2),
1(Z(82),CABLNI),	(Z(83),VISC),	(Z(84),T),	(Z(85),GMAX),
2(Z(86),W5GD),	(Z(87),W5GX),	(Z(88),GMADR),	(Z(89),GMAXR),
3(Z(90),S1),	(Z(91),S2),	(Z(92),S3),	(Z(93),S4),
4(Z(94),S5),	(Z(95),S6),	(Z(96),S7),	(Z(97),S8),
5(Z(98),S9),	(Z(99),S10),		

C

```

      X(I)=0.
      Y(J)=0.
2000 READ      ( 5,8102) IWSA, IWSB, N1, N2, N3, N4, ( AMX(K), K=1,4)
      L=1
      IF (N4) 2003, 2001, 2005
2001 IF (N3) 2004, 2002, 2004
2002 IF (N2) 2006, 2008, 2006
2003 L=L+1
2004 L=L+1
2006 L=L+1
C TEST TO CALC (X AND DX IF IWSB=0 OR Y AND DY IF IWSB=1)
2008 IF (IWSB) 2010, 2010, 2030
C CALC THE X AND DX VALUES
2010 DO 2014 N=1, L
      NK=I2(N+50)
      DO 2012 K=1, NK
      I=1+1
      DX(I)= AMX(N)
      X(I)=X(I-1)+DX(I)
2012 CONTINUE
2014 CONTINUE
      GO TO 2050
C CALC THE Y AND DY VALUES
2030 DO 2034 N=1, L
      NK=I2(N+50)
      DO 2032 K=1, NK
      J=1+1
      DY(J)= AMX(N)
      Y(J)=Y(J-1)+DY(J)
2032 CONTINUE
2034 CONTINUE
C TEST IF ANOTHER CARD SHOULD BE READ (YES IF IWSA=0, NO IF IWSA=1)
2050 IF (IWSA.EQ.0) GO TO 2000
      WS=X(1)**2
      TAU(1)=WS*P1DY
      DO 2054 I=2, IMAX
      WSA=X(I)**2
      TAU(I)=P1DY*(WSA-WS)
      WS=WSA
2054 CONTINUE
      WRITE (6,8066) IMAX, (DX(I), I=1, IMAX)
      WRITE (6,8067) JMAX, (DY(I), I=1, JMAX)
      WRITE (6,8092) IMAX, (TAU(I), I=1, IMAX)
C CLEAR ALL CELL ARRAYS.
      DO 1 K=1, KMAX
      U(K)=0.0
      V(K)=0.0
      P(K)=0.0
      AMX(K)=0.0
      AIX(K)=0.0
      THETA(K)=0.
      1 CONTINUE
      N1=0
      N2=0
      N3=0
      N4=0
      NF=1
      NN=ANN
      DO 10 N1=1, NN
10 NF=NF*N1
      NP=NN+1
      DO 20 MP=1, NP
      M=MP-1
      MF=1
      DO 20 N1=1, M

```

SETU1240

SETU1280

SETU1290

SETU1300

SETU1130

SETU1140

SETU1150

SETU1160

SETU1170

SETU1180

SETU1190

```

20 MF=MF*N1
   NMN=NN-M
   NMMF=1
   DO 30 N1=1,N/M
30 NMMF=NMMF*N1
   AMF=NF
   AMF=MF
   ANMF=NMMF
   AM=M
40 UNN=(-1.)*M*ANF/(AMF*ANMF*(2.*AM+1.))+BNN
   AAN=ANN
   IF(AAN.EQ.0.) AAN=1.
   TEMP(1)=1./2.**((1./AAN)
   IF(ANN.EQ.0.) TEMP(1)=0.
   TEMP(2)=1.-TEMP(1)
   SCDR=PW/TEMP(2)
   TEMP(3)=SQRT(PI/Y*2.*PW*CV/(CDUT*SVS*TEMP(2)))
   IF(CDUT.EQ.0.) TEMP(3)=0.
   TEMP(4)=CDUT*HCB/(2.*(1.-RFT)*CV)
   TEMP(5)=1./((ANN+1.)*UNN+EZERO)
   EXD= 1./((ANN+.5)
   TC = PW/(2.*TEMP(2))*(TEMP(3)*TEMP(4)*TEMP(5))*EXD
   EXD=1./((ANN+1.)
   IF(CDUT.EQ.0.) TC =SCDR/2.*(HCB*2./(EZERO*CAPS))*EXD
C CO=SOUND SPEED
CO=SQRT(GV*(GV+1.)*HCP)
HH=HVB+HCB-HCP*GV*(GV+1.)*HCP*.5
T=DY(J5)*(GV+1.)/((GV+1.)*CO)
DT=T/4.0
UTNA=DT/Z(139)
T=T+TC
TMT= T-TC
SCRT=.5*EZERO*(2.*T/SCDR)**((ANN+1.)/TMT)
IF(T.GT.0.5*SCDR) SCRT= EZERO*(1.-.5*(2.*(1.-T/SCDR))**((ANN+1.))
1 /TMT
SCRTC= .5*EZERO*(2.*TC/SCDR)**((ANN+1.)/TMT)
SCR=SCRT-SCRTC
HSCR=(1.-RFT)*SCRTC*(ANN+1.)*TMT/TC
TEMP(1)=(1.-RFT)*SCRTC*TMT*SVS/HCB*4.0/PIDY
TEMP(2)=TMT*SVS*SCR/(HH-HCB)
IF(CDUT.EQ.0.) TEMP(2)=0.
TEMP(3)=CDUT*HH*HCB/(CV*(HH-HCB)*(1.-RFT)*SCRTC)*PIDY/4.0
J=J5
DO 3050 I=1,ISR
K=(J-1)*IMAX+I+1
JB=(I-1)*20+1
V(K)=- CO*(GV+1.)/GV
AIX(K)=HH-0.5*V(K)**2
SOLID(JB+1)=TEMP(1)+(-TEMP(2)+TEMP(3))/(1.+TEMP(3)/(2.*TEMP(1)))
SOLID(JB+2)=(SCR-HCB*(SOLID(JB+1)-TEMP(1.)/(SVS*TMT))*(1.-HCB/HH)
SOLID(JB+3)=(1.-RFT)*SCRTC*TMT + HCB*(SOLID(JB+1)-TEMP(1.)/SVS
SOLID(JB+6)= SOLID(JB+2)/(HH-HCB)
AMX(K)=SOLID(JB+6)*(TMT)*TAU(I)
RHO(K)=AMX(K)/(TAU(I)*DY(J))
SCRE = SCRT*TMT*TAU(I) + SCRE
RADE=HFT*SCRTC*TMT*TAU(I) +RADE
CNDE=SOLID(JB+3)*TAU(I)+CNDE
W2(I)=SCR
SOLID(JB+7)=SOLID(JB+6)* TMT
VAPE = SOLID(JB+2)*TMT*TAU(I)+ VAPE+HCB*SOLID(JB+7)*TAU(I)
SOLID(JB+8)=SCRT*TMT
SOLID(JB+4)= SOLID(JB+8)
SOLID(JB+11)=SOLID(JB+6)*CO/GV
SOLID(JB+15)=-CO
SOLID(JB+12)=SOLID(JB+11)+SOLID(JB+6)*ABS(SOLID(JB+15))

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```

SOLID(JB+13)=SOLID(JB+12)*(TMTC)
IF(I.NE.ISR) GO TO 3040
AMX(K+1) = (GV-1.)/(GV+1.)*AMX(K)/(1.-DX(I)/(2.*X(I)))
1      * (2./(GV+1.))*2./(GV-1.)
AMX(K)=AMX(K)-AMX(K+1)
AIX(K+1)=HVB+HCB-HCP
U(K+1) = CO/(GV-1.)
U(K) =CO/8.
V(K+1)=-SQRT(2.*(HH-AIX(K+1)) -U(K+1)**2)
RHO(K)= AMX(K)/(TAU(I)*DY(J))
RHO(K+1)=AMX(K+1)/(TAU(I+1)*DY(J))
AIX(K)=AIX(K)-0.5*(U(K)**2)
ETH = ETH +(AIX(K+1)+ (V(K+1)**2 +U(K+1)**2)/2.)* AMX(K+1)
SV =1./RHO(K+1)
CALL ES(SV,AIX(K+1),THETA(K+1),P(K+1),CAP(K+1),GG)
CALL MFST(KFIT(K+1),1)
3040 ETH = ETH +(AIX(K)+(V(K)**2+U(K)**2)/2.)*AMX(K)
SV=1./RHO(K)
CALL ES(SV,AIX(K),THETA(K),P(K),CAP(K),GG)
CALL MFST(KFIT(K),1)
3050 CONTINUE
DO 2999 I=1,IMAX
CALL DJLOW(JLOW,JHIGH)
DO 2999 J=JLOW,JHIGH
K=(J-1)*IMAX+I+1
CALL FLAG(KFLAG,JLOW,JHIGH)
CALL KFST(KFIT(K),KFLAG)
2999 CONTINUE
CYCLE=0.0
DTH=1.E10
DTC=1.E10
XMAX=X(IMAX)
YMAX=Y(JMAX)
REWIND 10
WS=555.0
WRITE(10) WS,CYCLE,PROB
WRITE(10) (Z(I),I=1,150)
WRITE(10) (U(I),V(I),AMX(I),AIX(I),P(I),THETA(I),
1 RHO(I),FIOUT(I),CAP(I),KFIT(I),I=1,KMAX)
WRITE(10) (X(I),Y(I),TAU(I),I=1,IMAX)
WRITE(10) (Y(I),I=0,JMAX)
WS=666.0
WRITE(10) WS,WS,WS
REWIND 10
RETURN
8102 FORMAT(2I1,4I2,4E10.4)
8066 FORMAT(1H /11H DX(I) I=1,I2/(5F16.6))
8067 FORMAT(1H /11H DY(J) J=1,I3/(5F16.6))
8092 FORMAT(1H /13H AREA(I) I=1,I2/(5F16.6))
END

```

SETU1550

SETU1620

SETU1640

SETU1670

SETU1730

SETU1760

SETU1770

```

C      FOR ESK, ESK/FJ
C      SUBROUTINE ESK(THA,SV,H,CAPK)
C      COMMON // Z
C      I      O      U      I      V      A      L      I      H      C      I
C
C      UEQUVALENCE      (Z(17),PROB),      (Z(18),CYCLL),      (Z(19),DT),
C      1(Z(4),PRINTS),      (Z(15),FRIHIL),      (Z(6),DUMPT7),      (Z(7),LSTOP),
C      2(Z(11),PIDY),      (Z(9),IMZ),      (Z(10),SCYCLL),      (Z(11),SPROB),
C      3(Z(12),GAMX),      (Z(13),E110),      (Z(14),FFA),      (Z(15),FFH),
C      4(Z(16),IMDZ),      (Z(17),IMX2),      (Z(18),XMAX),      (Z(19),TXMAX),
C      5(Z(20),TYMAX),      (Z(21),AMOM),      (Z(22),AMAM),      (Z(23),ONN),
C      6(Z(24),OMINI),      (Z(25),FIF),      (Z(26),OTHIA),      (Z(27),CVIS),
C      7(Z(28),HPR),      (Z(29),HPR1),      (Z(30),HC),      (Z(31),HPC),
C      8(Z(32),HRC),      (Z(33),IMAX),      (Z(34),IMAXA),      (Z(35),JMAX),
C      9(Z(36),JMAXA),      (Z(37),KMAX),      (Z(38),KMAXA),      (Z(39),IMAX),
C      UEQUVALENCE      (Z(40),H1),      (Z(41),KOT),      (Z(42),IXMAX),
C      1(Z(43),HOD),      (Z(44),HOPR),      (Z(45),HOMAX),      (Z(46),HJMAX),
C      2(Z(47),I1),      (Z(48),I2),      (Z(49),I3),      (Z(50),I4),
C      3(Z(51),H1),      (Z(52),H2),      (Z(53),H3),      (Z(54),H4),
C      4(Z(55),H5),      (Z(56),H6),      (Z(57),H7),      (Z(58),H8),
C      5(Z(59),H9),      (Z(60),H10),      (Z(61),H11),      (Z(62),H12),
C      6(Z(63),THAD),      (Z(64),XIRG),      (Z(65),SN),      (Z(66),HXH),
C      7(Z(67),HADEH),      (Z(68),HADET),      (Z(69),HADEH),      (Z(70),OTHAD),
C      8(Z(71),HEZFC),      (Z(72),RSTOP),      (Z(73),SHELL),      (Z(74),HHOUNO),
C      9(Z(75),TUZONE),      (Z(76),ECK),      (Z(77),SHOUNO),      (Z(78),X1),
C      UEQUVALENCE      (Z(79),X2),      (Z(80),Y1),      (Z(81),Y2),
C      1(Z(82),CABLH),      (Z(83),VISC),      (Z(84),T),      (Z(85),GMAX),
C      2(Z(86),WSHO),      (Z(87),WSGX),      (Z(88),GMADR),      (Z(89),GMAXR),
C      3(Z(90),S1),      (Z(91),S2),      (Z(92),S3),      (Z(93),S4),
C      4(Z(94),S5),      (Z(95),S6),      (Z(96),S7),      (Z(97),S8),
C      5(Z(98),S9),      (Z(99),S10)
C
C      UEQUVALENCE      (Z(100),HVB),      (Z(101),HCB),      (Z(102),CD),
C      1(Z(103),SVS),      (Z(104),ATOM),      (Z(105),CV),      (Z(106),GV),
C      2(Z(107),SUMFE),      (Z(108),HETA),      (Z(109),ALCO),      (Z(110),ANN),
C      3(Z(111),EZERO),      (Z(112),PW),      (Z(113),CAP5),      (Z(114),HNU),
C      3(Z(115),COE),      (Z(116),SCR),      (Z(117),ISR),      (Z(118),SCDR),
C      4(Z(119),AHN),      (Z(120),DTH),      (Z(121),IH),      (Z(122),JH),
C      5(Z(123),UTC),      (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
C      X(Z(127),CDUT),      (Z(128),HCP),      (Z(129),HH),      (Z(130),CO),
C      6(Z(131),J1),      (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
C      7(Z(135),J5),      (Z(136),J6),      (Z(137),J7),      (Z(138),SVMAX),
C      8(Z(139),FRCUTC)
C      UEQUVALENCE      (Z(140),VAPE),      (Z(141),RADE),      (Z(142),CNDE),
C      1(Z(143),SCRE),      (Z(144),IV),      (Z(145),JV),      (Z(146),IU),
C      2(Z(147),JU),      (Z(148),DTVF),      (Z(149),DTUF),      (Z(150),E11)
C
C      REVISED CALCULATION OF CAPK IN ESK 7/19/66
C      ZBAR=CAPK
C      SCLIM=0.4*ZBAR/ATOM
C      IF(THA.GT.2.0) GO TO 10
C      CPL1=COE*(THA/SV)**2*THA**2
C      CAPL2=AMIN1(CPL1+SCLIM,CAP5)
C      IF(THA.GT.1.) GO TO 20
C      CAPK=CAPL2
C      GO TO 1000
C 10  CPL3=8.62E10*ZBAR**2*AMAX1(1.,ZBAR)*(FREXP(HNU/
C      1THA)-1.)/(SV*SQRT(THA)*ATOM**2*HNU**3)
C      CAPK=AMAX1(CPL3,SCLIM)
C      GO TO 1000
C 20  CPL4=8.81E8*THA*FREXP(-E11/THA)*(1.0-
C      1FREXP(-HNU/THA))/(ATOM*HNU**3)
C      CAPK=AMAX1(CAPL2,CPL4)
C 1000 RETURN
C      END

```

WI FOR SPRINT, SPRINT/FJ
SUBROUTINE SPRINT

C
C
C
D I M E N S I O N

DIMENSION
10(1200), V(1200), AMX(1200), AIX(1200), P(1200),
2THETA(1200), RHO(1200), FIOUT(1200), CAP(1200), KFIT(1200),
3PUL(255), IW1(50), W2(50), W3(50), TAILM(50),
4DX(52), X(53), XX(54), DY(100), Y(100), YY(101),
5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
6TAU(52), PL(200), PK(200), UL(200), UR(200),
7LEFT(100), YAMC(100), SIGC(100), GAMC(100),
8G(50), SOLID(400), TEMP(12), HEAD(12)

COMMON	Z	XX	UR	PR	THETA	YY
COMMON	AID	AIX	AM	AMD	AMX	AREA
COMMON	BIG	BOUNCE	DDXN	DDVK	DVK	DX
COMMON	DY	EL	FD	FS	FX	OUT
COMMON	P	PABOVE	PBLO	PTOTS	PPABOV	PRR
COMMON	PUL	QUT	RC	R	RHO	RL
COMMON	RR	SIG	G300FL	SWITCH	TAIL	TAU
COMMON	TAUDIS	TAUDTX	U	UK	URR	UT
COMMON	UU	UUU	UTEF	UVMAX	V	VABOVE
COMMON	VIBLO	VEL	VK	VT	VTEF	VV
COMMON	VVABOV	VVBLO	W2	W3	WPS	WS
COMMON	WSA	WSB	WSC	XL	XLF	XN
COMMON	XR	YL	YLW	YN	YU	ZMAX
COMMON	I	II	IN	IR	IWS	IWSA
COMMON	IWSB	IWSC	IW1	J	JN	JP
COMMON	JR	K	KN	KP	KR	KRM
COMMON	L	M	MA	MB	MC	MD
COMMON	ME	MZ	N	NK	NKMAX	NK1
COMMON	NO	NH	G	SOLID	TEMP	
COMMON	FIOUT	CAP	KFIT	ISEND	IGOT	HEAD

C
C
C
C

E Q U I V A L E N C E

0EQUIVALENCE	(Z(12),PROB),	(Z(2),CYCLE),	(Z(3),DT),
1(Z(4),PRINTS),	(Z(5),PRINTL),	(Z(6),DUMPT7),	(Z(7),CSTOP),
2(Z(8),PIDY),	(Z(9),TMZ),	(Z(10),SCYCLE),	(Z(11),SPROB),
3(Z(12),GAMX),	(Z(13),ETH),	(Z(14),FFA),	(Z(15),FFB),
4(Z(16),TMDZ),	(Z(17),TMXZ),	(Z(18),XMAX),	(Z(19),TXMAX),
5(Z(20),TYMAX),	(Z(21),ANDM),	(Z(22),AMXM),	(Z(23),DNN),
6(Z(24),DMIN),	(Z(25),FEF),	(Z(26),DTNA),	(Z(27),CVIS),
7(Z(28),NPR),	(Z(29),NPR1),	(Z(30),NC),	(Z(31),NPC),
8(Z(32),NRC),	(Z(33),IMAX),	(Z(34),IMAXA),	(Z(35),JMAX),
9(Z(36),JMAXA),	(Z(37),KMAX),	(Z(38),KMAXA),	(Z(39),NMAX),
0EQUIVALENCE	(Z(40),ND),	(Z(41),KUT),	(Z(42),IXMAX),
1(Z(43),NOD),	(Z(44),NOPR),	(Z(45),NIMAX),	(Z(46),NJMAX),
2(Z(47),I1),	(Z(48),I2),	(Z(49),I3),	(Z(50),I4),
3(Z(51),N1),	(Z(52),N2),	(Z(53),N3),	(Z(54),N4),
4(Z(55),N5),	(Z(56),N6),	(Z(57),N7),	(Z(58),N8),
5(Z(59),N9),	(Z(60),N10),	(Z(61),N11),	(Z(62),NRM),
6(Z(63),TRAD),	(Z(64),XNRG),	(Z(65),SN),	(Z(66),DXN),
7(Z(67),RADEK),	(Z(68),RADET),	(Z(69),RADEH),	(Z(70),DTRAD),
8(Z(71),RLZFC1),	(Z(72),RSTOP),	(Z(73),SHELL),	(Z(74),D90JND),
9(Z(75),TOZONE),	(Z(76),ECK),	(Z(77),SHOUND),	(Z(78),X1),
0EQUIVALENCE	(Z(79),X2),	(Z(80),Y1),	(Z(81),Y2),
1(Z(82),CAHLN),	(Z(83),VISC),	(Z(84),T),	(Z(85),GMAX),
2(Z(86),WS6U),	(Z(87),WS6X),	(Z(88),GMAUR),	(Z(89),GMAXR),
3(Z(90),S1),	(Z(91),S2),	(Z(92),S3),	(Z(93),S4),
4(Z(94),S5),	(Z(95),S6),	(Z(96),S7),	(Z(97),S8),
5(Z(98),S9),	(Z(99),S10)		

C

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DEQUIVALENC (Z(100),HVB), (Z(101),HCH), (Z(102),CB),
1(Z(103),SVS), (Z(104),ATOM), (Z(105),CV), (Z(106),GV),
2(Z(107),SUMFE), (Z(108),BETA), (Z(109),ALCO), (Z(110),ANN),
3(Z(111),EZERO), (Z(112),PW), (Z(113),CAPS), (Z(114),HNU),
4(Z(115),COE), (Z(116),SCR), (Z(117),ISR), (Z(118),SCOR),
5(Z(119),AHN), (Z(120),DTH), (Z(121),IH), (Z(122),JH),
6(Z(123),UTC), (Z(124),IC), (Z(125),JC), (Z(126),RFT),
7(Z(127),CDUT), (Z(128),HCP), (Z(129),HH), (Z(130),CO),
8(Z(131),J1), (Z(132),J2), (Z(133),J3), (Z(134),J4),
9(Z(135),J5), (Z(136),J6), (Z(137),J7), (Z(138),SVMAX),
DEQUIVALENCE (Z(140),VAPE), (Z(141),RADE), (Z(142),CNDE),
1(Z(143),SCRE), (Z(144),IV), (Z(145),JV), (Z(146),IU),
2(Z(147),JU), (Z(148),DTVF), (Z(149),DTUF), (Z(150),EI1)

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C

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DEQUIVALENCE (XX(2),X(1)), (UR,UL,FLLFT), (UR(100),YA4C),
1(PH(100),SIGC), (PH,PL,GAMC), (DKE,THETA), (UR,TAB),
2(UR(16),AMK), (UR(31),PK), (UR(46),GK), (YY(2),Y(1))
COMMON/HEADER/ TITLE(48), TITLE1(48), TITLE2(48), TITLE3(6)
DATA TITLE/288HPRB CYCLE DT PRINTSPRINTLDUMPT7CSTOP PIDY TM
12 SCYCLESPOB GAMX ETH FFA FFB TMDZ TMXZ XMAX TXMAX TY
2MAX AMDM AMXM UNN UMIN FEF DTNA CVIS NPR IPRI NC NP
3C NRC IMAX IMAXA JMAX JMAXA KMAX KMAXA NMAX ND KDT 1X
4MAX NOD NOPK NIMAX NJMAX I1 I2 /
DATA TITLE1/288HI3 I4 N1 N2 N3 N4 N5 N6 N7
1 N8 N9 N10 N11 NRM TRAD XNRG SN DXN RADER RA
2DET HADEB DTRAD REZFCTRSTOP SHELL BBOUNDTOZONECK SHOUNDX1 X2
3 Y1 Y2 CABLN VISC T GMAX WSGU WSGX GMADR GMAXR S1
4 S2 S3 S4 S5 S6 S7 /
DATA TITLE2/288HS8 S9 S10 HVB HCB CB SVS ATOM CV
1 GV SUMFE BETA ALCO ANN EZERO PW CAPS HNU COE SC
2K ISR SCUR AHN DTH IH JH DTC IC JC RFT CD
3UT HCP HH CO J1 J2 J3 J4 J5 J6
4MAX FRCUTCVAPE RADE CNDE SCRE IV /
DATA TITLE3/36HJV IU JU DTVF DTUF EI1 /
IGO=1
KOUNT=1
IFROM=1
ITO=8
WRITE(6,10) (HEAD(I),I=1,12),CYCLE
10 FORMAT(37H1 HECTIC PANIC DUMP OF PROBLEM . . . 12A6,5HCYCLEF6.0)
WRITE(6,3) S1
3 FORMAT(7H S1 = F10.4)
15 WRITE(6,20) (TITLE(I),I=IFROM,ITO)
20 FORMAT(1H0 / 5X,8A15)
GO TO (22,22,22,24,26,26),IGO
22 WRITE(6,23)KOUNT,(Z(I),I=IFROM,ITO)
GO TO 30
23 FORMAT(1X,15,1P8E15.7)
24 WRITE(6,25)KOUNT,(Z(I),I=IFROM,ITO)
25 FORMAT(1X,15,1P3E15.7,5(5X,I10))
GO TO 30
26 WRITE(6,27)KOUNT,(Z(I),I=IFROM,ITO)
27 FORMAT(1X,15,8(5X,I10))
30 IGO=IGO+1
KOUNT=KOUNT+8
IFROM=IFROM+8
ITO=ITO+8
IF(IGO.LT.7) GO TO 15
IGO=1
31 WRITE(6,20) (TITLE(I),I=IFROM,ITO)
GO TO (32,34,36,36,36,36),IGO
32 WRITE(6,27)KOUNT,(Z(I),I=IFROM,ITO)
GO TO 40
34 WRITE(6,35)KOUNT,(Z(I),I=IFROM,ITO)

```

```

35 FORMAT(1X,15,6(5X,110),1P2E15.7)
GO TO 40
36 WRITE(6,23)KOUNT,(Z(1),I=IFROM,ITO)
40 IGO=IGO+1
IFROM=IFROM+8
ITO=ITO+8
KOUNT=KOUNT+8
IF(IGO.LT.7) GO TO 31
IGO=1
41 WRITE(6,20) (TITLE(1),I=IFROM,ITO)
GO TO (42,42,44,46,48,42),IGO
42 WRITE(6,23)KOUNT,(Z(1),I=IFROM,ITO)
GO TO 50
44 WRITE(6,45)KOUNT,(Z(1),I=IFROM,ITO)
45 FORMAT(1X,15,1P4E15.7,5X,110,3E15.7)
GO TO 50
46 WRITE(6,47)KOUNT,(Z(1),I=IFROM,ITO)
47 FORMAT(1X,15,2(5X,110),1PE15.7,2(5X,110),3E15.7)
GO TO 50
48 WRITE(6,49)KOUNT,(Z(1),I=IFROM,ITO)
49 FORMAT(1X,15,1P2E15.7,6(5X,110))
50 IGO=IGO+1
IFROM=IFROM+8
ITO=ITO+8
KOUNT=KOUNT+8
IF(IGO.LT.7) GO TO 41
WRITE(6,20) (TITLE(1),I=145,150)
WRITE(6,23)KOUNT,(Z(1),I=145,150)
WRITE(6,111)
WRITE(6,112)
WRITE(6,113)
WRITE(6,114)
WRITE(6,115)
WRITE(6,116)
IF(S1-4.0108)53,54,52
52 IF(S1-4.0126)53,54,53
53 IF(AUS(ECK).GT.DMIN) WRITE(6,117) ECK,DMIN
111 FORMAT(79H1S1 ERROR NUMBER TO FLAG THE SUBROUTINE WH
11CH CALLED MACHINE EXIT)
112 FORMAT(53H0 4.0108 NORMAL EXIT AFTER MAX. CYCLE//)
113 FORMAT(89H 1. MAIN 5. CDT 9. PH2
1 13. ES 17. PAC )
114 FORMAT(89H 16 14. JMH 18. SETUP)
115 FORMAT(89H 10W 15. MFST 19. ESK )
116 FORMAT(89H 1EX 16. KFST 20. )
117 FORMAT(28H0 ENERGY CHECK ERROR. ECK =1PE15.7,7H DMIN =E15.7)
54 REWIND 10
IF(N7.EQ.10) GO TO 1000
REWIND N7
1000 CALL EXIT
END

```

REFERENCES

1. Tillotson, J. H. , "Metallic Equations of State for Hypervelocity Impact," General Atomic Report GA-3216, July, 1962, p. 12.
2. Carslaw, H. S. , and J. C. Jaeger, Conduction of Heat in Solids, Oxford Press, 2nd Ed. , 1959, p. 76.

SECTION III

EQUATIONS OF STATE FOR IONIZED VAPOR

3.1. INTRODUCTION

Theoretical studies of hydrodynamics and radiation transport require information about the thermodynamic state variables of the system. In many applications, local thermodynamic equilibrium (LTE) may be assumed. Under this assumption, the law of mass action can be used to solve for the equilibrium concentrations of every species present in the system.

The methods described in this section, and the EIONX computer routines based upon them, apply to equilibria involving neutral atoms, ions, and electrons. At low temperatures (generally less than 2 ev), molecular constituents may also be present. Their equilibria, however, are calculated by other methods. The EIONX codes provide for linkage of molecular equilibrium routines in such a way that the contribution of the latter to the thermodynamic properties of the system can be taken into account.

The law of mass action was applied by Saha in 1920 to the equilibrium



With concentrations, in cm^{-3} , of neutrals, ions, and electrons denoted, respectively, by $[Cs]$, $[Cs^+]$ and $[e^-]$, the law states that for equilibrium at $T^\circ\text{K}$,

$$\frac{[e^-] [Cs^+]}{[Cs]} = e^{-\Delta G(T)/kT}$$

where $\Delta G(T)$ is the free energy change in the reaction. Similar relationships hold for equilibrium concentrations of more highly ionized stages and excited ionic states. If the perfect gas law is assumed, the following general relationship can be shown to hold for the relative concentrations or mole fractions, X_j , of ions of some atomic species in stage j (ionic charge j):

$$\frac{X_j}{X_{j-1}} = \Gamma \frac{u_j}{u_{j-1}} e^{-V_j/kT}$$

where V_j is the j th ionization potential of the atom, u_j is the partition function for stage j , and Γ is a parameter which is inversely proportional to the electron density, and therefore depends on the concentrations of all ionization stages of every atomic species present.

The calculation of the state of the vapor at a given temperature and mass density therefore involves solution of a comparatively extensive system of coupled nonlinear equations for the concentrations of each constituent. The EIONX routines perform this task, with the aid of certain simplifying assumptions, and then proceed to the evaluation of the thermodynamic state variables of the system. These simplifying assumptions are most valid in those regions of phase space (essentially characterized by $\Gamma \gg 1$) in which particle interactions are sufficiently infrequent that the distribution of ionic states is sharply peaked. In other regions, not only these assumptions but also those more basic ones mentioned in the preceding paragraph are likely to be invalid.

3.2. FORMULATION OF THE LINEAR EIONX ROUTINES

3.2.1. Definitions

τ	Specific volume, $\text{cm}^3 \text{g}^{-1}$,
θ	Temperature, ev; $\theta = kT$,
P	Pressure, dynes cm^{-2} ,
E	Specific internal energy, ergs g^{-1} ,

α_i	Number fraction of element i in the material; $\sum_i \alpha_i = 1,$
Z^i	Atomic number of element $i,$
V_j^i	j^{th} ionization potential of element $i,$
X_j^i	Number fraction of element i in the j^{th} ionization stage; $\sum_j X_j^i = 1$
$\bar{Z}^i$	Mean ionic charge of element i ; $\bar{Z}^i = \sum_{j=1} Z^i X_j^i,$
$\bar{Z}$	Mean ionic charge of material; $\bar{Z} = \sum_i \alpha_i \bar{Z}^i,$
A_i	Atomic mass number of element $i,$
$\bar{A}$	Mean atomic mass number; $\bar{A} = \sum_i \alpha_i A_i,$
φ	Gas constant in ergs $g^{-1} \text{ev}^{-1}$; $\varphi = eR/k\bar{A} = eN_0/\bar{A}$ $\cong 9.65 \times 10^{11}/\bar{A},$
c	Constant in Saha equation; $c = 2h^{-3}(2\pi m_e)^{3/2} m_p eR/k$ $\cong e^{22.99} \text{ergs ev}^{-5/2} \text{cm}^{-3},$
Γ	Electronic "nondegeneracy" parameter; $\Gamma = c\tau\theta^{3/2}/\varphi\bar{Z},$
I^0	$I^0 = \theta \ln (c\tau\theta^{3/2}/\varphi),$
β_j^i	$\beta_j^i = \exp [(I^0 - V_j^i)/\theta],$
I	$I = \theta \ln \Gamma = I^0 - \theta \ln \bar{Z},$
$\bar{N}$	Mean number of atoms per molecule.

3.2.2. The Saha Equation for Ionic Equilibria

$$\frac{X_j^i}{X_{j-1}^i} = \Gamma e^{-V_j^i/\theta} = e^{(I-V_j^i)/\theta} = \frac{\beta_j^i}{\bar{Z}} \quad 1 \leq j \leq Z^i$$

The ratio of partition functions u_j/u_{j-1} has been omitted from this equation. It is usually of order unity, in contrast to Γ and the exponential factor. The effect of omitting this ratio is thus equivalent to a small shift in temperature. The pressure lowering of the ionization potential is also neglected.

It should be noted that the distribution of populations X_j^i is in general strongly peaked near those stages j for which $V_j^i \approx I$. For $V_j^i = I$, in particular, X_j^i and X_{j-1}^i are equal, while the adjacent terms X_{j+1}^i and X_{j-2}^i are smaller by factors such as $\exp(-\Delta V/\theta)$, where ΔV , the separation of the ionization potentials, is usually large compared with θ . The mean ionic charge $\bar{Z}^i$, for $I = V_j^i$, is thus approximately

$$\bar{Z}^i \approx (j-1) X_{j-1}^i + j X_j^i \approx j - 1/2$$

This fact is used as the basis for an approximate interpolation procedure which avoids the need for solving the entire coupled set of Saha equations yet preserves some of the basic characteristics of any such solution, namely, that $\bar{Z}^i$ is a continuous monotonic increasing function of I which assumes half-odd-integer values when I is close to an ionization potential.

3.2.3. The EONX Model for Mean Ionic Charge

$$\bar{Z}^i = j - \frac{3}{2} + \frac{I - V_{j-1}^i}{V_j^i - V_{j-1}^i}, \quad V_{j-1}^i < I \leq V_j^i, \quad j = 2, \dots, Z^i$$

$$\bar{Z}^i = \left[1 + \exp \left(\frac{V_1^i - I}{\theta} \right) \right]^{-1} = X_1^i = \frac{\beta_1^i}{\bar{Z} + \beta_1^i}, \quad I < V_1^i$$

$$X_Z^i = \left[1 + \exp \left(- \frac{I - V_Z^i}{\theta} \right) \right]^{-1} = \frac{\beta_Z^i}{\bar{Z} + \beta_Z^i}, \quad I > V_Z^i$$

$$\bar{Z}^i = Z^i - 1 + X_Z^i, \quad I > V_Z^i$$

That is, for I between two ionization potentials, $\bar{Z}^i(I)$ is the linear interpolant between the half-integer values defined above; and for I less than the first ionization potential or greater than the last, it is assumed that only two ionization stages are populated (the neutral or stripped stage, respectively, and the adjacent stage), in which case a single Saha equation determines the state.

These assumptions, together with the defining relations

$$\bar{Z} = \sum_i \alpha_i \bar{Z}^i$$

$$I = I^0 - \theta \ln \bar{Z}$$

form the basis for an iterative solution for I , $\bar{Z}$, and the $\bar{Z}^i$, given θ and r or I^0 .

3.2.4. Computation of P and E

The thermodynamic variables to be computed are the pressure P , the internal energy E , and their derivatives with respect to the independent variables τ and θ . All of these quantities depend upon $\bar{Z}$, as well. Since

$\bar{Z}$ is not an independent variable but a function of τ and θ determined by the model discussed above, it is necessary to impose a thermodynamic consistency condition of some sort on the definitions of P and E . A suitable choice is the thermodynamic relation

$$\left(\frac{\partial E}{\partial \tau}\right)_{\theta} = \theta \left(\frac{\partial P}{\partial \theta}\right)_{\tau} - P$$

For the pressure, the perfect gas law is assumed:

$$P = (\bar{N}^{-1} + \bar{Z}) \varphi \theta / \tau$$

and for the internal energy a sum of random kinetic, ionization, and dissociation terms:

$$E = \frac{3}{2} (\bar{N}^{-1} + \bar{Z}) \varphi \theta + \varphi \sum_i \alpha_i \xi_i + E_{\text{dis}}$$

where E_{dis} is the molecular dissociation contribution, and ξ_i , the mean ionization energy per atom of element i , is

$$\xi_i = \sum_{k=1}^{j-1} v_k^i + v_{j-1}^i (\bar{Z}^i - j + 1) + (v_j^i - v_{j-1}^i) (\bar{Z}^i - j + \frac{3}{2})^2 / 2$$

$$\xi_i = \bar{Z}^i v_1^i$$

$$\xi_i = \sum_{k=1}^{Z^i-1} v_k^i + (\bar{Z}^i - Z^i + 1) v_Z^i$$

$$v_{j-1}^i < I \leq v_j^i$$

$$I < v_1^i$$

$$I > v_Z^i$$

These definitions for ξ_i are the simplest which conform to the thermodynamic consistency condition and also to the assumptions made above for the X_j^i .

The derivatives of P and E are

$$\left(\frac{\partial P}{\partial \theta}\right)_{\tau} = P/\theta + \frac{\varphi\theta}{\tau} \left[\left(\frac{\partial \bar{Z}}{\partial \theta}\right)_{\tau} - \bar{N}^{-2} \left(\frac{\partial \bar{N}}{\partial \theta}\right)_{\tau} \right]$$

$$\left(\frac{\partial P}{\partial \tau}\right)_{\theta} = -\frac{P}{\tau} + \frac{\varphi\theta}{\tau} \left[\left(\frac{\partial \bar{Z}}{\partial \tau}\right)_{\theta} - \bar{N}^{-2} \left(\frac{\partial \bar{N}}{\partial \tau}\right)_{\theta} \right]$$

$$C_V = \left(\frac{\partial E}{\partial \theta}\right)_{\tau} = \frac{3}{2} \varphi (\bar{N}^{-1} + \bar{Z}) + \frac{3}{2} \varphi\theta \left[\left(\frac{\partial \bar{Z}}{\partial \theta}\right)_{\tau} - \bar{N}^{-2} \left(\frac{\partial \bar{N}}{\partial \theta}\right)_{\tau} \right]$$

$$+ \varphi \sum_i \alpha_i \left(\frac{\partial \xi_i}{\partial \theta}\right)_{\tau} + \left(\frac{\partial E_{\text{dis}}}{\partial \theta}\right)_{\tau}$$

$$\left(\frac{\partial E}{\partial \tau}\right)_{\theta} = \frac{3}{2} \varphi\theta \left[\left(\frac{\partial \bar{Z}}{\partial \tau}\right)_{\theta} - \bar{N}^{-2} \left(\frac{\partial \bar{N}}{\partial \tau}\right)_{\theta} \right] + \varphi \sum_i \alpha_i \left(\frac{\partial \xi_i}{\partial \tau}\right)_{\theta} + \left(\frac{\partial E_{\text{dis}}}{\partial \tau}\right)_{\theta}$$

$$\text{where } \left(\frac{\partial \bar{Z}}{\partial \theta}\right)_{\tau} = D^{-1} \sum_i \alpha_i \left(\frac{J_i}{\theta} + \frac{3}{2}\right) \left(\frac{\partial \bar{Z}^i}{\partial I}\right)_{\theta}$$

$$\left(\frac{\partial \bar{Z}}{\partial \tau}\right)_{\theta} = D^{-1} \frac{\theta}{\tau} \sum_i \alpha_i \left(\frac{\partial \bar{Z}^i}{\partial I}\right)_{\theta}$$

$$\left(\frac{\partial \xi_i}{\partial \tau}\right)_{\theta} = J_i \left(\frac{\partial \bar{Z}^i}{\partial \tau}\right)_{\theta} = J_i \left[\frac{\theta}{\tau} - \frac{\theta}{\bar{Z}} \left(\frac{\partial \bar{Z}}{\partial \xi}\right)_{\theta} \right] \left(\frac{\partial \bar{Z}^i}{\partial I}\right)_{\theta}$$

$$\left(\frac{\partial \xi_i}{\partial \theta}\right)_{\tau} = J_i \left(\frac{\partial \bar{Z}^i}{\partial \theta}\right)_{\tau} = J_i \left[\frac{J_i}{\theta} + \frac{3}{2} - \frac{\theta}{\bar{Z}} \left(\frac{\partial \bar{Z}}{\partial \theta}\right)_{\tau} \right] \left(\frac{\partial \bar{Z}^i}{\partial I}\right)_{\theta}$$

$$J_i = \text{Min} \left[V_Z^i, \text{Max} (V_I^i, 1) \right]$$

$$D = 1 + \frac{\theta}{\bar{Z}} \sum_i \alpha_i \left(\frac{\partial \bar{Z}^i}{\partial I}\right)_{\theta}$$

$$\begin{aligned}
 \left(\frac{\partial \bar{Z}^i}{\partial I} \right)_\theta &= \frac{1}{V_j^i - V_j^{i-1}}, \quad V_{j-1}^i < I \leq V_j^i, \quad j = 2, \dots, Z^i \\
 &= \frac{\beta_1^i \bar{Z}}{\theta (\bar{Z} + \beta_1^i)^2} = \frac{X_1^i (1 - X_1^i)}{\theta} \quad I < V_1^i \\
 &= \frac{\beta_Z^i \bar{Z}}{\theta (\bar{Z} + \beta_Z^i)^2} = \frac{X_Z^i (1 - X_Z^i)}{\theta} \quad I > V_Z^i
 \end{aligned}$$

E_{dis} , $\bar{N}$, and their derivatives are obtained from molecular equilibrium routines external to EIONX. If no such routines are used, $\bar{N}$ is taken to be 1 and its derivatives are taken to be zero; similarly, $E_{\text{dis}} = 0$.

The velocity of sound, c_o , is determined from these derivatives by using the thermodynamic relation

$$c_o^2 = \tau^2 \left[\frac{\theta}{C_V} \left(\frac{\partial P}{\partial \theta} \right)_\tau^2 - \left(\frac{\partial P}{\partial \tau} \right)_\theta \right]$$

3.3. PROCEDURES FOR ITERATIVE SOLUTION

When only one element is present in the material, a number of simplifications are possible in the formulation and in the program coding; furthermore a more efficient iterative procedure is available. Two versions of the linear EIONX routines were therefore prepared. The more general multi-element procedure is described first.

3.3.1. Multi-element Iterative Procedure

1. Initialize (i. e., iteration index $n = 1$): $\bar{Z}^{(n)} = 1$.
2. $I^0 - \theta \ln \bar{Z}_{(n)} \rightarrow I_{(n)}$.

3. Compute $\bar{Z}^i$.
4. $\sum_i x_i \bar{Z}^i \rightarrow \bar{Z}_{(n+1)}$.
5. Apply Aitken extrapolation every third pass.
6. If

$$\left| \frac{\bar{Z}_{(n+1)} - \bar{Z}_{(n)}}{\bar{Z}_{(n+1)}} \right| > \epsilon$$

then $n+1 \rightarrow n$ and repeat from step 2.

7. Otherwise, $I^0 - \theta \ln \bar{Z}_{(n+1)} \rightarrow I$.
8. Compute $\bar{Z}$, its derivatives, and all of the thermodynamic variables defined in Section 3.2.

The procedure converges unless, for some i ,

$$\frac{\theta/\bar{Z}}{V_j^i - V_{j-1}^i} > 1 \text{ and } 1/2 < \bar{Z} < \bar{Z}^i - 1/2$$

Since, usually, $V_j^i - V_{j-1}^i > 2\theta$, failures are exceptional. They have occasionally been noted for materials at moderately low temperature and very high density, essentially also the conditions for electron degeneracy and consequently for inapplicability of the entire formulation. If convergence does not occur in 20 iterations, a flag is set and the last iterate is used.

3.3.2. Single-element Iterative Procedure

For $V_1 < I \leq V_Z$,

$$\bar{Z} = j - 1.5 + \frac{I^0 - \theta \ln \bar{Z} - V_{j-1}}{V_j - V_{j-1}} = a - b \ln \bar{Z}$$

where

$$a = j - 1.5 + \frac{I^0 - V_{j-1}}{V_j - V_{j-1}}, \quad b = \frac{\theta}{V_j - V_{j-1}}$$

If $b/\bar{Z} < 1$, the iteration procedure

$$\bar{Z}_{(n+1)} = a - b \ln \bar{Z}_{(n)}$$

converges, since then

$$\begin{aligned} \bar{Z}_{(n+1)} - \bar{Z}_{(n)} &= -b \ln \left[1 + \frac{\bar{Z}_{(n)} - \bar{Z}_{(n-1)}}{\bar{Z}_{(n-1)}} \right] \\ &\approx -b \frac{\bar{Z}_{(n)} - \bar{Z}_{(n-1)}}{\bar{Z}_{(n-1)}} \end{aligned}$$

and the convergence ratio is

$$\left| \frac{\bar{Z}_{(n+1)} - \bar{Z}_{(n)}}{\bar{Z}_{(n)} - \bar{Z}_{(n-1)}} \right| \approx \frac{b}{\bar{Z}} < 1$$

By a similar argument it can be shown that if $b/\bar{Z} > 1$, the iteration procedure

$$\ln \bar{Z}_{(n+1)} = \frac{a - \bar{Z}_{(n)}}{b}$$

is convergent.

There is, however, a far more efficient procedure for the single-element case. For $V_{j-1} < I \leq V_j$, let $\alpha = j - 1/2$ and $x = (I - V_{j-1}) / (V_j - V_{j-1})$ so that $\bar{Z} = \alpha + x$ with $0 < x \leq 1$.

The equation

$$\bar{Z} = a - b \ln \bar{Z}$$

may then be written as

$$\alpha + x = a - b \ln (\alpha + x)$$

so that

$$x = -\alpha + a - b \left[\ln \alpha + 2 \sum_{k=0}^{\infty} \frac{1}{2k+1} \left(\frac{x}{2\alpha+x} \right)^{2k+1} \right]$$

or

$$x = \left(1 + \frac{2b}{2\alpha+x} \right)^{-1} \left[-\alpha + a - b \ln \alpha - 2b \sum_{k=1}^{\infty} \frac{1}{2k+1} \left(\frac{x}{2\alpha+x} \right)^{2k+1} \right]$$

This expansion of the logarithm converges provided that $\alpha > 0$ and $-\alpha < x < +\infty$; both conditions are satisfied in this application. The iterative solution for x is then straightforward:

$$x_{(1)} = -\alpha + a - b \ln \alpha - 2b \frac{x}{2\alpha+x}$$

$$x_{(n+1)} = \left(1 + \frac{2b}{2\alpha+x_{(n)}} \right)^{-1} \left[-\alpha + a - b \ln \alpha - 2b \sum_{k=1}^3 \frac{1}{2k+1} \left(\frac{x_{(n)}}{2\alpha+x_{(n)}} \right)^{2k+1} \right]$$

This procedure is more than twice as efficient as the general multi-element procedure for a single element, primarily owing to the elimination of most of the logarithm calculations and the bookkeeping required for additional elements.

3.4. PROGRAM FLOW

The EIONX routines are called by

CALL EIONX (X1,X2,M1,X3)

where X1 is the temperature θ in ev; X2 is the specific volume τ in cm^3/g ; M1 is a material identification integer discussed below; X3 on entry specifies any special options as discussed below; and X3 on exit contains an error parameter if a noncatastrophic error has occurred, or zero if no error has occurred. Catastrophic errors cause an immediate return with

a nonzero value for the error flag EION(14). The calling program should check both X3 and EION(14) on return, and take appropriate action if either flag was set.

On entry to EIONX, a nonzero value for EION(14) enables a call to one of three molecular equation-of-state routines, provided that the material identifier M1 is set to one of the following:

102	(air)
101	(polyethylene)
306 or 6	(carbon)

The subsequent procedure for air is as follows: M1 is changed from 102 to 208 and a return is made to the calling program, which then calls a specialized air routine. For carbon and polyethylene, the molecular subroutine CMOL (for carbon) or ES1LMS (for polyethylene) is called directly for calculation of E_{dis} , $\bar{N}$, and their derivatives. On return to EIONX, $\bar{Z}$ and the other ionic variables are calculated in the same way as in the monatomic case (an approach which is more valid for carbon than for polyethylene, but is considered satisfactory for both materials). The final results contain contributions of both molecular and ionic processes.

3.5. COMMUNICATIONS BLOCKS

Except for the four subroutine parameters, communication with EIONX is handled through arrays in named COMMON blocks. The contents of these are listed below. At the top of each list are the block name, array name, and array dimension; and for each element of the array, the index, equivalent names, and descriptive information, including variable type if different from the implicit type of the name, are given.

/LMS/EION(20): The main output communications region

- EION (1) THETA, θ , temperature, ev
 (2) TAU, τ , specific volume, cm^3/g
 (3) ZBAR, $\bar{Z}$, mean ionic charge, or free electrons per atom

- (4) ZBARI, $\bar{Z}^i$, mean ionic charge of a constituent element
- (5) PHI, ϕ , gas constant, erg/g/ev
- (6) ESUM
- (7) PRESHR, P, pressure, dyne/cm²
- (8) ENERGY, E, specific internal energy, erg/g
- (9) DEDTHT, $(\partial E / \partial \theta)_T = C_V$, specific heat at constant volume
- (10) DEDTAU, $(\partial E / \partial \tau)$
- (11) SNDSPPD, $\tau(-\partial P / \partial \tau)_S^{\frac{1}{2}} = c_o$, sound speed
- (12) DPDTAU, $(\partial P / \partial \tau)_\theta$
- (13) DPDTHT, $(\partial P / \partial \theta)_T$
- (14) If nonzero input, molecular EOS is called; if nonzero output, fatal error.
- (15)
- (16) ZMEAN, $\sum_i \alpha_i Z_i$, mean atomic number of elements in the material
- (17) NBAR, $\bar{N}$, mean number of atoms per molecule; REAL type
- (18) ZSUM1
- (19) ZSUM2
- (20) ZSUM3

/LMSB/U(1): A variable-length input block, supplied by the MARI routine. Any number of elements, greater or equal to those actually needed, may be represented, and in any order; preferably those used most should be first. In the MARI routine itself, each element is represented by an array of DATA statements, with the chemical symbol used for the array name (which must be REAL type). Each array contains, in order, the atomic number Z^i , the mass number A^i , and the ionization potentials V_j^i , $j=1,2,\dots, Z^i$. (Higher potentials which will not be needed in the calculation may be entered as zero.) In EIONX, /LMSB/ contains a single array name U, the contents of which are of course identical to those entered in MARI provided that the system loader uses MARI to define the COMMON block.

U(1), $Z^{(1)}$, charge number of first element
 (2), $A^{(1)}$, mass number of first element
 (3), $V_1^{(1)}$, first ionization potential of first element
 :

$(Z^{(1)} + 2), V_z^{(1)}$, last ionization potential of first element

$(Z^{(1)} + 3), Z^{(2)}$, charge number of second element
 etc.

/LMSC/M(51): Material definition and indexing information. M, Z and PART are equivalent array names.

M(1), NOLMNT, number of elements in the material. Note: INTEGER type.

Z(2), Z^i , charge number of first element in the material

PART(3), α_1 , number fraction of atoms of first element in the material

M(4) index in the U array of the first entry (Z^i) for this element.

Z(5), $\bar{Z}^i$, mean ionic charge for this element

Z(6), $(\frac{\partial \bar{Z}^i}{\partial I})_\theta$

Z(7), $(\frac{J_i}{\theta} + \frac{3}{2})$

Z(8), J_i

Z(9), $(\frac{\partial \bar{Z}^i}{\partial \theta})_\tau$

Z(10), $(\frac{\partial \bar{Z}^i}{\partial \tau})_\theta$

Z(11), $\mathcal{E}^i$

Z(12)

Z(51) } 10 word groups like Z(2)-Z(11) for up to 4 more elements

See Section 3.2.4 for definitions.

/LMSD/TLMS(30)

TLMS(1), BACK(1), $\bar{Z}^{(n)}$, previous iterate for $\bar{Z}$

(2), BACK(2), $\bar{Z}^{(n-1)}$, second previous iterate for $\bar{Z}$

(3) $\bar{A}$, mean atomic mass number

(4) temporary storage

- (5) $\ln(\Gamma \bar{Z})$
- (6), XBAR, X^i
- (7), ZBARLN, $\ln \bar{Z}$
- (8) temporary storage
- (9), XI, $\phi(\bar{N}^{-1} + \bar{Z})$
- (10) $I = \theta \ln \Gamma$
- (11) $\bar{Z}^{(n+1)} - 2\bar{Z}^{(n)} + \bar{Z}^{(n-1)}$
- (12) $\bar{Z}^{(n+1)} - \bar{Z}^{(n)}$ } terms for Aitken extrapolation
- (13) $V_j^i - V_{j-1}^i$
- (14) $V_1^i + V_2^i + \dots + V_{j-1}^i$
- (15), DZDTAU $(\partial \bar{Z} / \partial \tau)_\theta$
- (16), DZDTHT $(\partial \bar{Z} / \partial \theta)_\tau$
- (17)-(30) temporary storage

/LMSE/: Internal flags, DO-loop indices, etc.

MATERL , material Identifier, from subroutine parameter M1

ILEMNT atomic charge number, U(I1)

SNAFU, PATH, internal error flag, special option flag

I1 index of Z in U array

I2 j, upper ionization stage index

I3 index of V_j^i in U array

I4

I5 iteration counter

I6

I7

I8, NJUMP

19, BYPASS, internal flow flag; INTEGER type

I10, M2

J1

J2, L0

J3

J4

J5

J6

/EOSIN/EIONIN(30): Specifies material composition for nonstandard materials.

Elements are in order of increasing Z.

EIONIN(1) (=NOLMNT), number of elements in this material; REAL type

(2), $Z^{(1)}$, atomic charge number of first element

(3), $\alpha^{(1)}$, number fraction of first element

(4), $Z^{(2)}$, atomic charge number of second element

.

.

.

(2*NOLMNT+1), Last entry for first material

. } up to 2 additional materials, specified as above.

(28), FESTER(1), option flag for molecular routines

(29), ZBRMIN(1), for $\bar{Z}$ less than this, ionization is ignored.

(30), EPSI(1), convergence criterion for $\bar{Z}$ iteration

/LMSG/CARBENZ(10): Communications area for carbon molecular routine CMOL. The first six words contain molecular contributions to energy, pressure, $(\partial E / \partial \tau)_\theta$, $(\partial E / \partial \theta)_\tau$, $(\partial P / \partial \tau)_\theta$, $(\partial P / \partial \theta)_\tau$, respectively.

/LMSESN/TLMSB(15): Communications and working storage for polyethylene molecular routine ESILMS. Words 12, 13, and 14 are equivalenced to DNDTAU, DNDTHT, and DISNRG, i.e., to $(\partial \bar{N} / \partial \tau)_\theta$, $(\partial \bar{N} / \partial \theta)_\tau$, and E_{dis} respectively.

3.6. MATERIAL IDENTIFICATION

The third subroutine parameter, M1, identifies the material according to the following list:

1-100 Single-element materials; M1=Z, the atomic charge number,

101	Polyethylene
102	Air
103	Teflon
104	Nylon-Phenolic A
105	Wet tuff
106	Refrasil
107	Phenolic A
108	Lithium Hydride
109	Salt
110	Magnalium
111	HMX
112	Refrasil B
113	Phenolic B
114	Refrasil C
115	Carbon-phenolic
116	First material specified in /EOSIN/
117	Second material specified in /EOSIN/
118	Third material specified in /EOSIN/
119-200	Currently invalid but reserved for multi-element material specifications
201-300	Reserved for equation-of-state routines not under control of EIONX
301-400	Reserved for special isotopic compositions of single-element materials; $M1 = 306+Z$

Care should be taken to use the multi-element version of EIONX if $100 < M1 \leq 200$. In other cases the single-element version is recommended. All elements called for in the M1 specification must be represented in the table of ionization potentials in /LMSB/.

3.7. OPTIONS

The fourth subroutine parameter, X3, may be used to specify a limited part of the entire EIONX procedure. $X3=0$. gives the complete calculation and is the normal setting. $X^3=-1$. provides for computing only

the two quantities

$$\text{PHI} = 9.648679 \times 10^{11} / \bar{A}$$

$$\text{ZMEAN} = \sum_i \alpha_i Z^i$$

X3=-2. suppresses all contributions from ionization by bypassing the $\bar{Z}$ calculation and setting $\bar{Z}=0$. X3=-3. is designed to provide communication with non-equilibrium ionic routines; the latter supply as input the following quantities in /LMSC/ for each element in the material:

M(10*i-6) Index in the U array of the first entry (Z^i) for the i^{th} element.

Z(10*i-5) $\bar{Z}^i$, mean ionic charge of i^{th} element.

Z(10*i-8) Z^i , charge number of i^{th} element.

The EIONX routine then evaluates the thermodynamic variables P, E, C_V , etc., and returns control to the calling routine. For M1=101, 6 or 306, this option should instead be specified by X3=-4., which allows for molecular contributions.

3.8. ERROR RETURNS

For sufficiently mild error conditions, a normal return is made at the completion of the calculation with a nonzero value of the parameter X3. For example, in the calculation of sound velocity the quantity

$$\frac{c_o^2}{\tau} = \frac{\theta}{C_V} \left(\frac{\partial P}{\partial \theta} \right)_\tau^2 - \left(\frac{\partial P}{\partial \tau} \right)_\theta$$

may turn out to be negative (this only occurs when ESILMS is used at very high densities). If so, the sound speed is set to zero and the above quantity is returned in X3. More serious errors cause an immediate return with the catastrophic error flag EION(14) set. The following list of EION(14) settings may be used for diagnostic purposes:

- 97.0097 Invalid M1 (material identifier)
- 97.0150 $X1 = \theta < 0$ or $X2 = \tau < 10^{-30}$
- 97.0505 (Multi-element version): internal data statement altered incorrectly
- 97.0502 (Multi-element version): /EOSIN/data input (for M1=116, 117, or 118) incorrect
- 97.0012 (Multi version) } Needed element omitted from MARI
- 97.0003 (Single version) }
- 97.0607 (Multi version) } Needed ionization potential was zero.
- 97.0007 (Single version) }
- 97.0297 CMOL iteration did not converge.
- 97.0197 CMOL was called with $\tau < 0.1$

97.

3.9. APPENDIX: LISTING OF EIONX ROUTINES

```

C      WILT FOR SINGLE
C      SUBROUTINE EIONX (X1, X2, M1, X3 )
C
C
C      CODED MAY, 1965 BY LEW SCHAEFF
C      RECORDED ITERATION PROCEDURE FOR ZBAR MAY 6, 1966 BY G. LAKE
C      LAST COMPILED BY G. LAKE JUNE 8, 1966
C
C      ***** RATIONALE - THREE STATE Saha Equation Iterative
C      ***** SOLUTION.
C
C      ***** CODED FOR SINGLE-ELEMENT-MATERIALS ONLY *****
C      ***** CODED FOR SINGLE-ELEMENT-MATERIALS ONLY *****
C      ***** CODED FOR SINGLE-ELEMENT-MATERIALS ONLY *****
C      ***** CODED FOR SINGLE-ELEMENT-MATERIALS ONLY *****
C      ***** CODED FOR SINGLE-ELEMENT-MATERIALS ONLY *****
C
C      ***** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS *****
C      ***** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS *****
C      ***** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS *****
C      ***** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS *****
C      ***** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS *****
C
C      EION(14) MUST BE NONZERO TO CALL A MOLECULAR EQUATION OF STATE
C      LION(14) IS SET JUST BEFORE ENTRY TO THIS SUBROUTINE
C
C      COMMON/LMS/ EION(20)
C      VARIABLES (INPUT AND OUTPUT)
C
C      REAL NBAR
C      EQUIVALENCE (EION(1),THTA), (EION(2),TAU), (EION(3),ZBAR)
C      EQUIVALENCE (LION(4),ZBARI), (EION(5), PHI), (EION(6),ESIM)
C      EQUIVALENCE (EION(7),PRESHR), (EION(8),ENERGY), (EION(9),DIDTHT)
C      EQUIVALENCE (LION(10),DELTAU), (EION(11),SNDSPD), (EION(12),DPUTAU)
C      EQUIVALENCE (EION(13),DIDTHT)
C      EQUIVALENCE (LION(16),ZMLAN), (EION(17),NBAR)
C
C      COMMON/LMSD/MATERL, ILEMNT, SNAFU, I1, I2, I3, I4, I5, I6, I7, I8, I9, I10, J1,
2 J2, J3, J4, J5, J6
C      DATA MATERL, ILEMNT, SNAFU, I1, I2, I3, I4, I5, I6, I7, I8, I9, I10, J1,
2 J2, J3, J4, J5, J6/2*0.0, I6*0/
C      EQUIVALENCE (SNAFU, PATH)
C      EQUIVALENCE (I8, NJUMP)
C      EQUIVALENCE (I10, M2)
C      EQUIVALENCE (L0, J2)
C      EQUIVALENCE (BFORL, J6)
C      INTEGER BYPASS
C      INTEGER BFORE
C
C      MATERL IS INPUT AS M1
C
C      SNAFU IS THE INTERNAL SUBROUTINE ERROR FLAG CELL
C      X3 IS SET TO SNAFU ON SUBROUTINE EXIT
C      X3 IS SET TO 0. IF NO SUBROUTINE ERRORS ARE FOUND
C      TO BACK1 IF 15.GL.20 (THE ROUTINE USES THE
C      20TH ITERATE OF ZBARI AS ITS FINAL ANSWER.)
C
C      ABOVE ARE DO LOOP RUNNING INDICES OR JUMP NOS.
C      I1 SPECIFIES THE LOCATION OF THE ATOMIC NUMBER.
C      I2 SPECIFIES THE UPPER IONIZATION INDEX.
C      I3 SPECIFIES THE LOCATION OF THE UPPER IONIZATION POTEN-
C      TIAL.
C      I5 COUNTS ITERATIONS
C
C      COMMON/LMSD/ TLM5(J0)
C      TEMPORARY STORAGE

```

C	EQUIVALENCE (TLMS(1),BAC(1), (175(1),X1))	M5	0660
	EQUIVALENCE (XHA0,TLMS(1))	M5	0700
	EQUIVALENCE (TLMS(3),SIGMA), (175(1),X1)	M5	0710
	EQUIVALENCE (TLMS(15),DELTAU)	M5	0720
	EQUIVALENCE (TLMS(16),DELTAU)	M5	0730
	EQUIVALENCE (TLMS(27),XALFA1)	M5	0740
	EQUIVALENCE (TLMS(28),GAMMA)	M5	0750
	EQUIVALENCE (TLMS(29),CHI)		
C	COMMON/LMSC/ M(51)	M5	0760
	DIMENSION Z(51),PART(51)	M5	0770
C		M5	0780
C	EQUIVALENCE (M(1),NOLMNT), (M(2),Z(2)), (M(3),PART(3))	M5	0790
C		M5	0800
C		M5	0810
C	COMMON/LMSB/U(1)	M5	0820
C		M5	0830
C		M5	0840
C		M5	0850
C	ARRAY CONTAINING, FOR EACH ELEMENT, ATOMIC	M5	0860
C	NUMBER, ATOMIC MASS, IONIZATION POTENTIALS IN	M5	0870
C	INCREASING ORDER.	M5	0880
C	*** THE ORDER (OF ELEMENTS IN THE TABLE) IS NOT SIGNIFICANT. FOR	M5	0890
C	HIGHEST SPEED, THOSE ELEMENTS MOST FREQUENTLY CALLED SHOULD BE	M5	0900
C	PLACED FIRST.	M5	0910
C		M5	0920
C	ARRAY FORMAT	M5	0930
C	U(1) IS THE ATOMIC NUMBER OF THE FIRST ELEMENT, SAY ZAM	M5	0940
C	U(2) IS ITS ATOMIC WEIGHT.	M5	0950
C	U(3), ETC. ARE, IN MONOTONE INCREASING ORDER, ITS ION-	M5	0960
C	IZATION POTENTIALS. A MAXIMUM OF 2A SUCH ARE	M5	0970
C	ALLOWED ARRAY ELEMENTS FROM U(3) THRU U(2A+2).	M5	0980
C	ALL IONIZATION POTENTIALS REQUIRED BY THE INPUT	M5	0990
C	THETA, TAU VALUES MUST BE LOADED. HIGHER POTEN-	M5	1000
C	TIALS MAY BE INPUT AS ZERO OR MAY BE SKIPPED BY	M5	1010
C	THE INPUT DECK WITH A BSS CARD.	M5	1020
C	U(2A+3) IS THE ATOMIC NUMBER OF THE SECOND ELEMENT,	M5	1030
C	SAY ZB.	M5	1040
C	U(2A+4) IS THE ATOMIC WEIGHT OF THE SECOND ELEMENT.	M5	1050
C	U(2A+5) BEGINS ITS IONIZATION POTENTIAL TABLE.	M5	1060
C		M5	1070
C		M5	1080
C	COMMON/LMSG/CARJNZ(10)	M5	1090
C	COMMON/EOSIN/EIONIN(30)	M5	1100
C	DIMENSION EPSI(1)	M5	1110
C	EQUIVALENCE (EPSI(1),EIONIN(30))	M5	1120
C	DATA EPSI/.001/	M5	1130
C	DIMENSION ZURMIN(1)	M5	1140
C	EQUIVALENCE (ZURMIN(1),EIONIN(29))	M5	1150
C	DATA ZURMIN/.00001/	M5	1160
C	DIMENSION FASTER(1)	M5	1170
C	EQUIVALENCE (FASTER, EIONIN(28))	M5	1180
C	DATA FASTER/0./	M5	1190
C	DIMENSION ZLN(100)	M5	1200
C		M5	1210
C	EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.	M5	1220
C	OR IF A NEEDED IONIZATION POTENTIAL WAS FOUND TO BE ZERO	M5	1230
C	OR IF A NEEDED ELEMENT IS MISSING FROM THE MARI DECK	M5	1240
C	OR IF THETA(EV) WAS LESS THAN ZERO OR IF TAU(CC/G) WAS LESS THAN	M5	1250
C	1.E-30		
C		M5	1270
C	ENERGY= 0.	M5	1280
C	NBAR= 1.	M5	1290
C		M5	1300
C		M5	1310
C	PATH= X3	M5	1320
	THETA= X1	M5	1330
	TAU= X2	M5	1340

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IF (THETA.LT.0.,OR.TAU.LT.1.E-50) GO TO 150
IF (PATH.EQ.(-3.)) GO TO 6800
IF (M1.GE.I01.AND.M1.LE.300.OR.M1.GE.401.OR.M1.EQ.0) GO TO 97
IF (M1.LE.M2) GO TO 91
IF (PATH.EQ.-1.) GO TO 5033
DO 503 I= 1,51
Z(I)= 0.
IF (1.GT.10) GO TO 503
CARBONZ(1)= 0.
503 CONTINUE
5033 CONTINUE
M2= M1
ILEMNT= M1
C
IF (ILEMNT.GE.301) GO TO 401
IF (ILEMNT.EQ. 0) GO TO 97
ISOTOP= 1
402 CONTINUE
C
C
C
11= 1
NJUMP= 1
C
2 J1= U(11)
IF (J1-ILEMNT) 3,52,3
FOR SHORTEST SEARCH, PUT IN ORDER OF MOST-NEEDED FIRST
AT EXIT, 11= ARRAY LOCATION OF DESIRED Z=ATOMIC NO.
NEXT ARRAY ELEMENT IS THE ATOMIC WEIGHT. THIS IS FOLLOWED
BY THE SET OF IONIZATION POTENTIALS (MONOTONE INCREASING)
3 CONTINUE
11= 11+J1+2
NJUMP= NJUMP+1
IF (NJUMP.LT. 201) GO TO 2
EION(14)= 97.0003
RETURN
EION(14) IS SET IF A NEEDED ELEMENT HAS BEEN LEFT OUT OF THE
MARI DECK
401 CONTINUE
ISOTOP= 2
ILEMNT= ILEMNT-500
GO TO 402
404 CONTINUE
ISOTOP= 1
GO TO 3
C
97 EION(14)= 97.0097
RETURN
EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.
52 CONTINUE
IF (ISOTOP.LE.2) GO TO 404
PHI= 9.648679E11 / U(11+1)
M(1)= 1
Z(2)= U(11)
PART(3)= 1.
M(4)= 11
ZMEAN= U(11)
TLMS(3)= U(11+1)
THIS SECTION ALSO COMPUTES A MLAN ATOMIC NUMBER CALLED ZMEAN
91 CONTINUE
IF (PATH.EQ. (-1.)) GO TO 1
C
IF (PATH.EQ. (-2.)) GO TO 75

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M5 1360
M5 1370
M5 1380
M5 1390
M5 1400
M5 1410
M5 1420
M5 1430
M5 1440
M5 1450
M5 1460
M5 1470
M5 1480
M5 1490
M5 1500
M5 1510
M5 1520
M5 1530
M5 1540
M5 1550
M5 1560
M5 1570
M5 1580
M5 1590
M5 1600
M5 1610
M5 1620
M5 1630
M5 1640
M5 1650
M5 1660
M5 1670
M5 1680
M5 1690
M5 1700
M5 1710
M5 1720
M5 1730
M5 1740
M5 1750
M5 1760
M5 1770
M5 1780
M5 1790
M5 1800
M5 1810
M5 1820
M5 1830
M5 1840
M5 1850
M5 1860
M5 1870
M5 1880
M5 1890
M5 1900
M5 1910
M5 1920
M5 1930
M5 1940
M5 1950

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C	IF (LION(14) .EQ. 0.) GO TO 599	MS	1960
C	LION(14) IS TO BE SET BEFORE ENTRY TO FLOREN	MS	1970
C	LION(14) MUST BE SET BEFORE TO CALL THE MOL(CHEAP) OF STATE	MS	1980
C	CARBON ROPS USING LIONX AND CMOI MUST SET LCHY(017) = 5.00004	MS	1990
C	IF (ILEMNT .EQ. 0) CALL CHOI(TAB,THETA,FEET)	MS	2000
C	FEETER IS LION(28)	MS	2010
C	LIONIN(28) MUST BE SET .LT. 0. BY INPUT TO GET	MS	2020
C	TRANSCATION-ONLY CMOI	MS	2030
C	LIONIN(28) MUST BE SET .GT. 0. TO GET THAR .EQ. 0. WHEN	MS	2040
C	T (DEL. REEVIH) .LT. 0.00.	MS	2050
C	IF (CARBNZ(18) .EQ. 0.) GO TO 16	MS	2060
	LION(14)= CARBNZ(18)	MS	2070
	RETURN	MS	2080
16	CONTINUE	MS	2090
599	CONTINUE	MS	2100
	IF(PATH.EQ.(-4.)) GO TO 6000	MS	2110
	TLMS(5)= 22.9926 + ALOC(TAU/PHI) + 1.5* ALOC(THE TA)	MS	2120
C		MS	2130
	15= 1	MS	2140
	IF((BFORE.GT.0).AND.(BFORE.LE.ILEMNT)) GO TO 1030	MS	2150
	IF(BFORE.GT.ILEMNT) GO TO 1010	MS	2160
C		MS	2170
	DO 1000 K=1,100	MS	2180
	AK=K	MS	2190
	AK=AK-.5	MS	2200
	ZLN(K)= ALOC(AK)	MS	2210
1000	CONTINUE	MS	2220
C		MS	2230
1010	CONTINUE	MS	2240
	J4= ILEMNT	MS	2250
	J3= ILEMNT/2	MS	2260
	J3= MAX0(J3,1)	MS	2270
	IF(BFORE.EQ.0) J3= 1	MS	2280
	J5= 1	MS	2290
	GO TO 1050	MS	2300
C		MS	2310
1030	CONTINUE	MS	2320
	TLMS(10)= THETA+(TLMS(5) -ZLN(BFORE))	MS	2330
	I3= 11+1+BFORE	MS	2340
	I2= BFORE	MS	2350
	IF(TLMS(10).LE. 0(13)) GO TO 1040	MS	2360
	IF(I2 .EQ. ILEMNT) GO TO 7	MS	2370
C		MS	2380
	J3= BFORE +1	MS	2390
	J4= ILEMNT	MS	2400
	J5= 1	MS	2410
	GO TO 1050	MS	2420
C		MS	2430
1040	CONTINUE	MS	2440
	IF(I2.EQ.1) GO TO 14	MS	2450
	J3= BFORE -1	MS	2460
	J4= 2*J3 -1	MS	2470
	J5= 2	MS	2480
C		MS	2490
1050	CONTINUE	MS	2500
C		MS	2510
	DO 1060 K= J3,J4	MS	2520
	IF(J5.LE.2) GO TO 1061	MS	2530
	I2= K		
	TLMS(10)= THETA+(TLMS(5) -ZLN(I2))		
	I3= 11 +1 +I2		
	IF(TLMS(10).LE.0(13)) GO TO 1070		
C		MS	2580
1060	CONTINUE	MS	2620
C		MS	2630
	IF(J5.EQ.2) GO TO 14	MS	2640
	GO TO 7	MS	2650

C	1061 CONTINUE	M5	2660
	12= K= 2*(BFORE - 12)	M5	2660
	TLMS(10)= THETA*(TLMS(5) -ZLN(12))	M5	2660
	13= 11+12	M5	2670
	IF (TLMS(10).GT.0(13)) GO TO 1090		
	GO TO 1060		
C	1070 CONTINUE	M5	2680
	IF (12.EQ.1) GO TO 14	M5	2670
	TLMS(10)= THETA*(TLMS(5) -ZLN(12-1))	M5	2680
	BFORE= 12		
	GO TO 1100	M5	2690
C	1080 CONTINUE	M5	2700
	12= 12+1	M5	2710
	13= 13+1	M5	2720
	BFORE= 12	M5	2730
	GO TO 1100	M5	2740
C	7 CONTINUE	M5	2750
	IF (U(13) .NE. 0.) GO TO 601	M5	2760
	EION(14)= 97.0007	M5	2770
	RETURN	M5	2780
C	EION(14) IS SET IF A NEEDED IONIZATION POTENTIAL WAS ZERO	M5	2790
C	601 CONTINUE	M5	2800
	12= 1LLMNT	M5	2810
	BFORE= 12	M5	2820
	ZBAR1= U(11)	M5	2830
	LO= 2	M5	2840
	GO TO 9	M5	2850
C		M5	2860
C		M5	2870
	14 CONTINUE	M5	2880
	LO= 1	M5	2890
	BFORL= 1	M5	2900
C		M5	2910
	9 CONTINUE	M5	2920
	TLMS(27)= EXP(TLMS(5)- U(13)/THETA)	M5	2930
	GO TO (93, 94) , LO	M5	2940
C		M5	2950
	93 CONTINUE	M5	2960
	IF (ZBRMIN(1).LT.1.E-18) ZBRMIN(1)= 1.E-18	M5	2970
	IF (TLMS(27).LE.(ZBRMIN(1)**2)) GO TO 75	M5	2980
C	ZBRMIN(1) IS THE MINIMUM ALLOWED ZBAR	M5	2990
C		M5	3000
	ALPHA= TLMS(27)	M5	3010
	95 CONTINUE	M5	3020
	XBAR= .5* (-ALPHA+SQRT(ALPHA*ALPHA+4.*TLMS(27)))	M5	3030
	ZBAR1= XBAR	M5	3040
	IF (LO.EQ.2) ZBAR1 = ZBAR1 + U(11) - 1.	M5	3050
	IF (ZBAR1 .GT. ZMLAN) GO TO 98	M5	3060
	GO TO 13	M5	3070
C		M5	3080
	94 CONTINUE	M5	3090
	IF (TLMS(27).GT.1.E6) GO TO 13	M5	3100
	ALPHA= TLMS(27)+U(11) - 1.	M5	3110
	GO TO 95	M5	3120
C		M5	3130
	75 CONTINUE	M5	3140
C	PERFECT GAS PATH	M5	3150
	SNAFU= 0.	M5	3160
C	99 CONTINUE	M5	3170
	SIGMA= 0.	M5	3180
	ZBAR1= 0.	M5	3190
	ZBAR= 0.	M5	3200
	GAMMA= 0.	M5	3210
		M5	3220
		M5	3230
		M5	3240
		M5	3250

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CHI=	0.	M5	3260
XI=	PHI/NBAR	M5	3270
LO=	4	M5	3280
GO TO 73		M5	3290
C		M5	3300
98 CONTINUE		M5	3310
SNAFU=	ZBAR1	M5	3320
GO TO 99		M5	3330
C		M5	3340
1100 CONTINUE		M5	3350
TLMS(4)=	12	M5	3360
TLMS(13)=	U(13)-U(13-1)	M5	3370
TLMS(11)=	TLMS(4) -1.5	M5	3380
TLMS(12)=	THETA/TLMS(13)	M5	3390
TLMS(17)=	TLMS(11) + (THETA+TLMS(5)-U(13-1))/TLMS(13)	M5	3400
TLMS(19)=	TLMS(17) - TLMS(12)*LN(12-1)	M5	3410
TLMS(20)=	3.*TLMS(11) - TLMS(19) + 2.*TLMS(12)	M5	3420
TLMS(21)=	TLMS(11) - TLMS(19)	M5	3430
C		M5	3440
C		M5	3450
C		M5	3460
BACK1=	0.	M5	3470
BACK2=	0.	M5	3480
C		M5	3490
C		M5	3500
XALFA1=	.5*(-TLMS(20) + SQRT(TLMS(20)*TLMS(20) - 8.*TLMS(11)*TLMS(21)))	M5	3510
2		M5	3520
C		M5	3530
ZBAR1=	TLMS(11) + XALFA1	M5	3540
C		M5	3550
1130 CONTINUE		M5	3560
IF(15.GT.19) GO TO 1200		M5	3570
BACK2=	BACK1	M5	3580
BACK1=	ZBAR1	M5	3590
C		M5	3600
C		M5	3610
TLMS(23)=	XALFA1/(2.*TLMS(11) + XALFA1)	M5	3620
TLMS(24)=	TLMS(23)*TLMS(23)	M5	3630
TLMS(22)=	.66666667*TLMS(12)*TLMS(23)*TLMS(24)	M5	3640
TLMS(25)=	TLMS(22)*.6*TLMS(24)	M5	3650
TLMS(26)=	.71428571*TLMS(24)*TLMS(25)	M5	3660
C		M5	3670
15=	15+1	M5	3680
TLMS(18)=	TLMS(22) + TLMS(25) + TLMS(26)	M5	3690
C		M5	3700
XALFA1=	(-TLMS(21)-TLMS(18))/(1.+TLMS(12)/(XALFA1+.5+TLMS(11)))	M5	3710
ZBAR1=	TLMS(11) + XALFA1	M5	3720
IF(ABS(1.-BACK1/ZBAR1) - EPS1(1))	1300,1300,1130	M5	3730
C		M5	3740
1200 CONTINUE		M5	3750
SNAFU=	BACK1	M5	3760
LO=	3	M5	3770
GO TO 600		M5	3780
C		M5	3790
C		M5	3800
1300 CONTINUE		M5	3810
LO=	3	M5	3820
13 CONTINUE		M5	3830
SNAFU=	0.	M5	3840
600 CONTINUE		M5	3850
ZBAR=	ZBAR1	M5	3860
XI=	(1./NBAR+ZBAR)*PHI	M5	3870
C		M5	3880
GO TO (71,71,72),LO		M5	3890
71 CONTINUE		M5	3900
GAMMA=	XBAR+ZBAR/(2.*XBAR+ALPHA)	M5	3910
IF(ZBAR.EQ.U(11)) GAMMA=	0.	M5	3920
IF(ZBAR.EQ.U(11)) XBAR=	1.	M5	3930
		M5	3940
		M5	3950
		M5	3960

SIGMA=	XHAR + U(13)*PHI	M5	3970
CHI=	U(13) + 1.5 * THETA	M5	3980
GO TO 73		M5	3990
C		M5	4000
72 CONTINUE			
TLMS(30)=	TLMS(10) - TLMS(13) * (TLMS(18) + 2. * TLMS(12) * TLMS(23))	M5	4010
GAMMA=	THETA * ZBAR / (THETA + ZBAR + TLMS(13))	M5	4020
CHI=	TLMS(30) + 1.5 * THETA	M5	4030
SIGMA=	((ZBAR - TLMS(4) + 1.5) * 2) * TLMS(13) / 2. * PHI	M5	4040
2	+ U(13-1) * (XI - TLMS(4) * PHI)	M5	4050
C		M5	4060
C		M5	4070
73 CONTINUE		M5	4080
Z(5)=	ZBAR	M5	4090
C		M5	4100
DZDTAU=	GAMMA / TAU	M5	4110
DZDTHI=	GAMMA * CHI / THETA / THETA	M5	4120
PRESHR=	XI * THETA / TAU	M5	4130
DPDTHI=	PRESHR / THETA + PHI * THETA / TAU * DZDTHI	M5	4140
DPDTAU=	(PHI * THETA * DZDTAU - PRESHR) / TAU	M5	4150
DEDTAU=	PHI * CHI * DZDTAU	M5	4160
DEDTHT=	XI * 1.5 + PHI * CHI * DZDTHI	M5	4170
IF (EION(14) .EQ. 0.) GO TO 501		M5	4180
C	EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR EQN OF STATE	M5	4190
C	EION(14) IS TO BE SET BEFORE ENTRY TO EIONFN	M5	4200
IF (ILEMNT.EQ.6) GO TO 500		M5	4210
501 CONTINUE		M5	4220
SNDSPD=	TAU * SQRT (-DPDTAU + DPDTHI * DPDTHI * THETA / (DEDTHT))	M5	4230
C		M5	4240
ENERGY=	ENERGY + XI * THETA * 1.5 * SIGMA	M5	4250
GO TO (100,77,77,100), LO		M5	4260
C		M5	4270
77 TLMS(14)= 0.		M5	4280
16=	12 - 1		
IF (16.EQ.0) GO TO 51			
DO 50 14= 1, 16		M5	4300
J1=	11 + 14 + 1	M5	4310
TLMS(14)=	TLMS(14) + U(J1)	M5	4320
50 CONTINUE		M5	4330
51 CONTINUE			
C		M5	4340
C		M5	4350
ENERGY=	ENERGY + TLMS(14) * PHI	M5	4360
C		M5	4370
C		M5	4380
C		M5	4390
100 CONTINUE		M5	4400
X3=	SNAFU	M5	4410
C		M5	4420
1 CONTINUE		M5	4430
C		M5	4440
EION(14)= 0.		M5	4450
RETURN		M5	4460
C		M5	4470
C		M5	4480
C		M5	4490
150 CONTINUE		M5	4500
EION(14)=	97.0150	M5	4510
RETURN		M5	4520
C	SET EION(14) IF THETA.LT.ZERO OR TAU.LT. 1.E-30		
C		M5	4540
500 CONTINUE		M5	4550
ENERGY=	ENERGY + CARBNZ(1)	M5	4560
DEDTAU=	DEDTAU + CARBNZ(3)	M5	4570
DEDTHT=	DEDTHT + CARBNZ(4)	M5	4580
DPDTAU=	DPDTAU + CARBNZ(5)	M5	4590
DPDTHI=	DPDTHI + CARBNZ(6)	M5	4600
GO TO 501		M5	4610

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C		M5	4670
C	***** PAGE - 3,4. *****	M5	4680
	6000 CONTINUE	M5	4690
C	II1= M(4)	M5	4695
	IF(Z(5).GT.(U(II1)-.5)) GO TO 6010	M5	4696
C		M5	4670
	GL= Z(5)	M5	4680
	LAG= GL	M5	4690
	GAL= GL +FLOAT(LAG)	M5	4700
	IF(GAL.GT..5) II2= LAG +2	M5	4710
	IF(GAL.LE..5) II2= LAG +1	M5	4720
	GO TO 6020	M5	4730
C		M5	4740
	6010 CONTINUE	M5	4750
	II2= Z(2)	M5	4760
C		M5	4770
	6020 CONTINUE	M5	4780
	II3= II1 +II2 +1	M5	4790
C		M5	4800
	XI= PHI*(1./XBAR +ZBAR)	M5	4810
	IF(II2.EQ.1) GO TO 6030	M5	4820
	IF(II2.EQ.ILEMNT) GO TO 6040	M5	4830
C		M5	4840
	TLMS(4)= II2	M5	4850
	TLMS(13)= U(II3) -U(II3-1)	M5	4860
	SIGMA= ((ZBAR -TLMS(4) +1.5)*.7) +TLMS(13)/2.*PHI +	M5	4870
	2 U(II3-1)*(XI -TLMS(4)*PHI)	M5	4880
	GO TO 6060	M5	4890
C		M5	4900
	6030 CONTINUE	M5	4910
	XBAR= ZBAR	M5	4920
	GO TO 6050	M5	4930
C		M5	4940
	6040 CONTINUE	M5	4950
	XBAR= ZBAR -U(II1) +1.	M5	4960
C		M5	4970
	6050 CONTINUE	M5	4980
	SIGMA= XBAR*U(II3)*PHI	M5	4990
C		M5	5000
	6060 CONTINUE	M5	5010
	PRESHR= XI*THETA/TAU	M5	5020
	IF((PATH.EQ.(-4.)).AND.(ILEMNT.EQ.6)) ENERGY= ENERGY +CAPMIZ(1)	M5	5030
C		M5	5040
	6070 CONTINUE	M5	5050
	ENERGY= 1.5*THETA*XI +SIGMA +ENERGY	M5	5060
C		M5	5070
	TLMS(14)= 0.	M5	5080
	IF(II2.EQ.1) GO TO 6080	M5	5100
	II6= II2 -1	M5	5090
	DO 6075 II4= 1,II6	M5	5110
	JJ1= II1 +II4 +1	M5	5120
	TLMS(14)= TLMS(14) +U(JJ1)	M5	5130
	6075 CONTINUE	M5	5140
	6080 CONTINUE	M5	5150
C		M5	5160
	ENERGY= ENERGY +TLMS(14)*PHI	M5	5170
C		M5	5180
	SNAFU= 0.	M5	5190
	GO TO 100	M5	5200
	CALL MARI	M5	5210
	RETURN		
	END	M5	5220

WILT FOR MULTI

SUBROUTINE EIONX (X1, X2, M1, X3)

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CODED BY LEW SCHALIT
CODED DURING JUNE, 1965

LAST COMPILED BY G. LANE JUNE 8, 1966

***** RATIONALE - THREE STATE SARA EQUATION ITERATIVE *****
 ***** SOLUTION. *****
 EION(14) MUST BE NONZERO TO CALL A MOLECULAR EQUATION OF STATE
 EION(14) IS SET JUST BEFORE ENTRY TO THIS SUBROUTINE

***** ZBAR .LE. ZHRMIN REVERTS TO PERFECT GAS *****
 ***** ZBAR .LE. ZHRMIN REVERTS TO PERFECT GAS *****
 ***** ZBAR .LE. ZHRMIN REVERTS TO PERFECT GAS *****
 ***** ZBAR .LE. ZHRMIN REVERTS TO PERFECT GAS *****
 ***** ZBAR .LE. ZHRMIN REVERTS TO PERFECT GAS *****

ZHRMIN ORDINARILY SET .EQ. (.001) BUT MAY BE CHANGED BY INPUT
 ZHRMIN ORDINARILY SET .EQ. (.001) BUT MAY BE CHANGED BY INPUT

COMMON/LMS/ EION(20)

VARIABLES (INPUT AND OUTPUT)

EQUIVALENCE (EION(1), THETA), (EION(2), TAU), (EION(3), ZBAR)
 EQUIVALENCE (EION(4), ZBAR1), (EION(6), ESIM)
 EQUIVALENCE (EION(5), PHI)
 EQUIVALENCE (EION(7), PRESHR), (EION(8), ENERGY), (EION(9), DEUTHT)
 EQUIVALENCE (EION(10), DEDTAU), (EION(11), SMOSEP), (EION(12), DPUTAU)
 EQUIVALENCE (EION(13), DPUTHT)
 EQUIVALENCE (EION(16), ZMEAN)
 EQUIVALENCE (EION(17), NBAR)
 EQUIVALENCE (EION(18), ZSUM1), (EION(19), ZSUM2), (EION(20), ZSUM3)
 REAL NBAR

COMMON/LMSB/

U(1)

ARRAY CONTAINING, FOR EACH ELEMENT, ATOMIC
 NUMBER, ATOMIC MASS, IONIZATION POTENTIALS IN
 INCREASING ORDER.

*** THE ORDER (OF ELEMENTS IN THE TABLE) IS NOT SIGNIFICANT. FOR
 HIGHEST SPEED, THOSE ELEMENTS MOST FREQUENTLY CALLED SHOULD BE
 PLACED FIRST.

ARRAY FORMAT

U(1) IS THE ATOMIC NUMBER OF THE FIRST ELEMENT, SAY ZA
 U(2) IS ITS ATOMIC WEIGHT.

U(3), ETC. ARE, IN MONOTONE INCREASING ORDER, ITS ION-
 IZATION POTENTIALS. A MAXIMUM OF ZA SUCH ARE
 ALLOWED ARRAY ELEMENTS FROM U(3) THRU U(ZA+2).
 ALL IONIZATION POTENTIALS REQUIRED BY THE INPUT
 THETA, TAU VALUES MUST BE LOADED. HIGHER POTEN-
 TIALS MAY BE INPUT AS ZERO.

U(ZA+3) IS THE ATOMIC NUMBER OF THE SECOND ELEMENT,
 SAY ZB.

U(ZA+4) IS THE ATOMIC WEIGHT OF THE SECOND ELEMENT.
 U(ZA+5) BEGINS ITS IONIZATION POTENTIAL TABLE.

COMMON/LMSC/ M(51)

DIMENSION Z(51), PART(51)

0040

0050

0060

0070

0080

0090

0110

0120

0130

0140

0150

0160

0220

0230

0240

0250

0260

0270

0280

0290

0300

0310

0320

0330

0350

0360

0370

0380

0390

0400

0410

0420

0430

0440

0450

0460

0470

0480

0490

0500

0510

0520

0530

0540

0550

0560

0570

0580

0590

0610

0620

0630

0640

0650

0660

0670

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C      EQUIVALLNCL(M(1),NOLMNT), (DZ1(1),DZ1(2),DZ1(3),DZ1(4))
C
C      COMMON/LMSD/      TLM5(30)
C                        TEMPORARY STORAGE
C
C      EQUIVALENCE (TLM5(1),BACK(1),DZ1(2),BACK(2),TLM5(7),BACK(7))
C      EQUIVALENCE (XBAR,TLM5(6))
C      EQUIVALENCE (TLM5(9),X1)
C      EQUIVALENCE (TLM5(15),DZ1(TAU))
C      EQUIVALENCE (TLM5(16),DZ1(THT))
C
C      COMMON/LMSE/MATERL,ILEMNT,SNAFU(1),1,2,3,4,5,6,7,8,9,10,11,
2      J2,J3,J4,J5,J6
C      EQUIVALENCE (L0,J2)
C      DATA MATERL,ILEMNT,SNAFU(11,12,13,14,15,16,17,18,19,20,21,22,23,
2      J4,J5,J6/2*0.0,0.0,16*0/
C      EQUIVALENCE (SNAFU(1),ATIO)
C      EQUIVALENCE (18,NJUMP)
C      EQUIVALENCE (19,BYPASS)
C      INTEGER BYPASS
C      EQUIVALENCE (110,M2)
C
C      MATERL IS INPUT AS M1
C
C      SNAFU IS THE INTERNAL SUBROUTINE ERROR FLAG CELL
C      IS COUNTS ITERATIONS
C      X3 IS SET TO SNAFU ON SUBROUTINE EXIT
C      X3 IS SET TO 0. IF NO SUBROUTINE ERRORS ARE FOUND
C      TO BACK1 IF 05,06,20 (ROUTINE USES THE
C      20TH ITERATE OF ZBAR1 AS ITS FINAL ANSWER. HOWEVER, THIS
C      CASE MAY REQUIRE FURTHER INVESTIGATION, AS THE ITERATION
C      PROCEDURE MAY HAVE BEEN OSCILLATORY.)
C
C      ABOVE ARE DO LOOP RUNNING INDICES OR JUMP NOS.
C      11 SPECIFIES THE LOCATION OF THE ATOMIC NUMBER.
C      12 SPECIFIES THE UPPER IONIZATION INDEX.
C      13 SPECIFIES THE LOCATION OF THE UPPER IONIZATION POTEN-
C      TIAL.
C      15 COUNTS ITERATIONS
C
C      COMMON/LMSESN/TLM5H(15)
C      EQUIVALENCE (DNDTAU,TLM5H(12)), (DNDTH1,TLM5H(13))
C      EQUIVALENCE (TLM5H(14),DISNRG)
C
C      COMMON/LUSIN/EIONIN(30)
C      DIMENSION EPSI(1)
C      EQUIVALLNCE (EPSI(1),EIONIN(30))
C      DATA EPSI/.001/
C      DIMENSION ZBRMIN(1)
C      EQUIVALENCE (ZBRMIN(1),EIONIN(29))
C      DATA ZBRMIN/.001/
C      DIMENSION FLSTER(1)
C      EQUIVALENCE (FLSTER(1),EIONIN(28))
C      DATA FLSTER/0./
C      COMMON/LMSG/CARLONZ(10)
C      DIMENSION MATREL(11,15)
C      REAL MATREL
C
C      ARRAY FORMAT IS NO. OF ELEMENTS, SUCCESSIVE PAIRS OF
C      (ATOMIC NOS., ATOM NUMBER FRACTION) IN MONOTONIC
C      INCREASING ORDER. (FOR ENTRY CONVENIENCE ONLY)
C
C      DIMENSION      DY1 (11), DY2 (11), DY3 (11), DY4 (11), DY5 (11),
2      DY6 (11), DY7 (11), DY8 (11), DY9 (11), DY10(11),
3      DY11(11), DY12(11), DY13(11), DY14(11), DY15(11)
C
C      EQUIVALLNCL (MATREL(1,1), DY1(1))

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[illegible]

1820

113.50

2030

C
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C

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	DATA DY14/5.1. .248, 5. .007, 6. .292, 8. .321, 14. .132/ CARBON-PHENOLIC (R. SCHLAUG A) DATA DY15/3.1. .179, 6. .779, 8. .042, 4*0./	
		1110
		1120
		1130
		1140
	EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO. OR IF READ-IN INPUT IS INCORRECT OR IF A MATERIAL DATA STATEMENT WAS ALTERED INCORRECTLY OR IF A NEEDED IONIZATION POTENTIAL WAS FOUND TO BE ZERO OR IF A NEEDED ELEMENT IS MISSING FROM THE MARI DECK OR IF THETA(EV) WAS LESS THAN ZERO OR IF TAU(CC/G) WAS LESS THAN 1.E-30	1150 1160 1170
		1190
		1200
		1250
		1260
		1270
		1280
	PATH= X3	1290
	NBAR= 1.	1300
	THETA= X1	1310
	TAU= X2	1320
	IF(THETA.LT.0..OR.TAU.LT.1.E-30) GO TO 150	
	IF(PATH.EQ.(-3.)) GO TO 6000	
	IF (M1 .EQ. M2) GO TO 91	
	DO 503 I= 1,51	1340
	Z(I)= 0.	
	IF(I.GT.15) GO TO 503	
	TLMSB(I)= 0.	1360
	IF (I .GT. 10) GO TO 503	1370
	CARBNZ(I)= 0.	1380
503	CONTINUE	1390
	MATERL= M1	1400
	MATERL NAMES THE MATERIAL USED	1410
	M2= M1	1420
		1430
		1440
		1450
	IF(MATERL .LT. 101) GO TO 1	1460
	ABOVE PATH FOR IONIC SINGLE ELEMENT MATERIAL	1470
		1480
	IF (MATERL .LT. 201) GO TO 2	1490
	ABOVE PATH FOR IONIC MULTI-ELEMENT MATERIAL	1500
		1510
	IF (MATERL .LT. 301) GO TO 97	1520
	IF (MATERL .LT. 401) GO TO 401	1530
	MATERIAL NUMBERS FROM 301 TO 399 ARE TO BE USED FOR ISOTOPIC MIXES FOR SINGLE ELEMENT MATERIALS ONLY	1540 1550
	SUCH ISOTOPIC MIXES ARE TO BE ENTERED AFTER THE PURE ELEMENT ENTRY IF SUCH EXISTS	1560 1570
		1580
97	EION(14)= 97.0097	1590
	RETURN	1600
	EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.	1610
		1620
		1630
1	CONTINUE	1640
	IF (MATERL.EQ. 0) GO TO 97	1650
	ISOTOP= 1	1660
	Z(2)= MATERL	1670
402	CONTINUE	1680
	THIS PATH FOR ANY SINGLE ELEMENT MATERIAL	1690
	ILEMNT= Z(2)	1700
	NOLMNT= 1	1710
	PART(3)= 1.	1720

	GO TO 11	1730
C		1740
401	CONTINUE	1750
	ISOTOP= 2	1760
	Z(2)= MATERL-300	1770
	GO TO 402	1780
C		1790
2	CONTINUE	
	L = MATERL - 100	
	ILEMNT= 0	1810
	IF(L .GT. 15) GO TO 58	
	SUMPRT = 0.	
	NOLMNT = MATREL(1,L) + .5	
	DO 10 I=1,NOLMNT	
	MM = 2*I	
	Z(10*I-8) = MATREL(MM,L)	
	PART(10*I-7) = MATREL(MM+1,L)	
	SUMPRT = SUMPRT + PART(10*I-7)	
10	CONTINUE	
	IF(ABS(SUMPRT-1.) .LE. (.01)) GO TO 11	
505	CONTINUE	
C	AN INTERNAL DATA STATEMENT FOR MATERIAL PROPERTIES	
C	WAS ALTERED INCORRECTLY	
	EION(14) = 97.0505	
	RETURN	
C		
58	CONTINUE	4140
	IF(L .GT. 18) GO TO 97	
	IF(L - 17) 581,59,60	
C	PATH 58 FOR A FIRST MATERIAL USING READ-IN INPUT	4150
C	(INPUT TO BE ENTERED INTO THE EIONIN ARRAY IN	4160
C	FLOATING POINT FORM. NOLMNT TO BE ENTERED FIRST.	4170
C	THEN COME PAIRS OF ENTRIES FOR EACH ELEMENT OF	4180
C	ATOMIC NUMBER AND NUMBER FRACTION IN ORDER OF	4190
C	INCREASING ATOMIC NUMBER. FURTHER MATERIALS STACK	4200
C	ON TOP.)	4210
581	MOPSY = 0	
504	CONTINUE	4230
	SUMPRT = 0.	
	NOLMNT = EIONIN(MOPSY+1) + .5	4240
	IF(NOLMNT .GT. 5.0R.NOLMNT.LE.0) GO TO 502	4250
	DO 501 I=1,NOLMNT	4260
	MOPSI= 2*I+MOPSY	4270
	Z(10*I-8)= EIONIN(MOPSI)	4280
	PART(10*I-7)=EIONIN(MOPSI+1)	4290
	SUMPRT = SUMPRT + PART(10*I-7)	
501	CONTINUE	4300
	IF(ABS(SUMPRT-1.) .LE. (.01)) GO TO 11	
C		4320
502	CONTINUE	4330
C	AN INPUT DATA WAS ENTERED INCORRECTLY	
	EION(14) = 97.0502	4340
	RETURN	
C		4360
59	CONTINUE	4370
C	PATH 59 FOR A SECOND MATERIAL USING READ-IN INPUT.	4380
C	SEE PATH 58 FOR INPUT INSTRUCTIONS.	4390
	KRAZY = EIONIN(1) + .5	4400
	MOPSY= 2*KRAZY+1	4410
	GO TO 504	4420
C		4430
60	CONTINUE	4440
C	PATH 60 FOR A THIRD MATERIAL USING READ-IN INPUT.	4450
C	SEE PATH 58 FOR INPUT INSTRUCTIONS.	4460
	KRAZY= EIONIN(1) + .5	4470
	KAT= EIONIN(2*KRAZY+2) + .5	4480
	MOPSY= 2*(KRAZY+KAT+1)	4490
	GO TO 504	4500

C		4510
C		4520
C		4530
C		4540
C	404 CONTINUE	4550
	ISOTOP= 1	4560
	GO TO 403	4570
C		4580
C	11 CONTINUE	4590
C		4600
C		4610
C	THE FOLLOWING SECTION INSERTS INTO THE 4TH,ETC., CELLS IN THE	4620
C	M ARRAY THE LOCATION INDEX FOR THE U ARRAY OF THAT ELEMENT WHOSE	4630
C	ATOMIC NUMBER WAS IN THE 2ND,ETC., CELL OF THE M ARRAY	4640
C	THE FACTOR PHI , WHICH IS A COMBINATION OF CONVERSION FACTORS,	4650
C	AND WEIGHTED ATOMIC MASSES, IS ALSO COMPUTED HERE	4660
C	THIS SECTION ALSO COMPUTES A MEAN ATOMIC NUMBER CALLED ZMEAN	4670
C		4680
	TLMS(3)= 0.	4690
	ZMEAN= 0.	4700
	DO 14 I= 1, NOLMNT	4710
	I1= 1	4720
	NJUMP= 1	4730
	12 IF (U(I1).EQ.2(10*I-8)) GO TO 13	4740
C	403 CONTINUE	4750
	I1= I1 + 2 + INT(U(I1) + .5)	4760
	NJUMP= NJUMP+1	4770
	IF (NJUMP .LT. 201) GO TO 12	4780
	EION(14)= 97.0012	4790
	RETURN	4800
C	EION(14) IS SET IF A NEEDED ELEMENT HAS BEEN LEFT OUT OF THE	4810
C	MARI DECK	4820
C	13 CONTINUE	4830
	IF (ISOTOP .EQ. 2) GO TO 404	4840
	ZMEAN= ZMEAN+PART(10*I-7)*U(I1)	4850
	M(10*I-6)=I1	4860
	TLMS(3)= TLMS(3)+ PART(10*I-7) * U(I1+1)	4870
C	TLMS(3) IS THE MEAN PARTICLE WEIGHT	
C	14 CONTINUE	4880
	PHI= 9.648679E11/TLMS(3)	4890
C		4900
C		4910
C	91 CONTINUE	4920
C		4930
C	IF (PATH .EQ.(-1.)) GO TO 100	4940
C		4950
C		4960
	IF ((MATERL.EQ.6.OR.MATERL.EQ.306).AND.EION(14).NE.0.)CALL CMOL	
	1(TAU,THETA,FESTER)	
C	FESTER IS EIONIN(28)	
C	EIONIN(28) MUST BE SET .LT. 0. BY INPUT TO GET	
C	TRANSLATION-ONLY CMOL	
C	EIONIN(28) MUST BE SET .GT. 0. TO GET NIAR .EQ. 9. WHEN	
C	T (DEG. KELVIN) .LT. 1500.	
C	EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR EQN OF STATE	4980
C	CARBON RUNS USING EIONX AND CMOL MUST SET LCHCK(J+17) = 5.90566E11	
	IF (CARBNZ(8) .EQ. 0.) GO TO 16	4990
	EION(14)= CARBNZ(8)	5000
	RETURN	5010
C	EION(14) IS TO BE SET BEFORE ENTRY TO EIONFN	5020
C		5030
C		5040
C	16 CONTINUE	5050
C		5060
	IF (MATERL.NE.102) GO TO 700	5070
	IF (THETA .GT. EION(14)) GO TO 700	5080
C	IF THETA.LE.EION(14) (WHICH WAS SET BEFORE ENTRY TO EIONFN) RETURN	5090
C	TO A MOLECULAR AIR EQUATION OF STATE	5100

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C      EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR ION OF STATE      5110
C      EION(14) IS TO BE SET BEFORE ENTRY TO EIONFN                        5120
C      AIR RUNS USING EIONFN AND AIRS MUST SET ECHCK(J+17) TO AID
C      DISSOCIATION ENRGY (ABOUT 2.9E11)
C      MATERL= 208
C      GO TO 100
700 CONTINUE
C
C
C      IF (MATERL.NE.101) GO TO 92
C      EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR ION OF STATE      5180
C      EION(14) IS TO BE SET BEFORE ENTRY TO EIONFN                        5190
C      THE ESILMS SUBROUTINE IS CALLED WHENEVER THE MOLECULAR SPECIES      5200
C      CHARACTERISTIC OF CH2 DECOMPOSITION ARE BELIEVED PRESENT.          5210
C      TLMSB(1)= .78+.20833*ALOG(TAU)
C      CH2 RUNS USING ESILMS AND EIONF3 MUST HAVE ECHCK(J+17) = 9.63E11    5220
C      IF (THETA.LT..207107+1./TLMSB(1).AND. EION(14) .NE. 0.)CALL ESILMS  5230
C
C      92 CONTINUE
C
C      IF (PATH.EQ.(-2.)) GO TO 90
C
C      IF (PATH.EQ.(-4.)) GO TO 6000
C
C      DO 93 I=1,NOLMNT
C      Z(10*I)= 0.
C      93 CONTINUE
C
C
C
C      WHEN ABOVE DO LOOP FINISHES,M(1) =NOLMNT
C
C      M(2) = Z OF FIRST ELEMENT
C      M(12)= Z OF 2ND ELEMENT
C      M(22)= Z OF 3RD ELEMENT
C      M(32)= Z OF 4TH ELEMENT
C      M(42)= Z OF 5TH ELEMENT
C
C      M(13)=NUMBER FRACTION OF 1ST ELEMENT
C      M(13)=NUMBER FRACTION OF 2ND ELEMENT
C      M(23)=NUMBER FRACTION OF 3RD ELEMENT
C      M(33)=NUMBER FRACTION OF 4TH ELEMENT
C      M(43)=NUMBER FRACTION OF 5TH ELEMENT
C
C      M(14)=LOCATION OF Z OF FIRST ELEMENT
C      M(14)=LOCATION OF Z OF 2ND ELEMENT
C      M(24)=LOCATION OF Z OF 3RD ELEMENT
C      M(34)=LOCATION OF Z OF 4TH ELEMENT
C      M(44)=LOCATION OF Z OF 5TH ELEMENT
C
C      THE VALUE OF ZBAR FOR EACH SPECIES PRESENT IS STORED IN THE 5TH,
C      ETC., ARRAY ELEMENTS AFTER IT IS COMPUTED.
C
C      ZSUM1= 0.
C      ZSUM2= 1.
C      ZSUM3= 0.
C      ZBAR= 0.
C      ZBARLN= 0.
C      UACK1= 0.
C      IS= 1
C      BYPASS= 0
C
C      SETS ITERATION COUNTER
C
C      TLMS(5)= ALOG(TAU/PHI)+1.5*ALOG(THETA)+22.9926
C      21 CONTINUE
C      TLMS(10)= THETA*(TLMS(5)-ZBARLN)

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C	22 DO 23 I=1,NOLMNT	5770
C		5780
C		5790
C		5800
C		5810
C		5820
	I1= M(10*I-6)	5830
	I1EMNT= U(I1) + .5	5840
C		5850
C	AT ENTRY, I1= ARRAY LOCATION OF DESIRED Z=ATOMIC NO.	5860
C	IN THE U(250) ARRAY	5870
C	NEXT ARRAY ELEMENT IS THE ATOMIC WEIGHT. THIS IS FOLLOWED	5880
C	BY THE SET OF IONIZATION POTENTIALS (MONOTONE INCREASING)	5890
C		5900
	DO 607 I2=1,I1EMNT	5910
	I3= I2+I1+1	5920
	IF (TLMS(10).LE.U(I3)) GO TO 608	5930
607	CONTINUE	5940
	IF (U(I3) .NL. 0.) GO TO 601	5950
	LION(14)= 97.0607	5960
	RETURN	5970
C	EION(14) IS SET IF A NEEDED IONIZATION POTENTIAL WAS ZERO	5980
601	CONTINUE	5990
	I2= I1EMNT	6000
C		6010
	IF (I5 .EQ. 1) BACK1 = U(I1)	6020
	LO= 2	6030
	GO TO 609	6040
C		6050
C		6060
C		6070
608	CONTINUE	6080
	IF (I2.EQ.1) GO TO 614	6090
C		6100
C		6110
620	TLMS(13)= U(I3)-U(I3-1)	6120
	TLMS(4)= I2	6130
	LO= 3	6140
	ZBAR1= TLMS(4) - 1.5 + (TLMS(10)-U(I3-1)) / TLMS(13)	6150
	GO TO 641	6160
C		6170
C		6180
95	CONTINUE	6190
	IF (NOLMNT .EQ. 1) BACK1 = 1.E-20	6200
	XBAR= 1.E-20	6210
	ZBAR1= 1.E-20	6220
	IF (NOLMNT .EQ. 1) GO TO 90	6230
	GO TO 641	6240
C		6250
96	CONTINUE	6260
	XBAR= 1.	6270
	ZBAR1= U(I1)	6280
	GO TO 641	6290
C		6300
614	CONTINUE	6310
	LO= 1	6320
C		6330
609	CONTINUE	6340
	I4= 10*I	6350
	IF (Z(I4) .EQ. 0.) Z(I4)= EXP(TLMS(5)-U(I3)/THETA)	6360
	ZBRLOW= (ZBRMIN(1)+.1)**2	6370
	IF(ZBRLOW.EQ.0.) ZBRLOW= 1.E-38	
C	ZBRMIN(1) IS THE MINIMUM ALLOWED ZBAR	
	IF (Z(I4).LT.ZBRLOW.AND.LO.EQ.1) GO TO 95	
	IF (Z(I4).GT.(1.E6).AND.LO.EQ.2) GO TO 96	
	IF (I5.EQ.1 .AND. LO.EQ.1) BACK1= SORT (.5*Z(I4))	6400
	XBAR= Z(I4)/(Z(I4)+BACK1)	6410

ZBAR1=	XBAR	6420
IF (12.NE.1)	ZBAR1= ZBAR1 + U(11)-1.	6430
641	CONTINUE	6440
C		6450
I6=	10*1-7	6460
C	16 IS PART INDEX	6470
C		6480
ZBAR=	ZBAR+ PART(I6) + ZBAR1	6490
C		6500
C		6510
C		6520
C		6530
C		6540
IF (BYPASS.EQ.0)	GO TO 23	6550
C		6560
ESUM=	0.	6570
IF (12.EQ.1)	GO TO 664	6580
I7=	12-1	6590
DO 660	J1=1,17	6600
I8=	J1+1,1+1	6610
ESUM=	ESUM +U(I8)	6620
660	CONTINUE	6630
664	CONTINUE	6640
C		6650
C		6660
C		6670
Z(10+1-5)=ZBAR1		6680
C		6690
EQUIVALLNCE(M(1),Z(1))		6700
C		6710
C		6720
C		6730
C		6740
C		6750
C		6760
C		6770
GO TO (650,650,651),LO		6780
650	CONTINUE	6790
TLMS(4)=	XBAR-XBAR*XBAR	6800
Z(10+1-4)=TLMS(4)/THETA		6810
Z(10+1-3)=U(13)/THETA+1.5		6820
Z(10+1-2)=U(13)		6830
Z(10+1+1)=XBAR +U(13)		6840
ZSUM1=	ZSUM1+PART(I6)*Z(10+1-4)+Z(10+1-3)	6850
ZSUM2=	ZSUM2+PART(I6)*XBAR/(Z(14) +BACK1)	6860
ZSUM3=	ZSUM3+PART(I6) + TLMS(4)/TAU	6870
GO TO 653		6880
651	CONTINUE	6890
Z(10+1-4)=1./TLMS(13)		6900
Z(10+1-3)=TLMS(10)/THETA +1.5		6910
Z(10+1-2)=TLMS(10)		6920
Z(10+1+1)=U(13-1)*(ZBAR1-TLMS(4)+1.)+.5+ TLMS(13)	*(ZBAR1-	6930
2	TLMS(4)+1.5)**2	6940
ZSUM1=	ZSUM1+PART(I6)*Z(10+1-3)/TLMS(13)	6950
ZSUM2=	ZSUM2+ PART(I6) / TLMS(13) +THETA /BACK1	6960
ZSUM3=	ZSUM3+ PART(I6)/ TLMS(13)+THETA/TAU	6970
653	CONTINUE	6980
Z(10+1+1)=ESUM+Z(10+1+1)		6990
23	CONTINUE	7000
IF(ZBAR .GT. ZMEAN)	GO TO 94	
C		7010
C		7020
IF (ABS(1.- BACK1/ZBAR)-EPS1(1).LE. 0.)	HYPASS= 1+HYPASS	7030
IF(BYPASS .GE. 2)	GO TO 41	
30	CONTINUE	7050
IF (I5 .GT. 2)	GO TO 40	7060
31	BACK2= BACK1	7070
BACK1=	ZBAR	7080

	IS=	IS+I	7090
	ZBARLN=	ALOG(ZBAR)	7100
	ZBAR=	0.	7110
	GO TO 21		7120
C			7130
C			7140
	32 CONTINUE		
	SNAFU=	ZBAR	
	BYPASS=	2	
	GO TO 31		
C			7170
	40 CONTINUE		7180
	IF(ZBAR.LT.ZHRMIN(1)) GO TO 90		
C	ZHRMIN(1) IS THE MINIMUM ALLOWED ZBAR		
C	EXIT IF ZBAR IS TOO SMALL		
	TLMS(11)= ZBAR -2.* BACK1 + BACK2		7210
	HOLDZ= ZBAR		7220
	TLMS(12)= ZBAR -BACK1		7230
	ZBAR= ZBAR -(TLMS(12)**2) / TLMS(11)		7240
C	ABOVE IS AITKENS DEL-SQUARE ITERATION CONVERGENCE IMPROVEMENT		7250
C	PROCEDURE		7260
	IF((ZBAR.LE.0.).OR.(ZBAR.GT.ZMEAN)) ZBAR=.5*(HOLDZ+BACK1)		
	IF(15 .GT. 18) GO TO 32		
	GO TO 31		7290
C			7300
	94 CONTINUE		
	SNAFU=	ZBAR	
	GO TO 98		
C			7310
	50 CONTINUE		7320
C	PERFECT GAS PATH		7330
	SNAFU=	0.	7380
	98 CONTINUE		
	LO=	4	
	ZBAR=	0.	7340
	XI=	PHI/NBAR	7350
	DZDHT=	0.	7360
	DZDTAU=	0.	7370
	GO TO 43		7390
C			7400
	101 CONTINUE		7410
	IF (THETA.GE..207107+1./TLMSH(1)) GO TO 80		7420
C			7430
C	LOW TEMPERATURE POLYETHYLENE PATH		7440
	ENERGY= ENERGY + DISNRG * (TLMSH(4)-1.)		7450
	DEDHT= DEDHT + DNDHT*THETA* 1.5 *PHI + DISNRG *TLMSH(11)		7460
	DEDTAU= DEDTAU + DNDTAU*THETA* 1.5 *PHI+DISNRG*TLMSH(10)		7470
	DPDHT= DPDHT + DNDHT*THETA/ TAU*PHI		7480
	DPDTAU= DPDTAU + DNDTAU*THETA/ TAU*PHI		7490
	GO TO 80		7500
	500 CONTINUE		7510
	ENERGY= ENERGY+CARBNZ(1)		7520
	DEDTAU= DEDTAU+CARBNZ(3)		7530
	DEDHT= DEDHT+CARBNZ(4)		7540
	DPDTAU= DPDTAU+CARBNZ(5)		7550
	DPDHT= DPDHT+CARBNZ(6)		7560
	GO TO 80		7570
C			7580
C			7590
	41 CONTINUE		7600
	IF(ZBAR.LT.ZBRMIN(1)) GO TO 90		
C	ZBRMIN(1) IS THE MINIMUM ALLOWED ZBAR		
C	EXIT IF ZBAR IS TOO SMALL		
	42 CONTINUE		7630
	DZDHT= ZSUM1/ZSUM2		7640
	DZDTAU= ZSUM3/ZSUM2		7650
	XI= PHI*(1./NBAR+ZBAR)		7660
	43 CONTINUE		7670

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PRESHR= XI*THETA/TAU                                7680
DPDTHT= PRESHR/THETA + THETA/TAU*DPDTHT + PHI      7690
DPDTAU= ( THETA*PHI*DPDTAU-PRESHR ) / TAU          7700
ENERGY= 1.5*XI*THETA                                7710
DEDTHT= 1.5*(XI*THETA*DPDTHT + PHI)                7720
DEDTAU= 1.5*THETA*DPDTAU*PHI                       7730
IF ( EION(14) .EQ. 0. ) GO TO 80                   7740
C EION(14) IS TO BE SET BEFORE ENTRY TO EION(14)    7750
C EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR ION OF STATE 7760
IF (MATERL.EQ.6.OR.MATERL.EQ.306) GO TO 500        7770
IF (MATERL.EQ.101) GO TO 101                       7780
80 CONTINUE                                         7790
IF(ZBAR .EQ. 0.) GO TO 669                          7800
DO 662 I= 1,NOLMNT                                  7810
I6= 10*I-7                                           7820
C I6 INDEXES PART ARRAY                           7830
Z(10*I-1)=Z(10*I-4)* ( Z(10*I-3) -THETA/ZBAR*DPDTHT) 7840
Z(10*I)= Z(10*I-4) *THETA * ( 1./TAU - DPDTAU/ZBAR) 7850
ENERGY= ENERGY+PART(I6)*PHI+Z(10*I+1)            7860
DEDTHT= DEDTHT+PART(I6)*PHI+Z(10*I-2)*Z(10*I-1)    7870
DEDTAU= DEDTAU+PART(I6)*PHI+Z(10*I-2)*Z(10*I)      7880
662 CONTINUE                                         7890
669 CONTINUE                                         7900
ARGSQ= -DPDTAU +DPDTHT*DPDTHT*THETA/DEDTHT
IF(ARGSQ.GT.0.) GO TO 1669
IF(SNAFU.EQ.0.) SNAFU= ARGSQ
ARGSQ= 0.
1669 CONTINUE
SNDSQD= TAU*SQRT(ARGSQ)
C
670 CONTINUE                                         7920
X3= SNAFU                                           7930
100 CONTINUE                                         7940
EION(14)= 0.                                         7950
C
C
C RETURN                                             7960
C
C
C RETURN                                             7970
C
C
C RETURN                                             7980
C
C
C RETURN                                             7990
150 CONTINUE                                         8000
EION(14)= 97.0150                                   8010
RETURN                                              8020
C SET EION(14) IF THETA.LT.ZERO OR TAU.LT. 1.E-30
C
C
C
C***** SPECIAL PATH *****
C***** PATH= -3. *****
C
6000 CONTINUE
DO 6010 II= 1,NOLMNT
III= M(10*II-6)
C
IF(Z(10*II-5).GT.(U(III)-.5)) GO TO 6005
GL= Z(10*II-5)
LAG= GL
GAL= GL -FLOAT(LAG)
IF(GAL.GT..5) II2= LAG +2
IF(GAL.LE..5) II2= LAG +1
GO TO 6007
6005 CONTINUE
II2= Z(10*II-8)
C
6007 CONTINUE
II3= II2 +III +1
C
ESUM= 0.
IF(II2.EQ.1) GO TO 6060
II7= II2 -1
DO 6050 JJ1= 1,II7

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        I18=      JJ1 +I11 +1
        LSUM=      ESUM +U(I18)
6050 CONTINUE
6060 CONTINUE
      IF(Z(10*I1-5).LE..5) GO TO 6100
      IF(Z(10*I1-5).GT.(U(I11) -.5)) GO TO 6110
      GO TO 6130
C
6100 CONTINUE
      XBAR=      Z(10*I1-5)
      GO TO 6120
6110 CONTINUE
      XBAR=      Z(10*I1-5) -U(I11) +1.
6120 CONTINUE
      Z(10*I1+1)= XBAR+U(I13)
      GO TO 6140
6130 CONTINUE
      ZBAR1=      Z(10*I1-5)
      TLMS(4)=      FLOAT(I12)
      TLMS(13)= U(I13) -U(I13-1)
      Z(10*I1+1)= U(I13-1)+(ZBAR1 -TLMS(4) +1.) +.5*TLMS(13)*(ZBAR1 -
2          TLMS(4) +1.5)*+2
6140 CONTINUE
      Z(10*I1+1)= Z(10*I1+1) +ESUM
6010 CONTINUE
C
C
6143 CONTINUE
      XI=      PHI*(1./XBAR +ZBAR)
C
      PRESIR=      XI*THETA/1AU
C
      ENERGY=      1.5*XI*THETA
C
      IF(PATH.EQ.(-3.)) GO TO 6150
      IF(MATERL.EQ.6.OR.MATERL.EQ.306) ENERGY= ENERGY +CARIN7(1)
      IF(MATERL.EQ.101) GO TO 6200
6150 CONTINUE
      DO 6160 I1= 1,NOLMNT
      I16=      10*I1-7
      ENERGY=      ENERGY +PART(I16)*PHI*Z(10*I1+1)
6160 CONTINUE
C
      SNAFU=      0.
      GO TO 670
6200 CONTINUE
      IF(THETA.GE..207107+1./TLMSB(1)) GO TO 6150
      ENERGY=      ENERGY +DISNRG*(TLMSB(4)-1.)
      GO TO 6150
      CALL MARI
      RETURN
      END

```

8050

SECTION IV

EQUATION OF STATE INVERSION FROM TEMPERATURE-DENSITY
TO SPECIFIC ENERGY-DENSITY BY TABLE LOOK-UP4.1. INTRODUCTION

In order to obtain solutions to the general equations for inviscid, compressible fluid flow with radiation and/or conduction energy transport mechanisms, it is necessary to specify at least the following thermodynamic variables: pressure, P ; temperature, θ ; specific internal energy, E ; and density, ρ . The equations which relate these four thermodynamic quantities are usually referred to as the equations of state. If local thermodynamic equilibrium (LTE) is assumed, the equations for the thermodynamic variables can be completely specified by only two independent variables (e.g., temperature and density).

Some computer programs use equations of state with θ and ρ as the independent variables and others use E and ρ . Comparison of problems calculated using both types of programs can be extremely difficult unless completely consistent representations are used. The inversion of an equation of state given in terms of the temperature and density to the (E, ρ) form is thus required. For many materials of interest, analytic inversion from (θ, ρ) to (E, ρ) is not a trivial matter.

4.2. METHOD

One method of inverting equations of state from (θ, ρ) space to (E, ρ) space is to use a table look-up procedure to interpolate from one set of variables to the other. In the scheme reported here a two step process is used to obtain the necessary conversion. First, a table is generated from data given (or calculated) with θ and ρ as independent variables. This

table is punched on card; in DATA STATEMENT form. Second, these DATA STATEMENTS become part of a code which can be used as a subroutine to determine the temperature and pressure given E , and ρ or $\tau = 1/\rho$.

The actual values of θ and P are not tabulated. Instead, the table entries have been chosen to be $\bar{Z}$, the mean number of free electrons per atom, and $\ln I$ where I is the internal energy due to ionization and excitation. The quantities $\bar{Z}$ and $\ln I$ are both rather weak functions of density and energy over most of their range, which gives rise to a minimum error when interpolating between table entries.

The other thermodynamic variables are easily expressed in terms $\bar{Z}$ and I . In addition, other material properties, such as absorption coefficients, can be conveniently calculated from $\bar{Z}$.

The method of preparing the tables of $\bar{Z}$ and $\ln I$ is fairly straightforward. The range of E and τ is determined by available data or as needed for a particular application. The tabular entries are picked such that

$$E_m = E_Z \cdot 10^{(m-1)/T}$$

$$\tau_n = \tau_Z \cdot 10^{(n-1)/S}$$

where E_Z = minimum value of E ,

τ_Z = minimum value of τ ,

T = desired number of points per decade for E ,

S = desired number of points per decade for τ .

The values of $\bar{Z}$ and $\ln I$ at the desired value of E and τ are obtained from the existing (θ, ρ) equation of state. If interpolation is required, the energy is forced to be within 0.1% of the desired value. The values of τ and E at each point do not have to be saved.

For any arbitrary pair of values of (E, τ) , the proper region on the table can easily be calculated. Let

$$N = (\log_{10} (\tau / \tau_Z) * S + 1)$$

and

$$M = (\log_{10} (E/E_Z) * T + 1) \quad (103)$$

and let

$$n = \text{truncated value of } N$$

and

$$m = \text{truncated value of } M. \quad (104)$$

Entries at (n, m) , $(n, m + 1)$, $(n + 1, m)$, and $(n + 1, m + 1)$ can then be used to obtain interpolated values for $\bar{Z}$ and $\ln I$ at the desired value of (E, τ) .

4.3. PROGRAM GEST

The program GEST generates a table of $\bar{Z}$ and $\ln I$ for the values of E, τ specified by input data. If the minimum value of E is specified as zero by the input data, then the program will calculate E_Z as $E_Z(\theta_o, \tau_{\max})$, where $\tau_{\max}$ is specified by input and θ_o is chosen such that

$$\bar{Z}(\theta_o, \tau_{\max}) < \frac{0.2 \theta_o}{V_1}$$

where V_1 is the first ionization potential of the given material.

To generate this table, an interpolation must be performed between an initial guess at a temperature θ' which will produce E' and an unknown temperature θ which will produce the desired value of E indicated by the input data. Newton's method of linear interpolation is used repeatedly until a relative error of 0.1% is obtained between successive interpolations. Then the values of $\bar{Z}$ and I are obtained using the final value of θ . If I is found to be less than 10^{-10} ev, then I is set equal to 10^{-10} ev. The

process is repeated for each value of E and τ specified. Once the table of $\bar{Z}$ and $\ln I$ is generated, the DATA STATEMENTS for the program EST are punched. (NOTE: For punching DATA STATEMENTS on an IBM-7044, the IBM FORTRAN IV print and punch routine ECV must be used.)

4.3.1. Input

Card 1 and 2 have a floating point field width of 10, and card 3 had an integer field width of 5.

	<u>Mnemonic</u>	<u>Comment</u>
Card 1	Z	Atomic number
	A	Atomic mass number
	V1	First ionization potential
	VZ	Last ionization potential
	S	Number of tabular pts./decade of τ
	T	Number of tabular pts./decade of E
Card 2	DN	Number of decades of τ
	DM	Number of decades of E
	TAUZ	Min. value of τ in table
Card 3	EZ	Min. value of E in table. If zero, program will calculate an EZ.
	IS	Source of information used to generate table. (NOTE: At this writing an IS of 1 indicating the use of EIONX (see Section III) is the only option available.)

	<u>Mnemonic</u>	<u>Comment</u>
Card 3 (Continued)	I1 → I8	Flags to indicate the use of a special treatment at the boundaries of the table. If the flag is a 1, the calculation will stop when the region is entered. If zero, the calculation will proceed with the available analytic equation in the general EOS program.

Regions of the table as defined by I1 through I8:

	3	4	5
$E_{\max}$			
$E \uparrow$	2		6
$E_{\min}$			
	1	8	7
	$\tau_{\min}$	$\tau_{\max}$	
	$\tau \rightarrow$		

4.3.2. Output

The output appears in two forms: printed output (for checking input data and the calculations of the table), and punched card output. The punched cards are in DATA STATEMENT form for immediate placement into the program EST, which performs further equation of state calculations from this data.

4.4. PROGRAM EST

The program EST performs a two-dimensional linear interpolation within the limits of the table supplied it by the program GEST. If a region is entered which is outside the limits of the table, the calculation will either stop or go to an analytic solution which is based on the values of the table at the boundary.

Within the limits of the table, Eqs. (103) and (104) are used to find indices (as functions of E and τ) for use in an interpolation formula to find $\bar{Z}$ and $\ln I$. The interpolation formula used is as follows:

$$\begin{aligned} \bar{Z}(E, \tau) = & \bar{Z}_{n,m} + (\bar{Z}_{n+1,m} - \bar{Z}_{n,m}) D1 + (\bar{Z}_{n,m+1} - \bar{Z}_{n,m}) D2 \\ & + (\bar{Z}_{n+1,m+1} + \bar{Z}_{n,m} - \bar{Z}_{n+1,m} - \bar{Z}_{n,m+1}) D1 \times D2 \end{aligned} \quad (105)$$

where

$$D1 = N - n \text{ and } D2 = M - m \quad (106)$$

The interpolation used to obtain $\ln I$ is performed in the same manner as for $\bar{Z}$ by replacing $\bar{Z}$ with $\ln I$ in Eq. (105). The quantity I is then evaluated as $\exp(\ln I)$.

At this writing only regions 7 and 8 referred to in Section 4.3.1 have been supplied with analytic solutions. These solutions are based on using a crude approximation to the Saha equation. For $\theta \gg 1$ the value of $\bar{Z}^2$ is proportional to

$$\tau \theta^{3/2} e^{-V_1/\theta} \quad (107)$$

where V_1 is the first ionization potential of the material being described. Therefore, given $\bar{Z}(E_o, \tau_o)$ from the table boundary, where $E_o = E_Z$,

$$\left(\frac{\bar{Z}(E, \tau)}{\bar{Z}(E_o, \tau_o)} \right)^2 = \left(\frac{\theta'}{\theta_o} \right)^{3/2} \left(\frac{\tau}{\tau_o} \right) \exp \left[\left(\frac{1}{\theta_o} - \frac{1}{\theta'} \right) V_1 \right] \quad (108)$$

In both regions 7 and 8, θ' is set to $(E/E_Z)\theta_o$. In region 8, $\tau = \tau_o$, $\theta_o = f(E_Z, \tau)$, and Eq. (108) can be written

$$\bar{Z}(E, \tau) = \bar{Z}(E_Z, \tau) \left(\frac{\theta'}{\theta_o} \right)^{3/4} \exp \left[\left(\frac{1}{\theta_o} - \frac{1}{\theta'} \right) \frac{V_1}{2} \right] \quad (109)$$

For region 7, $\tau_o = \tau_{\max}$ on the boundary of the table, $\theta_o = f(E_Z, \tau_{\max})$, and Eq. (108) is written

$$\bar{Z}(E, \tau) = \bar{Z}(E_Z, \tau_{\max}) \left(\frac{\tau}{\tau_{\max}} \right)^{1/2} \left(\frac{\theta'}{\theta_0} \right)^{3/4} \exp \left[\left(\frac{1}{\theta_0} - \frac{1}{\theta'} \right) \frac{V_1}{2} \right] \quad (110)$$

For both regions 7 and 8, the value for I is approximated as $\bar{Z}$ times V_1 .

The temperature and pressure are obtained, given $\bar{Z}$ and I , from the relations

$$\theta = (E/\varphi - I) / \left[1.5(1 + \bar{Z}) \right] \quad (111)$$

where

$$\varphi = 9.648679 \times 10^{11} / A$$

$$P = \varphi (1 + \bar{Z}) \theta / \tau$$

Section 4.5 contains the mnemonics used for both GEST and EST. Section 4.6 contains a listing of GEST and EST and an error routine, ERR, used by GEST. EST also includes a list of the DATA STATEMENTS produced by the program GEST. E , τ , and P are in cgs units, and θ and I are in ev.

4.5. APPENDIX: MNEMONICS FOR GEST AND EST

A	*
AIN	I , in ev
ALGE	$\log_{10} E$
ALGT	$\log_{10} \tau$
ALIN	$\ln I$
DLGE	$\log_{10} (E/E_0)$
DLGT	$\log_{10} (\tau/\tau_0)$
DMLE	ΔE above position n, m in table
DNLT	$\Delta \tau$ above position n, m in table
E	Specific internal energy
EILN1D	Array of $\ln I$
EL	$\log_{10} E$

*See input for GEST

EM	Max value of E for table
EMAX	Value of E used in interpolation
EMIN	Value of E used in interpolation
EZ	*
I	Ionization energy
I1-I8	*
IS	*
M	Index for table entries
N	Index for table entries
PHI	φ (see Eq. (111))
T	*
τ	Specific volume
TAUL	$\log_{10} \tau$
TAUM	Max value of τ for table
TAUZ	*
THETA	θ (temperature in ev)
THMAX	θ max used in interpolation
THMIN	θ min used in interpolation
V1	*
VF	*
Z	*
ZBAR	$\bar{Z}$, mean number of free electrons
ZBID	Array of ZBAR

*See input for GEST

4.6. APPENDIX: LISTING OF GEST AND EST

```

Q1  FOR  GEST/A, GEST/HSE1, GEST/R1
C    GENERATE EQUATION OF STATE TABLES
C
      DIMENSION  THETA(50,50),CARD(14)
      DIMENSION  TAUL(50),TAU(50),EL(50),E(50),ZB1D(2500),EILN1D(2500)
      COMMON/LMS/  EION(20)
      COMMON/LMSD/  TLMS(16)
      EXPT(Q)=EXP(2.3026*Q)
1    FORMAT (12A6)
      READ (5,1) (CARD(I), I = 1, 12)
      WRITE (6,1) (CARD(I), I = 1, 12)
9000 FORMAT (7F10.5)
9001 FORMAT(14I5)
9002 FORMAT(1X,1P7E10.4)
9003 FORMAT(6X14H DIMENSION ZB(12,1H,12,7H),EILN(12,1H,12,1H))
9004 FORMAT(6X35H EQUIVALENCE (ZB,ZB1), (EILN,EILN1) )
9005 FORMAT(5X11,6(1P1E10.3,1H,))
9006 FORMAT(6X24H DATA TAULZ,EZ,Z,S,T,PHI/ )
9007 FORMAT(6X36H DATA NN,MM,I1,I2,I3,I4,I5,I6,I7,I8/ .)
9008 FORMAT(5X11,1H/)
9009 FORMAT(6X16HCOMMON/EST/EILN(12,1H) )
9010 FORMAT (4H  EL)
9011 FORMAT (6H  TAUL)
9012 FORMAT (6H  ZBAR)
9013 FORMAT (7H  THETA)
9014 FORMAT(5X11,1P1E10.3,5(1H,1P1E10.3),1H/)
9015 FORMAT(6X,8H DATA ZB12,1H/)
9016 FORMAT(6X14H COMMON/EST/ZB12,1H(12,1H) )
9017 FORMAT(6H  EILN)
9018 FORMAT(6X28H DATA TAUM,EM,TAUZ,EZ,V1,VZ/)
9019 FORMAT(5X11,9(I3,1H,),I3,1H/)
9020 FORMAT(6X11H DATA EILN/)
9021 FORMAT(6X10H DATA EILN12,1H/)
9022 FORMAT(6X16H COMMON/EST/EILN12,1H(12,1H) )
9031 FORMAT(5X11,1P1E10.3,1H/)
9032 FORMAT(5X11,1P1E10.3, 1H,1P1E10.3 ,1H/)
9033 FORMAT(5X11,1P1E10.3,2(1H,1P1E10.3),1H/)
9034 FORMAT(5X11,1P1E10.3,3(1H,1P1E10.3),1H/)
9035 FORMAT(5X11,1P1E10.3,4(1H,1P1E10.3),1H/)
9036 FORMAT(5X11,1P1E10.3,5(1H,1P1E10.3),1H/)
C    READ AND STORE INPUT
      READ(5,9000) Z,A,V1,VZ,S,T,DN,DM,TAUZ,EZ
      WRITE(6,9002) Z,A,V1,VZ,S,T,DN,DM,TAUZ,EZ
      READ(5,9001) IS,I1,I2,I3,I4,I5,I6,I7,I8
      WRITE(6,9001)IS,I1,I2,I3,I4,I5,I6,I7,I8
C      Z = ATOMIC CHARGE NO.
C      A = ATOMIC MASS NO.
C      V1 = FIRST IONIZATION POTENTIAL
C      VZ = LAST IONIZATION POTENTIAL
C      S = NO. OF TABULAR PTS/DECADE OF TAU
C      T = NO. OF TABULAR FTS/DECADE OF E
C      DN = NO. OF DECADES OF TAU
C      DM = NO OF DECADES OF E
C      TAUZ = MIN VALUE OF TAU IN TABLE
C      EZ = MIN VALUE OF E IN TABLE
C      IS = SOURCE USED FOR TABLE GENERATION
C          = 1 USE EIONX
C      I1 THRU I8 FLAGS INDICATING TREATMENT AT BOUNDARIES OF TABLE
C      IN = 1 STOP IF REGION IS ENTERED
C          = 0 CALCULATE WITH AVAILABLE ANALYTIC EQS
C      3 * 4 * 5
C      *****
C      *      *
C      E 2 *   * 6
C      *      *
C      *****

```

```

C      1 * 8 * 7
C      TAU
      L=Z
      PHI=9.648679L11/A
      AM=T*DM+1.0
      AN=S*DN+1.0
      NN=AN
      MM=AM
      TAUM=TAUZ*10.0**DN
      TAUL(1)=ALOG10(TAUZ)
      DTAUL=1./S
      TAU(1) = TAUZ
      IF(EZ.NE.0.) GO TO 30
      THA = 1.1
      DO 20 I=1,10
10    THA = THA - .1
      CALL EIONX(THA,TAUM,L,0.)
      S1 = EION(14)
      IF(S1.NE.0.) CALL ERR(S1)
      IF(EION(3).GT. .2 * THA/V1) GO TO 20
      EZ = EION(8)
      GO TO 30
20    CONTINUE
      S1 = 10.20
      CALL ERR(S1)
30    CONTINUE
C      PREPARE TABLES OF SPECIFIC DENSITY AND ENERGY
C      IN REAL SPACE AND IN LOG BASE 10.
      DO 50 I=2,NN
      TAUL(I)=TAUL(I-1)+DTAUL
      TAU(I)=EXPT(TAUL(I))
50    CONTINUE
      EM=EZ*10.0**DM
      EL(1)=ALOG10(EZ)
      DEL=1./T
      E(1) = EZ
      DO 60 I=2,MM
      EL(I)=EL(I-1)+DEL
      E(I)=EXPT(EL(I))
60    CONTINUE
      WRITE (6,9011)
      WRITE (6,9002) (TAUL(N), N = 1,NN)
      WRITE (6,9010)
      WRITE (6,9002) (EL(M), M = 1,MM)
C      DETERMINE SOURCE OF EOS DATA
      GO TO (100,200,300,400),IS
100   CONTINUE
      DO 149 M=1,MM
      DO 149 N=1,NN
      K=(M-1)*NN+N
C      INITIAL GUESS AT THE TEMPERATURE
      THMIN = THETA(N,M-1)
      THMAX = THETA(N-1,M)
      IF(N.EQ.1) THMAX=E(M)/PHI
      IF( (N.EQ.1).AND.(M.GT.1) ) THMAX=3.*THETA(N,M-1)
      IF(M.EQ.1) THMIN =1.E-3
      THETA(N,M) =THMIN
      DO 120 I=1,20
      CALL EIONX(THMIN,TAU(N),L,0.)
      S1=EION(14)
      IF(S1.NE.0.) CALL ERR(S1)
      EMIN=EION(8)
      CALL EIONX(THMAX,TAU(N),L,0.)
      EMAX=EION(8)
      S1=EION(14)

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      IF(S1.NE.0.) CALL ERR(S1)
      CALL EIONX(THETA(N,M),TAU(N),L,0.)
C     NEWTON'S INTERPOLATION
      THETA(N,M)=THETA(N,M)+(THMAX-THMIN)*(E(M)-EION(8))
      1 / (EMAX-EMIN)
      IF(ABS(EION(8)-E(M)) / E(M).LE..001) GO TO 130
      IF(EION(8).LT.E(M)) THMIN=THETA(N,M)
      IF(EION(8).GT.E(M)) THMAX=THETA(N,M)
120  CONTINUE
      S1=10.120
      CALL ERR(S1)
130  CONTINUE
C     ZBAR AND EION OBTAINED FROM EIONX
      ZB1D(K)=EION(3)
      AEI=(EION(8)-1.5*EION(1)*TLMS(9))/PHI
      IF( AEI.LE. 1.E-10) AEI=1.E-10
      EILN1D(K) =ALOG(AEI)
149  CONTINUE
C     RESERVED FOR FUTURE SOURCES OF EOS DATA
200  CONTINUE
300  CONTINUE
400  CONTINUE
C
C     PUNCH DATA STATEMENTS FOR PROGRAM EST
500  CONTINUE
      ID=1
      PUNCH 9018
      PUNCH 9036,ID,TAUM,EM,TAUZ,EZ,V1,VZ
      PUNCH 9006
      PUNCH 9035,ID,TAUL(1),EL(1),S,T,PHI
      PUNCH 9007
      PUNCH 9019,ID,NN,MM,I1,I2,I3,I4,I5,I6,I7,I8
      PUNCH 9003,NN,MM,NN,MM
      PUNCH 9004
      KM=NN*MM
      NM=KM
      IF(NN*MM.GT.54) NM=54
      PUNCH 9016,ID,NM
      PUNCH 9015,ID
      ICNT=0
      DO 549 I=1,KM,6
      I6=I+5
      ICNT=ICNT+1
      IP=I
      IF((I6.LT.KM).OR.(ICNT.EQ.10) ) GO TO 539
530  I6=KM
      KI=KM-I+1
      GO TO (531,532,533,534,535),KI
531  PUNCH 9031,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
532  PUNCH 9032,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
533  PUNCH 9033,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
534  PUNCH 9034,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
535  PUNCH 9035,ICNT,(ZB1D(K),K=IP,I6 )
      GO TO 548
539  IF(ICNT.LT.10) GO TO 540
      ID=ID+1
      NM=54
      IF((ID )+54.GT.KM) NM=KM-(ID-1)*54
      PUNCH 9016,ID,NM
      PUNCH 9015,ID
      ICNT=1

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      IF(16.GT.KM) GO TO 530
      GO TO 545
540 IF(ICNT.NE.9) GO TO 545
      PUNCH 9036,ICNT,(ZB1D(K),K=1,16)
      GO TO 548
545 PUNCH 9005,ICNT,(ZB1D(K),K=1,16)
548 CONTINUE
549 CONTINUE
      NM=KM
      IF(1.NN*MM.GT.54) NM=54
      ID=1
      PUNCH 9022,ID,NM
      PUNCH 9021,ID
      ICNT =0
      DO 599 I=1,KM,6
      I6=I+5
      ICNT=ICNT+1
      IP=I
      IF((16.LT.KM).OR.(ICNT.EQ.10) ) GO TO 570
560 I6=KM
      KI=KM-I+1
      GO TO (561,562,563,564,565),KI
561 PUNCH 9031,ICNT,(EILN1D(K),K=IP,16)
      GO TO 598
562 PUNCH 9032,ICNT,(EILN1D(K),K=IP,16)
      GO TO 598
563 PUNCH 9033,ICNT,(EILN1D(K),K=IP,16)
      GO TO 598
564 PUNCH 9034,ICNT,(EILN1D(K),K=IP,16)
      GO TO 598
565 PUNCH 9035,ICNT,(EILN1D(K),K=IP,16)
      GO TO 598
570 IF(ICNT.LT.10) GO TO 580
      ID=ID+1
      NM=54
      IF((ID )*54.GT.KM) NM=KM-(ID-1)*54
      PUNCH 9022,ID,NM
      PUNCH 9021,ID
      ICNT=1
      IF(16.GT.KM) GO TO 560
      GO TO 585
580 IF(ICNT.NE.9) GO TO 585
      PUNCH 9036,ICNT,(EILN1D(K),K=1,16)
      GO TO 598
585 PUNCH 9005,ICNT,(EILN1D(K),K=1,16)
598 CONTINUE
599 CONTINUE
C      EDIT PRINTS
600 CONTINUE
      WRITE (6,9012)
      WRITE(6,9002) (ZB1D(K),K=1,KM)
      WRITE(6,9017)
      WRITE(6,9002) (EILN1D(K),K=1,KM)
      WRITE (6,9013)
      WRITE (6,9002) ((THETA(N,M), N = 1,NN), M = 1,MM)
700 CONTINUE
      CALL EXIT
      END
01  FOR ERR/A, ERR/RSE1, ERR/R1
      SUBROUTINE ERR(S1)
      3 FORMAT (6H S1 = F10.4)
      WRITE(6,3) S1
      CALL EXIT
      END
01  FOR LIBEX, LIBEX/FJ

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SUBROUTINE LIBEX(TAU,E,THA,P,ZHAR,GG)
COMMON Z(90)
EQUIVALLNCE (Z(90),S1)
C*****PLACE DATA STATEMENTS PRODUCED BY PROGRAM GEST HERE *****
DATA TAU,EM,TAUZ,EZ,V1,VZ/
1 5.000E+10, 1.583E+12, 5.000E-02, 1.583E+09, 7.980E+00, 1.126E+03/
DATA TAUZ,ELZ,S,T,PHI/
1 -1.301E+0, 9.2, 2.000E+0, 8.000E+0, 5.244E+9/
DATA NN,MM,I1,I2,I3,I4,I5,I6,I7,I8/
1 25, 25, 1, 1, 1, 1, 1, 1, 0, 0/
DIMENSION ZB(25,25),EILN(25,25)
EQUIVALENCE (ZB,ZB1), (EILN,EILN1)
COMMON/EST/ZB 1(54)
DATA ZB 1/
1 2.200E-10, 3.912E-10, 6.957E-10, 1.237E-09, 2.200E-09, 3.912E-09,
2 6.957E-09, 1.237E-08, 2.200E-08, 3.912E-08, 6.957E-08, 1.237E-07,
3 2.200E-07, 3.911E-07, 6.955E-07, 1.236E-06, 2.197E-06, 3.904E-06,
4 6.930E-06, 1.229E-05, 2.173E-05, 3.828E-05, 6.694E-05, 1.156E-04,
5 1.957E-04, 3.911E-08, 6.956E-08, 1.237E-07, 2.200E-07, 3.911E-07,
6 6.955E-07, 1.237E-06, 2.198E-06, 3.907E-06, 6.941E-06, 1.232E-05,
7 2.184E-05, 3.863E-05, 6.803E-05, 1.189E-04, 2.054E-04, 3.475E-04,
8 5.694E-04, 9.132E-04, 1.382E-03, 1.984E-03, 2.722E-03, 3.553E-03,
9 4.455E-03, 5.399E-03, 2.001E-06, 3.563E-06, 6.333E-06, 1.125E-05/
COMMON/EST/ZB 2(54)
DATA ZB 2/
1 1.997E-05, 3.542E-05, 6.265E-05, 1.104E-04, 1.932E-04, 3.342E-04,
2 5.669E-04, 9.331E-04, 1.499E-03, 2.279E-03, 3.284E-03, 4.485E-03,
3 5.898E-03, 7.394E-03, 8.953E-03, 1.054E-02, 1.217E-02, 1.375E-02,
4 1.529E-02, 1.679E-02, 1.823E-02, 4.031E-05, 7.149E-05, 1.263E-04,
5 2.223E-04, 3.879E-04, 6.677E-04, 1.124E-03, 1.847E-03, 2.903E-03,
6 4.337E-03, 6.138E-03, 8.283E-03, 1.064E-02, 1.312E-02, 1.566E-02,
7 1.820E-02, 2.075E-02, 2.318E-02, 2.552E-02, 2.776E-02, 2.989E-02,
8 3.192E-02, 3.384E-02, 3.567E-02, 3.739E-02, 3.950E-04, 6.918E-04,
9 1.189E-03, 1.996E-03, 3.264E-03, 5.096E-03, 7.557E-03, 1.060E-02/
COMMON/EST/ZB 3(54)
DATA ZB 3/
1 1.416E-02, 1.801E-02, 2.200E-02, 2.601E-02, 2.995E-02, 3.382E-02,
2 3.747E-02, 4.093E-02, 4.419E-02, 4.725E-02, 5.013E-02, 5.283E-02,
3 5.535E-02, 5.772E-02, 5.994E-02, 6.203E-02, 6.399E-02, 6.581E-02,
4 6.697E-03, 5.987E-03, 9.230E-03, 1.348E-02, 1.861E-02, 2.446E-02,
5 3.061E-02, 3.685E-02, 4.298E-02, 4.887E-02, 5.446E-02, 5.981E-02,
6 6.471E-02, 6.927E-02, 7.349E-02, 7.741E-02, 8.103E-02, 8.439E-02,
7 8.751E-02, 9.041E-02, 9.310E-02, 9.561E-02, 9.795E-02, 1.001E-01,
8 7.936E-03, 1.251E-02, 1.867E-02, 2.629E-02, 3.501E-02, 4.446E-02,
9 5.399E-02, 6.331E-02, 7.220E-02, 8.052E-02, 8.823E-02, 9.533E-02/
COMMON/EST/ZB 4(54)
DATA ZB 4/
1 1.018E-01, 1.079E-01, 1.134E-01, 1.184E-01, 1.230E-01, 1.272E-01,
2 1.311E-01, 1.346E-01, 1.379E-01, 1.410E-01, 1.438E-01, 1.464E-01,
3 1.489E-01, 2.062E-02, 3.056E-02, 4.261E-02, 5.613E-02, 7.047E-02,
4 8.465E-02, 9.826E-02, 1.110E-01, 1.227E-01, 1.334E-01, 1.431E-01,
5 1.518E-01, 1.597E-01, 1.668E-01, 1.733E-01, 1.792E-01, 1.845E-01,
6 1.894E-01, 1.938E-01, 1.979E-01, 2.016E-01, 2.051E-01, 2.083E-01,
7 2.112E-01, 2.140E-01, 4.294E-02, 6.053E-02, 8.040E-02, 1.013E-01,
8 1.223E-01, 1.421E-01, 1.605E-01, 1.772E-01, 1.922E-01, 2.057E-01,
9 2.177E-01, 2.284E-01, 2.380E-01, 2.465E-01, 2.542E-01, 2.612E-01/
COMMON/EST/ZB 5(54)
DATA ZB 5/
1 2.674E-01, 2.731E-01, 2.783E-01, 2.830E-01, 2.873E-01, 2.913E-01,
2 2.950E-01, 2.983E-01, 3.015E-01, 7.700E-02, 1.047E-01, 1.346E-01,
3 1.647E-01, 1.936E-01, 2.207E-01, 2.450E-01, 2.667E-01, 2.859E-01,
4 3.029E-01, 3.178E-01, 3.310E-01, 3.426E-01, 3.537E-01, 3.624E-01,
5 3.708E-01, 3.782E-01, 3.850E-01, 3.911E-01, 3.968E-01, 4.016E-01,
6 4.061E-01, 4.103E-01, 4.146E-01, 4.182E-01, 1.244E-01, 1.652E-01,
7 2.078E-01, 2.497E-01, 2.891E-01, 3.250E-01, 3.570E-01, 3.850E-01,

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8 4.100E-01, 4.316E-01, 4.505E-01, 4.671E-01, 4.817E-01, 4.948E-01,
 9 5.054E-01, 5.145E-01, 5.226E-01, 5.299E-01, 5.368E-01, 5.427E-01/
 COMMON/EST/ZB 6(54)
 DATA ZB 6/
 1 5.481E-01, 5.530E-01, 5.575E-01, 5.616E-01, 5.654E-01, 1.863E-01,
 2 2.434E-01, 3.020E-01, 3.588E-01, 4.117E-01, 4.595E-01, 5.017E-01,
 3 5.345E-01, 5.624E-01, 5.855E-01, 6.052E-01, 6.218E-01, 6.370E-01,
 4 6.499E-01, 6.613E-01, 6.715E-01, 6.806E-01, 6.887E-01, 6.960E-01,
 5 7.026E-01, 7.087E-01, 7.142E-01, 7.192E-01, 7.239E-01, 7.281E-01,
 6 2.629E-01, 3.396E-01, 4.174E-01, 4.923E-01, 5.592E-01, 6.139E-01,
 7 6.593E-01, 6.960E-01, 7.272E-01, 7.534E-01, 7.758E-01, 7.950E-01,
 8 8.117E-01, 8.262E-01, 8.390E-01, 8.504E-01, 8.605E-01, 8.695E-01,
 9 8.777E-01, 8.851E-01, 8.918E-01, 8.979E-01, 9.035E-01, 9.087E-01/
 COMMON/EST/ZB 7(54)
 DATA ZB 7/
 1 9.135E-01, 3.533E-01, 4.511E-01, 5.555E-01, 6.501E-01, 7.268E-01,
 2 7.895E-01, 8.404E-01, 8.818E-01, 9.168E-01, 9.463E-01, 9.714E-01,
 3 9.929E-01, 1.012E 00, 1.028E 00, 1.042E 00, 1.055E 00, 1.066E 00,
 4 1.076E 00, 1.085E 00, 1.093E 00, 1.101E 00, 1.108E 00, 1.114E 00,
 5 1.120E 00, 1.125E 00, 4.540E-01, 5.919E-01, 7.244E-01, 8.329E-01,
 6 9.206E-01, 9.913E-01, 1.049E 00, 1.096E 00, 1.135E 00, 1.168E 00,
 7 1.196E 00, 1.220E 00, 1.241E 00, 1.259E 00, 1.275E 00, 1.289E 00,
 8 1.302E 00, 1.313E 00, 1.323E 00, 1.332E 00, 1.340E 00, 1.348E 00,
 9 1.355E 00, 1.361E 00, 1.367E 00, 6.232E-01, 7.683E-01, 9.209E-01/
 COMMON/EST/ZB 8(47)
 DATA ZB 8/
 1 1.045E 00, 1.144E 00, 1.224E 00, 1.289E 00, 1.341E 00, 1.386E 00,
 2 1.422E 00, 1.453E 00, 1.480E 00, 1.504E 00, 1.525E 00, 1.544E 00,
 3 1.560E 00, 1.575E 00, 1.588E 00, 1.600E 00, 1.611E 00, 1.621E 00,
 4 1.628E 00, 1.636E 00, 1.644E 00, 1.650E 00, 8.692E-01, 9.739E-01,
 5 1.149E 00, 1.290E 00, 1.402E 00, 1.492E 00, 1.569E 00, 1.633E 00,
 6 1.686E 00, 1.730E 00, 1.768E 00, 1.799E 00, 1.827E 00, 1.851E 00,
 7 1.872E 00, 1.890E 00, 1.907E 00, 1.922E 00, 1.935E 00, 1.947E 00,
 8 1.958E 00, 1.968E 00, 1.977E 00, 1.985E 00, 1.993E 00/
 COMMON/EST/ZB 9(29)
 DATA ZB 9/
 5 9.721E-1, 1.216E+0, 1.415E+0, 1.580E+0, 1.718E+0,
 6 1.829E+0, 1.918E+0, 1.991E+0, 2.051E+0, 2.100E+0, 2.143E+0,
 7 2.180E+0, 2.211E+0, 2.239E+0, 2.263E+0, 2.284E+0, 2.303E+0,
 8 2.320E+0, 2.335E+0, 2.348E+0, 2.361E+0, 2.372E+0, 2.382E+0,
 9 2.391E+0, 2.401E+0, 1.217E+0, 1.497E+0, 1.743E+0, 1.944E+0/
 COMMON/EST/ZB10(54)
 DATA ZB10/
 1 2.103E+0, 2.229E+0, 2.331E+0, 2.415E+0, 2.485E+0, 2.538E+0,
 2 2.584E+0, 2.623E+0, 2.656E+0, 2.685E+0, 2.711E+0, 2.733E+0,
 3 2.754E+0, 2.772E+0, 2.788E+0, 2.803E+0, 2.817E+0, 2.828E+0,
 4 2.839E+0, 2.850E+0, 2.859E+0, 1.505E+0, 1.854E+0, 2.143E+0,
 5 2.373E+0, 2.550E+0, 2.681E+0, 2.786E+0, 2.872E+0, 2.943E+0,
 6 3.003E+0, 3.054E+0, 3.097E+0, 3.135E+0, 3.168E+0, 3.197E+0,
 7 3.223E+0, 3.246E+0, 3.266E+0, 3.285E+0, 3.301E+0, 3.317E+0,
 8 3.331E+0, 3.343E+0, 3.355E+0, 3.366E+0, 1.870E+0, 2.278E+0,
 9 2.600E+0, 2.834E+0, 3.019E+0, 3.164E+0, 3.284E+0, 3.381E+0/
 COMMON/EST/ZB11(54)
 DATA ZB11/
 1 3.461E+0, 3.527E+0, 3.582E+0, 3.630E+0, 3.672E+0, 3.708E+0,
 2 3.739E+0, 3.768E+0, 3.793E+0, 3.815E+0, 3.836E+0, 3.854E+0,
 3 3.871E+0, 3.886E+0, 3.900E+0, 3.913E+0, 3.925E+0, 2.303E+0,
 4 2.746E+0, 3.082E+0, 3.344E+0, 3.548E+0, 3.706E+0, 3.834E+0,
 5 3.938E+0, 4.025E+0, 4.098E+0, 4.161E+0, 4.214E+0, 4.261E+0,
 6 4.301E+0, 4.337E+0, 4.369E+0, 4.397E+0, 4.422E+0, 4.445E+0,
 7 4.466E+0, 4.485E+0, 4.502E+0, 4.518E+0, 4.532E+0, 4.545E+0,
 8 2.780E+0, 3.256E+0, 3.627E+0, 3.909E+0, 4.130E+0, 4.307E+0,
 9 4.449E+0, 4.566E+0, 4.661E+0, 4.743E+0, 4.812E+0, 4.872E+0/
 COMMON/EST/ZB12(54)
 DATA ZB12/

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1 4.924E+0, 4.969E+0, 5.009E+0, 5.045E+0, 5.076E+0, 5.105E+0,
2 5.130E+0, 5.153E+0, 5.174E+0, 5.194E+0, 5.211E+0, 5.228E+0,
3 5.243E+0, 5.307E+0, 5.828E+0, 4.230E+0, 4.544E+0, 4.789E+0,
4 4.986E+0, 5.145E+0, 5.274E+0, 5.383E+0, 5.474E+0, 5.536E+0,
5 5.582E+0, 5.623E+0, 5.659E+0, 5.692E+0, 5.721E+0, 5.748E+0,
6 5.772E+0, 5.794E+0, 5.814E+0, 5.833E+0, 5.850E+0, 5.866E+0,
7 5.880E+0, 5.894E+0, 3.901E+0, 4.474E+0, 4.921E+0, 5.267E+0,
8 5.526E+0, 5.658E+0, 5.767E+0, 5.859E+0, 5.939E+0, 6.007E+0,
9 6.067E+0, 6.119E+0, 6.166E+0, 6.207E+0, 6.244E+0, 6.277E+0/
COMMON/EST/ZB13( 9)
DATA ZB13/
1 6.306E+0, 6.334E+0, 6.358E+0, 6.381E+0, 6.402E+0, 6.419E+0,
2 6.437E+0, 6.453E+0, 6.468E+0/
COMMON/EST/EILN 1(54)
DATA EILN 1/
1-1.961E 01,-1.961E 01,-1.961E 01,-1.822E 01,-1.782E 01,-1.731E 01,
2-1.672E 01,-1.614E 01,-1.555E 01,-1.498E 01,-1.440E 01,-1.383E 01,
3-1.325E 01,-1.266E 01,-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,
4-9.802E 00,-9.229E 00,-8.659E 00,-8.093E 00,-7.534E 00,-6.987E 00,
5-6.461E 00,-1.499E 01,-1.440E 01,-1.383E 01,-1.325E 01,-1.268E 01,
6-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,-9.802E 00,-9.227E 00,
7-8.654E 00,-8.084E 00,-7.518E 00,-6.959E 00,-6.413E 00,-5.887E 00,
8-5.393E 00,-4.921E 00,-4.507E 00,-4.145E 00,-3.829E 00,-3.562E 00,
9-3.336E 00,-3.144E 00,-1.104E 01,-1.047E 01,-9.892E 00,-9.317E 00/
COMMON/EST/EILN 2(54)
DATA EILN 2/
1-8.743E 00,-8.171E 00,-7.600E 00,-7.034E 00,-6.474E 00,-5.926E 00,
2-5.998E 00,-4.899E 00,-4.425E 00,-4.006E 00,-3.641E 00,-3.329E 00,
3-3.055E 00,-2.829E 00,-2.638E 00,-2.475E 00,-2.331E 00,-2.209E 00,
4-2.103E 00,-2.009E 00,-1.927E 00,-1.804E 00,-1.746E 00,-1.689E 00,
5-6.334E 00,-5.777E 00,-5.234E 00,-4.713E 00,-4.216E 00,-3.764E 00,
6-3.363E 00,-3.016E 00,-2.716E 00,-2.466E 00,-2.256E 00,-2.079E 00,
7-1.929E 00,-1.797E 00,-1.687E 00,-1.591E 00,-1.506E 00,-1.432E 00,
8-1.367E 00,-1.308E 00,-1.256E 00,-1.209E 00,-1.159E 00,-1.109E 00,
9-4.657E 00,-4.139E 00,-3.647E 00,-3.202E 00,-2.808E 00,-2.469E 00/
COMMON/EST/EILN 3(54)
DATA EILN 3/
1-2.179E 00,-1.939E 00,-1.739E 00,-1.572E 00,-1.431E 00,-1.309E 00,
2-1.207E 00,-1.118E 00,-1.042E 00,-9.745E-01,-9.154E-01,-8.630E-01,
3-8.163E-01,-7.744E-01,-7.366E-01,-7.024E-01,-6.714E-01,-6.435E-01,
4-3.523E 00,-3.040E 00,-2.608E 00,-2.229E 00,-1.906E 00,-1.633E 00,
5-1.409E 00,-1.223E 00,-1.069E 00,-9.409E-01,-8.327E-01,-7.390E-01,
6-6.601E-01,-5.921E-01,-5.329E-01,-4.810E-01,-4.352E-01,-3.946E-01,
7-3.583E-01,-3.257E-01,-2.964E-01,-2.698E-01,-2.456E-01,-2.235E-01,
8-2.759E 00,-2.303E 00,-1.903E 00,-1.561E 00,-1.275E 00,-1.035E 00,
9-8.412E-01,-6.819E-01,-5.506E-01,-4.415E-01,-3.501E-01,-2.727E-01/
COMMON/EST/EILN 4(54)
DATA EILN 4/
1-2.067E-01,-1.484E-01,-9.905E-02,-5.591E-02,-1.794E-02, 1.568E-02,
2 4.563E-02, 7.246E-02, 9.660E-02, 1.184E-01, 1.383E-01, 1.564E-01,
3 1.729E-01,-1.804E 00,-1.411E 00,-1.078E 00,-8.024E-01,-5.749E-01,
4-3.915E-01,-2.424E-01,-1.206E-01,-2.026E-02, 6.316E-02, 1.332E-01,
5 1.925E-01, 2.432E-01, 2.870E-01, 3.250E-01, 3.583E-01, 3.876E-01,
6 4.136E-01, 4.368E-01, 4.576E-01, 4.764E-01, 4.934E-01, 5.088E-01,
7 5.229E-01, 5.358E-01,-1.070E 00,-7.269E-01,-4.430E-01,-2.121E-01,
8-2.386E-02, 1.265E-01, 2.481E-01, 3.471E-01, 4.286E-01, 4.962E-01,
9 5.529E-01, 6.010E-01, 6.420E-01, 6.774E-01, 7.082E-01, 7.351E-01/
COMMON/EST/EILN 5(54)
DATA EILN 5/
1 7.588E-01, 7.799E-01, 7.986E-01, 8.154E-01, 8.306E-01, 8.443E-01,
2 8.568E-01, 8.682E-01, 8.786E-01,-4.863E-01,-1.788E-01, 7.220E-02,
3 2.742E-01, 4.359E-01, 5.668E-01, 6.712E-01, 7.560E-01, 8.256E-01,
4 8.832E-01, 9.314E-01, 9.722E-01, 1.006E 00, 1.037E 00, 1.063E 00,
5 1.086E 00, 1.105E 00, 1.123E 00, 1.139E 00, 1.153E 00, 1.165E 00,
6 1.177E 00, 1.187E 00, 1.197E 00, 1.206E 00,-6.935E-03, 2.768E-01,

```

7 5.063E-01, 6.901E-01, 8.367E-01, 9.538E-01, 1.048E 00, 1.123E 00,
 8 1.186E 00, 1.238E 00, 1.280E 00, 1.317E 00, 1.347E 00, 1.374E 00,
 9 1.395E 00, 1.413E 00, 1.429E 00, 1.444E 00, 1.457E 00, 1.469E 00/

COMMON/EST/EILN 6(54)

DATA EILN 6/

1 1.479E 00, 1.488E 00, 1.497E 00, 1.505E 00, 1.512E 00, 3.972E-01,
 2 6.645E-01, 8.802E-01, 1.053E 00, 1.190E 00, 1.300E 00, 1.388E 00,
 3 1.453E 00, 1.506E 00, 1.550E 00, 1.587E 00, 1.617E 00, 1.644E 00,
 4 1.668E 00, 1.688E 00, 1.706E 00, 1.722E 00, 1.736E 00, 1.748E 00,
 5 1.760E 00, 1.770E 00, 1.779E 00, 1.788E 00, 1.796E 00, 1.803E 00,
 6 7.419E-01, 9.976E-01, 1.204E 00, 1.369E 00, 1.500E 00, 1.603E 00,
 7 1.684E 00, 1.748E 00, 1.801E 00, 1.845E 00, 1.882E 00, 1.913E 00,
 8 1.939E 00, 1.962E 00, 1.982E 00, 2.000E 00, 2.015E 00, 2.029E 00,
 9 2.042E 00, 2.053E 00, 2.063E 00, 2.072E 00, 2.080E 00, 2.088E 00/

COMMON/EST/EILN 7(54)

DATA EILN 7/

1 2.095E 00, 1.037E 00, 1.282E 00, 1.493E 00, 1.668E 00, 1.801E 00,
 2 1.904E 00, 1.985E 00, 2.048E 00, 2.100E 00, 2.143E 00, 2.179E 00,
 3 2.209E 00, 2.235E 00, 2.258E 00, 2.277E 00, 2.295E 00, 2.310E 00,
 4 2.323E 00, 2.335E 00, 2.346E 00, 2.356E 00, 2.365E 00, 2.373E 00,
 5 2.381E 00, 2.387E 00, 1.288E 00, 1.562E 00, 1.797E 00, 1.973E 00,
 6 2.106E 00, 2.207E 00, 2.286E 00, 2.349E 00, 2.400E 00, 2.442E 00,
 7 2.477E 00, 2.506E 00, 2.532E 00, 2.554E 00, 2.573E 00, 2.589E 00,
 8 2.604E 00, 2.617E 00, 2.629E 00, 2.640E 00, 2.649E 00, 2.658E 00,
 9 2.666E 00, 2.673E 00, 2.680E 00, 1.619E 00, 1.870E 00, 2.106E 00/

COMMON/EST/EILN 8(47)

DATA EILN 8/

1 2.281E 00, 2.412E 00, 2.512E 00, 2.589E 00, 2.650E 00, 2.700E 00,
 2 2.741E 00, 2.774E 00, 2.803E 00, 2.828E 00, 2.850E 00, 2.869E 00,
 3 2.886E 00, 2.901E 00, 2.914E 00, 2.926E 00, 2.936E 00, 2.944E 00,
 4 2.953E 00, 2.961E 00, 2.968E 00, 2.974E 00, 2.979E 00, 2.983E 00,
 5 2.989E 00, 2.991E 00, 2.718E 00, 2.815E 00, 2.895E 00, 2.958E 00,
 6 3.008E 00, 3.049E 00, 3.082E 00, 3.110E 00, 3.134E 00, 3.154E 00,
 7 3.172E 00, 3.188E 00, 3.202E 00, 3.214E 00, 3.225E 00, 3.234E 00,
 8 3.243E 00, 3.251E 00, 3.258E 00, 3.265E 00, 3.271E 00/

COMMON/EST/EILN 9(29)

DATA EILN 9/

5 2.180E+0, 2.501E+0, 2.732E+0, 2.906E+0, 3.036E+0,
 6 3.136E+0, 3.211E+0, 3.270E+0, 3.318E+0, 3.354E+0, 3.386E+0,
 7 3.412E+0, 3.435E+0, 3.455E+0, 3.472E+0, 3.487E+0, 3.500E+0,
 8 3.511E+0, 3.522E+0, 3.530E+0, 3.539E+0, 3.546E+0, 3.553E+0,
 9 3.559E+0, 3.565E+0, 2.504E+0, 2.820E+0, 3.061E+0, 3.232E+0/

COMMON/EST/EILN10(54)

DATA EILN10/

1 3.356E+0, 3.447E+0, 3.519E+0, 3.575E+0, 3.620E+0, 3.654E+0,
 2 3.683E+0, 3.707E+0, 3.728E+0, 3.746E+0, 3.762E+0, 3.775E+0,
 3 3.788E+0, 3.799E+0, 3.808E+0, 3.817E+0, 3.826E+0, 3.833E+0,
 4 3.839E+0, 3.846E+0, 3.851E+0, 2.829E+0, 3.157E+0, 3.385E+0,
 5 3.547E+0, 3.662E+0, 3.744E+0, 3.807E+0, 3.858E+0, 3.900E+0,
 6 3.935E+0, 3.955E+0, 3.989E+0, 4.011E+0, 4.029E+0, 4.045E+0,
 7 4.060E+0, 4.072E+0, 4.083E+0, 4.093E+0, 4.103E+0, 4.111E+0,
 8 4.118E+0, 4.125E+0, 4.131E+0, 4.137E+0, 3.171E+0, 3.482E+0,
 9 3.693E+0, 3.836E+0, 3.945E+0, 4.027E+0, 4.093E+0, 4.145E+0/

COMMON/EST/EILN11(54)

DATA EILN11/

1 4.188E+0, 4.222E+0, 4.251E+0, 4.275E+0, 4.296E+0, 4.315E+0,
 2 4.331E+0, 4.345E+0, 4.357E+0, 4.369E+0, 4.379E+0, 4.388E+0,
 3 4.396E+0, 4.403E+0, 4.410E+0, 4.417E+0, 4.422E+0, 3.500E+0,
 4 3.783E+0, 3.980E+0, 4.125E+0, 4.233E+0, 4.314E+0, 4.378E+0,
 5 4.429E+0, 4.471E+0, 4.506E+0, 4.535E+0, 4.560E+0, 4.581E+0,
 6 4.600E+0, 4.616E+0, 4.630E+0, 4.643E+0, 4.655E+0, 4.665E+0,
 7 4.674E+0, 4.682E+0, 4.690E+0, 4.697E+0, 4.703E+0, 4.709E+0,
 8 3.804E+0, 4.078E+0, 4.274E+0, 4.415E+0, 4.521E+0, 4.602E+0,
 9 4.667E+0, 4.718E+0, 4.759E+0, 4.794E+0, 4.823E+0, 4.848E+0/

COMMON/EST/EILN12(54)

```

DATA EILN12/
1 4.870E+0, 4.888E+0, 4.905E+0, 4.919E+0, 4.932E+0, 4.943E+0,
2 4.953E+0, 4.962E+0, 4.971E+0, 4.978E+0, 4.985E+0, 4.992E+0,
3 4.997E+0, 4.105E+0, 4.375E+0, 4.567E+0, 4.709E+0, 4.814E+0,
4 4.895E+0, 4.959E+0, 5.010E+0, 5.052E+0, 5.086E+0, 5.109E+0,
5 5.127E+0, 5.143E+0, 5.158E+0, 5.171E+0, 5.183E+0, 5.194E+0,
6 5.204E+0, 5.214E+0, 5.222E+0, 5.230E+0, 5.238E+0, 5.245E+0,
7 5.251E+0, 5.257E+0, 4.411E+0, 4.678E+0, 4.869E+0, 5.007E+0,
8 5.105E+0, 5.157E+0, 5.202E+0, 5.242E+0, 5.277E+0, 5.308E+0,
9 5.335E+0, 5.359E+0, 5.380E+0, 5.399E+0, 5.416E+0, 5.432E+0/
COMMON/EST/EILN13( 9)
DATA EILN13/
1 5.446E+0, 5.458E+0, 5.470E+0, 5.481E+0, 5.490E+0, 5.499E+0,
2 5.507E+0, 5.515E+0, 5.522E+0/
IF(E.NE.0.) GO TO 5
THA = 1.E-3
ZBAR=0.
GO TO 950
5 CONTINUE
ALGT=ALOG10(TAU)
ALGE=ALOG10(E)
DLGT=ALGT-TAULZ
DLGE=ALGE-ELZ
AN=DLGT*S+1.
AM=DLGE*T+1.
IF (DLGT.LT.0.) AN=0.
IF (DLGE.LT.0.) AM=0.
N=IFIX(AN)
M=IFIX(AM)
IN=0
EO=E
IF(N.LE.0) GO TO 10
IF(N.GE.NN) GO TO 20
IF(M.LE.0) GO TO 800
IF(M.GE.MM) GO TO 400
8 CONTINUE
DNLT=AN-AINT(AN)
DMLE=AM-AINT(AM)
ZBAR=ZB(N,M)+(ZB(N+1,M)-ZB(N,M))* DNLT
1 + (ZB(N,M+1)-ZB(N,M))* DMLE
2 + (ZB(N+1,M+1)+ZB(N,M)-ZB(N+1,M)-ZB(N,M+1))
3 *(DNLT*DMLE)
ALIN=EILN(N,M)+(EILN(N+1,M)-EILN(N,M))*DNLT
1 +(EILN(N,M+1)-EILN(N,M))*DMLE
3 *(DNLT*DMLE)
2 +(EILN(N+1,M+1)+EILN(N,M)-EILN(N+1,M)-EILN(N,M+1))
THA=(EO/PHI-EXP(ALIN))/(1.5*(1.+ZBAR ))
IF(IN.NE.0)GO TO (150,250,350,450,550,650,750,850),IN
GO TO 950
10 IF(M.LE.0) GO TO 100
IF(M.GE.MM) GO TO 300
GO TO 200
20 IF(M.LE.0) GO TO 700
IF(M.GE.MM) GO TO 500
GO TO 600
100 CONTINUE
IF(I1.EQ.1) GO TO 9901
150 CONTINUE
RETURN
200 CONTINUE
IF(I2.EQ.1) GO TO 9902
250 CONTINUE
RETURN
300 CONTINUE
IF(I3.EQ.1) GO TO 9903

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```

350 CONTINUE
    RETURN
400 CONTINUE
    IF(14.EQ.1) GO TO 9904
450 CONTINUE
    RETURN
500 CONTINUE
    IF(15.EQ.1) GO TO 9905
550 CONTINUE
    RETURN
600 CONTINUE
    IF(16.EQ.1) GO TO 9906
650 CONTINUE
    RETURN
700 CONTINUE
    IF(17.EQ.1) GO TO 9907
    IN = 7
    M = 1
    N = NN
    EO=EZ
    GO TO 8
750 THAP = E * THA / EZ
    ZBAR = ZBAR * (THAP/THA)**.75 * SQRT(TAUM/TAU)*EXP(V1*(THAP-THA) /
    1 (THA*THAP*2.))
    AIN=V1*ZBAR
    GO TO 900
800 CONTINUE
    IF(18.EQ.1) GO TO 9908
    IN = 8
    M = 1
    EO=EZ
    GO TO 8
850 THAP = E * THA / EZ
    ZBAR = ZBAR * (THAP/THA)**.75 * EXP(V1*( THAP - THA) /
    1 (THA * THAP*2.))
    AIN=V1*ZBAR
900 CONTINUE
    THA=(E/PHI-AIN)/(1.5*(1.+ZBAR))
950 P=PHI*(1.+ZBAR )*THA/TAU
    RETURN
9901 S1=12.0100
    GO TO 9999
9902 S1=12.0200
    GO TO 9999
9903 S1=12.0300
    GO TO 9999
9904 S1=12.0400
    GO TO 9999
9905 S1=12.0500
    GO TO 9999
9906 S1=12.0600
    GO TO 9999
9907 S1=12.0700
    GO TO 9999
9908 S1=12.0800
9999 WRITE(6,1000)TAU,E,THA,P,ZBAR,GG,ALGT
1000 FORMAT(1H1,12X,6HTAU ,9X,6HE ,9X,6HTHA ,9X,6HP ,9X,6HZ
    1UAR ,9X,6HGG ,9X,6HALGT /7X,1P7E15.7)
    WRITE(6,1001)ALGE,DLGT,DLGE,AN,AM
1001 FORMAT(1H0,12X,6HALGE ,9X,6HDLGT ,9X,6HDLGE ,9X,6HAN ,9X,6HA
    1M /7X,1P5E15.7)
    WRITE(6,1002)N,M,NN,MM,S1
1002 FORMAT(1H0,12X,6HN ,9X,6HM ,9X,6HNN ,9X,6HMM ,9X,6HS
    11 /7X,1P3(6X,19),1P5E15.7)
    CALL EDIT
    END

```

SECTION V

EQUATION OF STATE FOR MOLECULAR CARBON5. 1. INTRODUCTION

In the theoretical analysis of certain experimental systems, it is convenient to treat the vapor phase of a graphite-carbon vapor system as though it were in local thermodynamic equilibrium. It is then possible to calculate the equilibrium composition of the vapor. In this section a FORTRAN subroutine, CMOL, is described which, given the local temperature and specific volume, will calculate the composition and thermodynamic properties of molecular carbon vapor.

Two gross assumptions must first be stated: (1) it is assumed that only the species $C_1, C_2, \dots, C_{10}$ are present, and (2) the perfect gas law is assumed at several places. In addition to these assumptions, an extrapolation past the known data to the limiting high-temperature values of monatomic carbon vapor permits the user to bridge, in a physically consistent manner, the region where the free energies of the system have not yet been determined.

Finally, the systems of interest are metastable in that the carbon vapor formed is not expected to condense to graphite within the time period under study. Thus, the routine permits the calculation of the system composition under the assumption that only vapor is present.

5. 2. SYMBOLS

$A_{\alpha, j}$ j^{th} coefficient in the least-square fit to the enthalpy and
free energy of species α ,
 a_{α} A^{th} coefficient in $f(\xi_1)$; see Eq. (122e)

C_j	Molecule in carbon vapor containing j atoms of carbon,
E_{sp}	Specific internal energy in calories/gram,
E_α	Internal energy per mole of species α in calories/mole,
$f(\xi_1)$	See Eq. (122e),
$G_\alpha^0(0)$	Gibbs free energy of species α at $0^\circ K$,
$G_\alpha^0(T)$	Gibbs free energy of species α at $T^\circ K$,
G_α	$G_\alpha \equiv G_\alpha^0(T)$,
ΔG_α^0	Change in free energy due to reaction, for the reaction $\alpha C_1 = C_\alpha : \Delta G_\alpha^0 = G_\alpha - \alpha G_1$,
$H_\alpha^0(0)$	Enthalpy of species α at $0^\circ K$,
$H_\alpha^0(T)$	Enthalpy of species α at $T^\circ K$,
H_α	$H_\alpha \equiv H_\alpha^0(T)$,
K_c^α	Equilibrium constant, i. t. o. concentrations, for the reaction $\alpha C_1 = C_\alpha : K_c^\alpha = (RT)^{\alpha-1} K_p^\alpha ; K_c^\alpha = K_c^\alpha(T, \xi_\alpha)$,
K_p^α	Equilibrium constant i. t. o. partial pressures, for the reaction $\alpha C_1 = C_\alpha : K_p^\alpha = \exp(-\Delta G_\alpha^0/RT) ; K_p^\alpha = K_p^\alpha(T)$,
M	Mass of the system; $M = \sum_\alpha M_\alpha = \sum_\alpha n_\alpha M_\alpha^0$ in grams,
M_α^0	Gram-molecular weight of species α in grams/mole,
$\bar{N}$	Mean number of atoms/molecule; see Eq. (140a),
n_α	Number of moles of species α ,
n	$n = \sum_\alpha n_\alpha$, the total number of moles,
P	$P = \sum_\alpha P_\alpha = RT \sum_\alpha \xi_\alpha$; system pressure in dynes/cm ² ,
P_α	Pressure of component α ,

R	Gas constant. The units of R are consistent with the other factors in the equation in which it appears; for example, in Eqs. (120), (132), etc., $R = 1.9876$ calorie/mole-°K; in Eqs. (114), etc., $R = 8.3143 \times 10^7$ erg/mole-°K,
T	Temperature in °K,
V	Total system volume in cm^3 ,
α	Molecular species index: $1 \leq \alpha \leq 10$,
ρ	Mass density in g/cm^3 ; $\rho = M/V = 1/\tau$,
τ	Specific volume in cm/g ; $\tau = V/M = 1/\rho$,
θ	Temperature in ev,
ξ_α	$\xi_\alpha = n_\alpha/V$, the number density in moles/ cm^3 of species α .

5.3. THE SYSTEM COMPOSITION

The equilibria assumed can be written as

$$\alpha C_1 = C_\alpha; \quad \alpha = 2, 3, \dots, 10 \quad (112)$$

and they lead to

$$\frac{P_\alpha}{(P_1)^\alpha} = K_p^\alpha(T) \quad (113)$$

Or, assuming that

$$\begin{aligned} P_\alpha V &= n_\alpha RT \\ P_\alpha &= \frac{n_\alpha}{V} RT = \xi_\alpha RT \end{aligned} \quad (114)$$

where $\xi_\alpha = n_\alpha/V$, we obtain

$$\begin{aligned} \xi_\alpha &= (RT)^{\alpha-1} (\xi_1)^\alpha K_p^\alpha(T) \\ &= [K_c^\alpha(T, \xi_\alpha)] [\xi_1]^\alpha \end{aligned} \quad (115)$$

where

$$\begin{aligned} K_p^\alpha &= \exp(-\Delta G_\alpha/RT) \\ &= \exp\left(\left[\alpha G_1 - G_\alpha\right]/RT\right) \end{aligned} \quad (116)$$

and G_α is the Gibbs free energy of species α :

$$\frac{G_\alpha}{RT} \equiv \frac{G_\alpha^0(T)}{RT} \quad (117)$$

These free energy functions, and others, appear in a paper by Duff and Bauer (Ref. 1)* in the form of a least-square fit to the data over two overlapping ranges and are written as

$$\frac{G_\alpha^0(T)}{RT} = A_{\alpha,1} (1 - \ln T) - \left(\sum_{j=2}^{j=4} \left[A_{\alpha,j} T^j \right] / j \right) - A_{\alpha,5} + H_\alpha^0(0)/RT \quad (118)$$

This fit simultaneously gives the enthalpy of species α as

$$\frac{H_\alpha}{RT} \equiv \frac{H_\alpha^0(T)}{RT} = \left(\sum_{j=1}^{j=4} A_{\alpha,j} T^{j-1} \right) + H_\alpha^0(0)/RT \quad (119)$$

and thus satisfies the thermodynamic consistency relation:

$$-T \left(\frac{dG_\alpha/RT}{dT} \right) = (H_\alpha/RT) \quad (120)$$

We thus have 9 equations in the 10 species. The final equation needed is given by the mass conservation relation:

$$M = \sum_\alpha n_\alpha M_\alpha^0 \quad (121)$$

* It should be noted that the thermodynamic function table titles are inverted in this reference; i. e., the table titled "from 300° K-1500° K" actually is the table for 1500° K-6000° K, and vice versa.

which transforms to

$$\rho = \frac{M}{V} = \sum_{\alpha} \frac{n_{\alpha}}{V} M_{\alpha}^o \quad (122a)$$

$$= \sum_{\alpha} \xi_{\alpha} M_{\alpha}^o \quad (122b)$$

$$= \sum_{\alpha} \xi_{\alpha} (12\alpha) \quad (122c)$$

or

$$0 = \sum_{\alpha=1}^{10} \alpha e^{-\Delta G_{\alpha}/RT} (RT)^{\alpha-1} (\xi_1)^{\alpha} - \rho/12 \quad (122d)$$

which we immediately recognize as a tenth-order polynomial in ξ_1 , the number density, in moles/cm³, of carbon atoms. For convenience we assume the standard polynomial form:

$$0 = f(\xi_1) = \sum_{\alpha=0}^{\alpha=10} a_{\alpha} (\xi_1)^{\alpha} \quad (122e)$$

We note that, by definition of the variables ξ_{α} ,

$$0 < \xi_1 < \rho/12 \quad (123a)$$

For these limiting values of the argument, the polynomial assumes the values

$$f(0) = -\rho/12 \quad (123b)$$

and

$$f(\rho/12) > 0 \quad (123c)$$

Further, Descartes' rule of signs permits, at most, one real root. Since there is at least one real root, this root must be unique. We thus have all the information needed to find the root.

Because of limitations imposed by the permissible exponent range inherent in most computer systems, Eq. (122e) was rewritten as

$$0 = \sum_{\alpha=0}^{\alpha=10} a_{\alpha} X^{\alpha} \quad (124a)$$

where

$$X = \left[\xi_1 e^{G_1/RT} \right] = \frac{\xi_1}{a_1} \quad (124b)$$

$$a'_\alpha = \alpha e^{-G_\alpha/RT} / RT ; \quad 1 \leq \alpha \leq 10 \quad (124c)$$

$$a'_0 = -\rho/12 = a_0 \quad (124d)$$

The bounds on X are stated immediately in terms of those previously stated for ξ_1 in Eq. (123a):

$$0 < X < -a'_0/a'_1 \quad (124e)$$

A series of numerical experiments was performed to establish the most efficient manner of solving for this root. The techniques considered were:

- (a) Interval halving,
- (b) regula falsi (the n^{th} iterate is the inverse linear interpolate between iterates $n-1$ and $n-2$),
- (c) Newton-Raphson,
- (d) The analogue of Newton-Raphson which uses the first and second derivatives.

Numerical experiments showed that the expected gain in the rate of convergence with the higher order methods (c and d) did not occur over much of the (T, ρ) domain of interest. This would clearly not be true if an initial estimate sufficiently close to the final iterate could be found. However, the estimates which were used were not always within this desirable domain:

1. If $Z_1 \equiv (-a'_{10})/a'_1 \leq 1$, $X < Z_1$.
2. If $Z_1 > 1$, and $a'_j \neq 0$ where $j = 9, 8, 7, \dots, 1$ (and $a'_j \neq 0$ for $j = 9, 8, 7, \dots, 2$), $Z_2 \equiv 1 + \left| -a'_0/a'_j \right|^{1/j}$ and $X < Z_2$.
3. If $Z_2 < 2$, $Z_3 \equiv Z_2 - 1$ and $X < Z_3$.

Thus, techniques (c) and (d) were often useless.

For a tenth order polynomial with the constant term as the only negative coefficient, an upper bound on the root is

$$X < 1 + \left| a'_0/a'_{10} \right|^{1/10}$$

However, numerical experiments have shown that the bound Z_2 given above is better; this is easily understood when one examines the behavior of the functions $\left| (G_\alpha/RT) \right| 1 \leq \alpha \leq 10$, for ξ_9 always dominates ξ_{10} .

Technique (c) requires almost twice as much computation as techniques (a) and (b), and technique (d) requires almost three times as much computation. Thus, if second or third order convergence is not rapidly achieved, one is much better off with the lower order methods. For this reason, a careful study of the best way to use techniques (a) and (b) was performed.

Regula falsi and interval halving both require computation of $f(X^{(n)})$ where $X^{(n)}$ is the n^{th} iterate. In addition, interval halving requires comparison of $f(X^{(n)})$ with the upper and lower bounds determined at the $(n-1)^{\text{st}}$ iteration stage. If $f(X^{(n)}) > 0$, $X^{(n)}$ replaces the previous upper bound. If $f(X^{(n)}) < 0$, $X^{(n)}$ replaces the previous lower bound. If $|f(X^{(n)})| < \epsilon$, we are sufficiently close to the desired answer and can use $X^{(n)}$ as our final iterate. This process is clearly convergent; approximately

three iterations are required to reduce the error by a factor of 10. Regula falsi will permit a much faster asymptotic convergence rate; however, the initial rate of convergence may be much slower. Therefore, interval halving is used until the criterion

$$\left| \sum_{\alpha=1}^{\alpha=10} a_{\alpha} \left[X^{(k)} \right]^{\alpha} \right| < + 0.1 (\rho/12) \quad (125)$$

is met; from this iteration stage on, regula falsi is used until $|f(X^{(n)})| < \delta$. However, if regula falsi predicts a new iterate outside the current upper and lower bounds, interval halving is used at that iteration stage. The upper and lower bounds are updated at every iteration stage. Twenty-five iterations are allowed; if the accuracy test is not satisfied, the cell CARBNZ (8) is set to 97.0297 and a return is made to the calling program.

When X has been determined to the desired accuracy, the ξ_{α} , $\alpha = 1, \dots, 10$ are computed using Eqs. (115) and (116).

5.4. THERMODYNAMIC VARIABLES

The thermodynamic variables computed are:

$$P = RT \sum_{\alpha} \xi_{\alpha} \quad (126)$$

$$\left(\frac{\partial P}{\partial T} \right)_{\tau} = RT \sum_{\alpha} \left(\frac{d\xi_{\alpha}}{dT} \right)_{\tau} + \frac{P}{T} \quad (127)$$

$$\left(\frac{dP}{d\tau} \right)_{\tau} = RT \sum_{\alpha} \left(\frac{d\xi_{\alpha}}{d\tau} \right)_{\tau} \quad (128)$$

$$E_{sp} = \tau \sum_{\alpha} E_{\alpha} \xi_{\alpha} = \sum_{\alpha} E_{\alpha} \xi_{\alpha} / (12N \sum_{\alpha} \xi_{\alpha}) \quad (129)$$

$$\left(\frac{\partial E_{sp}}{\partial \tau} \right)_{\tau} = \tau \left[\sum_{\alpha} E_{\alpha} \left(\frac{\partial \xi_{\alpha}}{\partial \tau} \right)_{\tau} - 12 E_{sp} \left[\sum_{\alpha} \alpha \left(\frac{\partial \xi_{\alpha}}{\partial \tau} \right)_{\tau} \right] \right] \quad (130)$$

$$\left(\frac{\partial E_{sp}}{\partial T}\right)_\tau = \tau \left\{ \sum_\alpha \left[E_\alpha \left(\frac{\partial \xi_\alpha}{\partial \tau}\right) + \left(\frac{dE_\alpha}{dT}\right) \xi_\alpha \right] - 12 E_{sp} \right. \\ \left. \left[\sum_\alpha \alpha \left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau \right] \right\} \quad (131)$$

$$E_\alpha = RT \left[\frac{H_\alpha}{RT} - 1 \right] \quad (132)$$

$$\frac{dE_\alpha}{dT} = R \left[\frac{H_\alpha}{RT} - 1 \right] + RT \left(\frac{dH_\alpha/RT}{dT} \right) \quad (133)$$

where

$$RT \left(\frac{dH_\alpha/RT}{dT} \right) = R \left[\sum_{j=2}^{j=4} (j-1) A_{\alpha,j} T^{j-1} \right] - \frac{H_\alpha^0(0)}{RT} \quad (134)$$

so

$$\frac{dE_\alpha}{dT} = R \left[\sum_{j=1}^{j=4} (j) A_{\alpha,j} T^{(j-1)} - 1 \right] \quad (135)$$

$$\left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau = \xi_\alpha \left\{ \alpha (\xi_1)^{-1} \left(\frac{d\xi_1}{dT}\right)_\tau + T^{-1} \left[\alpha \left(T \frac{dG/RT}{dT}\right) \right. \right. \\ \left. \left. - \left(T \frac{dG_\alpha/RT}{dT}\right) + (\alpha - 1) \right] \right\} \quad (136)$$

$$\left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T = \alpha \left(\frac{\partial \xi_1}{\partial T}\right)_\tau \frac{\xi_\alpha}{\xi_1} \quad (137)$$

$$\left(\frac{\partial \xi_1}{\partial T}\right)_\tau = \xi_1 T^{-1} \left\{ \left[(\rho/12) - (\sum_\alpha \alpha \xi_\alpha \left[\alpha \left(T \frac{dG_1/RT}{dT}\right) \right. \right. \right. \right. \right. \\ \left. \left. \left. - \left(T \frac{dG_\alpha/RT}{dT}\right) \right] / \sum_\alpha \alpha^2 \xi_\alpha \right] - 1 \right\} \quad (138)$$

$$\left(\frac{\partial \xi_1}{\partial \tau}\right)_T = -(\rho^2/12) \xi_1 / \sum_\alpha \alpha^2 \xi_\alpha \quad (139)$$

$$\bar{N} = \sum_\alpha \alpha \xi_\alpha / \sum_\alpha \xi_\alpha \quad (140a)$$

$$\left(\frac{\partial \bar{N}}{\partial \tau}\right)_T = \left[\alpha \left(\frac{d\xi_\alpha}{d\tau} \right)_T / \sum_\alpha \xi_\alpha \right] + \left[\left(\frac{\partial \xi_\alpha}{\partial \tau} \right)_T (-\rho/12) / (\sum_\alpha \xi_\alpha)^2 \right] \quad (140b)$$

$$\left(\frac{\partial \bar{N}}{\partial T}\right)_\tau = \left[\alpha \left(\frac{\partial \xi_\alpha}{\partial T} \right)_\tau / \sum_\alpha \xi_\alpha \right] + \left[\left(\frac{\partial \xi_\alpha}{\partial T} \right)_\tau (-\rho/12) / (\sum_\alpha \xi_\alpha)^2 \right] \quad (140c)$$

5.5. THERMODYNAMICS AND COMPOSITIONS ABOVE 7000° K

Reliable data for the free energies and enthalpies for the species C_α , $2 \leq \alpha \leq 10$, have not yet been calculated above 7000° K. However, at all densities of interest the system composition can be calculated at 7000° K. Further, we know that, at all densities of interest, at a sufficiently high temperature there will only be carbon atoms present. In order to bridge this gap, the following equations are assumed (in which we denote all quantities relevant to the point $(\tau, T_o \equiv 7000^\circ \text{K})$ with the subscript "o" and all quantities at the upper limiting value with the subscript "u"):

$$\bar{N} = \bar{N}_o + (T - T_o) \left(\frac{\partial \bar{N}_o}{\partial T} \right)_\tau \quad (141)$$

$$\left(\frac{\partial \bar{N}}{\partial T} \right)_\tau = \left(\frac{\partial \bar{N}_o}{\partial T} \right)_\tau \quad (142)$$

$$\bar{N}_u \equiv 1 \quad (143)$$

$$T_u = T_o - (\bar{N}_o - \bar{N}_u) / \left(\frac{\partial \bar{N}_o}{\partial T} \right)_\tau \quad (144)$$

Thus, since T_o and $\bar{N}_u$ are constants,

$$(\partial T_u / \partial \tau)_T = - \left(\frac{\partial \bar{N}}{\partial \tau} \right)_T / \left(\partial \bar{N}_o / \partial T \right)_\tau \quad (145)$$

$$E = (\bar{N})^{-1} \bar{N}_o E_o + (T_o - T)(T_u - T_o)^{-1} (\bar{N}_o E_o - E_u) \quad (146)$$

$$E_u = E_1(T_u) \quad (147)$$

$$\left(\frac{\partial E}{\partial T}\right)_T = \left| \left| -E \left(\frac{\partial \bar{N}}{\partial T}\right)_T - (T_u - T_o)^{-1} (\bar{N}_o E_o - E_1) \right| / \bar{N} \right| - \frac{3R}{2\bar{N}} \quad (148)$$

$$\left(\frac{\partial E}{\partial \tau}\right)_T = - \left(\frac{\partial \bar{N}}{\partial \tau}\right)_T \frac{E}{\bar{N}} + (\bar{N})^{-1} \left| \left| \left(\frac{\partial \bar{N}_o}{\partial \tau}\right)_T E_o + \bar{N}_o \right| \right| \quad (149)$$

$$\left(\frac{\partial E_o}{\partial \tau}\right)_T \left| 1 + \frac{T_o - T}{T_u - T_o} \right|$$

$$\frac{[\bar{N}E - \bar{N}_o E_o]}{(T_u - T_o)} \left(\frac{\partial T_u}{\partial \tau}\right)_T$$

To be consistent with the technique used above 7000° K, if $T > T_u$, we assume that

$$\xi_1 = \rho/12 \quad (150)$$

$$\left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T = \left(\frac{\partial \xi_\alpha}{\partial T}\right)_T = \left(\frac{\partial E_{sp}}{\partial \tau}\right)_T = 0 \quad (151)$$

$$\bar{N} = 1 \quad (152)$$

$$P = RT(\rho/12) \quad (153)$$

$$E_{sp} = E_1/12 \quad (154)$$

$$(\partial E_{sp}/\partial T)_T = \frac{dE_1}{dT} / 12 \quad (155)$$

$$\left(\frac{\partial P}{\partial T}\right)_T = P/T \quad (156)$$

$$\left(\frac{\partial P}{\partial \tau}\right)_T = -P/\tau \quad (157)$$

5. 6. LOW TEMPERATURE RESULTS

Preliminary numerical calculations indicated that for $T < 1000^\circ \text{K}$, it is satisfactory to assume that

$$\xi_9 = \rho / 108 \quad (158)$$

$$N = 9 \quad (159)$$

$$\xi_{\alpha \neq 9} = 0 \quad (160)$$

$$\left(\frac{\partial P}{\partial T} \right)_\tau = P/T \quad (161)$$

$$\left(\frac{\partial E_{sp}}{\partial T} \right)_\tau = \frac{dE_9/dT}{108} \quad (162)$$

$$\left(\frac{\partial P}{\partial \tau} \right)_T = - P/\tau \quad (163)$$

$$P = \frac{RT}{108\tau} \quad (164)$$

$$E_{sp} = E_9/108 \quad (165)$$

$$\left(\frac{\partial \xi_\alpha}{\partial \tau} \right)_T = \left(\frac{\partial \xi_\alpha}{\partial T} \right)_\tau = \left(\frac{\partial E_{sp}}{\partial \tau} \right)_T = 0 \quad (166)$$

5. 7. COEFFICIENTS OF FITS TO THERMODYNAMIC FUNCTIONS

Table IV contains the $A_{\alpha,j}$, $\alpha = 1 \dots 10$, $j = 1 \dots 6$ used to fit

$$\begin{aligned} \left(\frac{G^0(T) - H^0(0)}{RT} \right)_\alpha &= A_{\alpha,1} (1 - \ln T) - A_{\alpha,2} T - A_{\alpha,3} \frac{T^2}{2} \\ &\quad - A_{\alpha,4} \frac{T^3}{3} - A_{\alpha,5} \frac{T^4}{4} - A_{\alpha,6} \end{aligned} \quad (167)$$

Table IV
IDEAL GAS THERMODYNAMIC FUNCTIONS FOR C_a

C_a	$A_{a,1}$	$A_{a,2}$	$A_{a,3}$	$A_{a,4}$	$A_{a,5}$	$A_{a,0}$	$\Delta H^0(O)$ (cal/mole)	Range of Fit ($\times 10^3$ °K)
C	2.616739-00	-1.075931-04	3.860104-08	-4.508465-12	1.825810-16	4.114400-00	1.69580-05	0.3-6
C ₂	4.608300-00	-4.309474-04	2.553405-07	-5.060553-11	3.488775-15	-1.851498-00	1.97000-05	0.3-0
C ₃	4.061127-00	2.501656-03	-1.491669-06	5.338941-10	-7.682421-14	1.015292-00	1.88104-05	0.3-2
C ₄	5.670072-00	2.941491-03	-1.583799-06	5.873590-10	-9.296338-14	-4.252196-00	2.40500-05	0.3-2
C ₅	7.279097-00	3.381009-03	-1.675500-06	6.405815-10	-1.090542-13	-1.310398-01	2.40298-05	0.3-2
C ₆	8.887801-00	3.821788-03	-1.768910-06	6.947653-10	-1.253361-13	-1.837056-01	2.87000-05	0.3-2
C ₇	1.049661-01	4.262157-03	-1.861752-06	7.486224-10	-1.415519-13	-2.722151-01	2.8500-05	0.3-2
C ₈	1.210560-01	4.701797-03	-1.953615-06	8.019347-10	-1.576603-13	-3.248919-01	3.39000-05	0.3-2
C ₉	1.371412-01	5.143305-03	-2.048004-06	8.566633-10	-1.740497-13	-4.133905-01	3.34000-05	0.3-2
C ₁₀	1.532298-01	5.583472-03	-2.140608-06	9.104058-10	-1.902459-12	-4.660623-01	3.93000-05	0.3-2
C ₃	4.577017-00	1.135460-03	-2.083718-07	1.709699-11	-4.957820-16	-9.902669-01	1.88104-05	1.5-0
C ₄	6.077354-00	1.721887-03	-3.159955-07	2.336921-11	-3.583350-16	-5.883521-00	2.40500-05	1.5-0
C ₅	7.577380-00	2.308765-03	-4.238504-07	2.969125-11	-2.247249-16	-1.436729-01	2.40298-05	1.5-0
C ₆	9.077268-00	2.895836-03	-5.318001-07	3.603287-11	-9.256675-17	-1.926238-01	2.87000-05	1.5-0
C ₇	1.057812-01	3.481519-03	-6.390447-07	4.222393-11	5.109466-17	-2.774611-01	2.87000-05	1.5-0
C ₈	1.207925-01	4.066801-03	-7.460864-07	4.837172-11	1.980545-16	-3.264719-01	3.39000-05	1.5-0
C ₉	1.357901-01	4.654071-03	-8.541425-07	5.473711-11	3.283272-16	-4.112566-01	3.34000-05	1.5-0
C ₁₀	1.507952-01	5.240247-03	-9.616407-07	6.098287-11	4.677693-16	-4.602377-01	3.93000-05	1.5-0

and

$$\left(\frac{H^0(T) - H^0(0)}{RT} \right)_\alpha = A_{\alpha,1} + A_{\alpha,2} T + A_{\alpha,3} T^2 + A_{\alpha,4} T^3 + A_{\alpha,5} T^4 \quad (168)$$

(The above equations are the same as Eqs. (118) and (119), respectively.)

5.8. INTERFACE OF CMOL WITH OTHER EQUATION OF STATE SUBROUTINES

In the SPUTTER code, the generalized ionic equation of state subroutines "EIONX"* are designed to interface with molecular equations of state in the following manner:

1. All ionization contributions are calculated by the EIONX routine
2. All translation contributions are calculated by the EIONX routine. If a molecular E. O. S. is not called by the EIONX routine, EIONX sets $\bar{N} = 1$, $(\partial \bar{N} / \partial \theta)_T = 0$, and $(\partial \bar{N} / \partial \tau)_\theta = 0$, where θ is the temperature in ev (see below). If a molecular E. O. S. is called, these quantities are calculated by that routine and returned to EIONX to be used.
3. The reference state for energy is assumed to contain only atoms.

The equations which have been presented have included the translational contributions, and the temperature scale has been in degrees Kelvin. The code actually uses a temperature scale in ev ($1 \text{ ev} \cong 11605^\circ \text{K}$). The translational contributions to E and $(\partial E / \partial \theta)_T$ are subtracted before these quantities are passed on by CMOL to the EIONX code. This gives

$$E_{\text{EIONX input}} = E_{\text{CMOL}} - \frac{3}{2} RT C / \bar{N} - E_0 \quad (169)$$

$$\left(\frac{\partial E}{\partial \theta} \right)_T, \text{ EIONX input} = \left(\frac{\partial E}{\partial \theta} \right)_T, \text{ CMOL} - C^1 / \bar{N} \quad (170)$$

* See Section III of this report.

where C and C^1 are the appropriate conversion factors. The corresponding factor does not have to be subtracted out of P since only $\bar{N}$ is transferred to the EIONX code. The derivatives of P that are calculated and transferred to the EIONX code also exclude the translational contribution since they are calculated as

$$\left(\frac{\partial P}{\partial \theta}\right)_\tau = \left(\frac{\partial P}{\partial \bar{N}}\right)_{T,\tau} \left(\frac{\partial \bar{N}}{\partial T}\right)_\tau \left(\frac{\partial T}{\partial \theta}\right) \quad (171)$$

$$\left(\frac{\partial P}{\partial \tau}\right)_\theta = \left(\frac{\partial P}{\partial \bar{N}}\right)_{T,\tau} \left(\frac{\partial \bar{N}}{\partial \tau}\right)_T \quad (172)$$

5.9. FUTURE IMPROVEMENTS

Several of the assumptions will be replaced by a more extended treatment as soon as possible:

1. A program is under way to (a) compute high temperature partition functions, and (b) fit the resultant free energies and enthalpies in a thermodynamically consistent least-square manner. As soon as this is done, the "bridging" section will be removed from the code. This will be done initially for C_α , $1 \leq \alpha \leq 10$.
2. Following this, an attempt will be made to estimate the thermodynamic quantities for C_β , $11 \leq \beta \leq 20$. Calculations with the present system show that $\xi_9 \gg \xi_\alpha \neq 9$ at $T \leq 1000^\circ \text{K}$. However, this is only an artifice due to the exclusion of $C_{\beta > 10}$ from the calculations. Inclusion of these species is expected to change the results at low temperatures so that $\bar{N} > 9$ at low temperatures.
3. An attempt will be made to add "real gas" correction factors for the various species.

5. 10. VARIABLE NAMES USED IN CMOL

1. A(10)	$A_{\alpha, 1}; 1 \leq \alpha \leq 10$ in Eq. (167) for $T \geq 1750^\circ \text{K}$.
2. A2(10)	$A_{\alpha, 1}; 1 \leq \alpha \leq 10$ in Eq. (167); for $T < 1750^\circ \text{K}$.
3. B(10)	$A_{\alpha, 2}; 1 \leq \alpha \leq 10$ in Eq. (167); for $T \geq 1750^\circ \text{K}$.
4. B2(10)	$A_{\alpha, 2}; 1 \leq \alpha \leq 10$ in Eq. (167); for $T < 1750^\circ \text{K}$.
5. BACK1	Previous Iterate.
6. C(10)	$A_{\alpha, 3}; 1 \leq \alpha \leq 10$ in Eq. (167); $T \geq 1750^\circ \text{K}$.
7. C2(10)	$A_{\alpha, 3}; 1 \leq \alpha \leq 10$ in Eq. (167); $T < 1750^\circ \text{K}$.
8. CARBNZ(10)	Routine out put array; see section 5. 9.
9. COEF(11)	$a_{\alpha}^1; 1 \leq \alpha \leq 11$; see Eqs. (124c) and (124d).
10. CONST	$a_{11}^1 = -\rho/12$; see Eqs. (122e) and (124d).
11. D(10)	$A_{\alpha, 4}; 1 \leq \alpha \leq 10$ in Eq. (167); $T \geq 1750^\circ \text{K}$.
12. DZ(10)	$A_{\alpha, 4}; 1 \leq \alpha \leq 10$ in Eq. (167); $T < 1750^\circ \text{K}$.
13. DCONDT	$\Sigma_{\alpha} (\partial \xi_{\alpha} / \partial T)_{\tau}$.
14. DEDT(10)	$dE_{\alpha}/dT = R \left[A_{\alpha, 1} - 1 + \Sigma_{j=2}^{j=5} \alpha A_{\alpha, j} T^j \right]$.
15. DEDTAU	$(\partial E / \partial \tau)_{\theta}$.
16. DEDTHT	$(\partial E / \partial \theta)_{\tau}$.
17. DELH(10)	$H_{\alpha}^0(0)$.
18. DNNDT	$(\partial N / \partial T)_{\tau}$.
19. DNNDTAU	$(\partial N / \partial \tau)_{T}$.
20. DPDN	$(\partial P / \partial N)_{T, \rho}$.
21. DPOTAU	$(\partial P / \partial \tau)_{\theta}$.
22. DPDTHT	$(\partial P / \partial \theta)_{\tau}$.

23. DREACT(10) $-\alpha H_1^0(T)/RT - H_\alpha^0(T)/RT.$
24. DXDT(10) $(\partial \xi_\alpha / \partial T) \tau; 1 \leq \alpha \leq 10.$
25. DXDTAU(10) $(\partial \xi_\alpha / \partial \tau) T; 1 \leq \alpha \leq 10.$
26. E(10) $A_{\alpha, 5}; 1 \leq \alpha \leq 10 \text{ in Eq. (167); } T < 1750^\circ \text{K.}$
27. E2(10) $A_{\alpha, 5}; 1 \leq \alpha \leq 10 \text{ in Eq. (167); } T < 1750^\circ \text{K.}$
28. EDIF $E_o \bar{N}_o - E_1.$
29. EION(20) EIONX input - out put array; see Section III of this report.
30. ENERGY Specific energy in ergs/g; see Eq. (129).
31. E0 $E_o = E(7000^\circ \text{K}, \rho).$
32. E0NBAR $E_o \bar{N}_o.$
33. ESPECZ(10) $E_\alpha^0(T) = H_\alpha^0(T) - RT.$
34. EI $E(T_u).$
35. EZERO Assumed specific energy of atomization (of graphite) ; 5.98566 Ell ergs/g.
36. FK(10) $A_{\alpha, 6}; 1 \leq \alpha \leq 10 \text{ in Eq. (167); } T \geq 1750^\circ \text{K.}$
37. FK2(10) $A_{\alpha, 6}; 1 \leq \alpha \leq 10 \text{ in Eq. (167); } T < 1750^\circ \text{K.}$
38. FOFX See Eq. (11e).
39. FOFXM1 f (previous iterate); see Eq. (122e).
40. FRENRG(10) $[G_\alpha^0(T)] RT; 1 \leq \alpha \leq 10.$
41. HSPECZ(10) $H_\alpha^0(T).$
42. NBAR Mean number of atoms per molecule; see Eq. (140a).
43. NBAR0 $\bar{N}_o = \bar{N}(7000^\circ \text{K}, \rho).$

44.	PRESHR	P ; see Eq. (126).
45.	RTKEL	RT with $R = 1.98726 \text{ cal/mole-}^\circ\text{K}$.
46.	R2TKEL	RT with $R = 82.06 \text{ cm}^3/\text{atm-}^\circ\text{K}$.
47.	SUMCON	$\sum_{\alpha} \xi_{\alpha}$.
48.	SUMNRG	$\sum_{\alpha} \xi_{\alpha} E_{\alpha}^{\circ}(T)$.
49.	SUM1DX	$-\left[\sum_{\alpha} \alpha \xi_{\alpha} \left[\alpha H_{\alpha}^{\circ}(T) + H_{\alpha}^{\circ}(T) \right] \right] / RT$.
50.	SUM2DX	$\sum_{\alpha} \alpha^2 \xi_{\alpha}$.
51.	SUM3DX	$\sum_{\alpha} (\partial \xi_{\alpha} / \partial \tau) T$.
52.	SUM4DX	$\sum_{\alpha} (\partial \xi_{\alpha} / \partial \tau) T \left[E_{\alpha}^{\circ}(T) \right]$.
53.	SUM5DX	$\sum_{\alpha} (\partial \xi_{\alpha} / \partial T) \tau \left[E_{\alpha}^{\circ}(T) \right]$.
54.	SUM6DX	$\sum_{\alpha} \xi_{\alpha} (dE_{\alpha} / dT)$.
55.	SUM7DX	$\sum_{\alpha} \alpha (\partial \xi_{\alpha} / \partial T) \tau$.
56.	SUM8DX	$\sum_{\alpha} \alpha (\partial \xi_{\alpha} / d\tau) T$.
57.	T	Storage cell for T in computations above 7000°K .
58.	TAU	Specific volume in cm^3/g .
59.	TDGDT(10)	$-[H_{\alpha}^{\circ}(T)] / RT$.
60.	TDIF	$T - 7000^\circ\text{K}$.
61.	TKEL	Temperature in $^\circ\text{K}$.
62.	TKELN	$\ln T$.
63.	TUPM7	$T_u - 7000^\circ\text{K}$.
64.	UPPERT	t_u ; see Eq. (144).
65.	X	$X = \xi_1 e^{G_1/RT} / RT$.
66.	XSET(10)	ξ_{α} ; $1 \leq \alpha \leq 10$.

- | | | |
|-----|------|---|
| 67. | XTRY | <u>Regula falsi</u> prediction of next iterate in Eq. (124a). |
| 68. | Y | Lower bound on X; $0 \leq Y$. |
| 69. | Z | Upper bound on X; $Z \leq \phi / 12)(RT)(e^{G_1/RT})$. |

5.11. APPENDIX: LISTING OF CMOL

WIT FOR HESTER/A,HESTER/A,HESTER/A1

SUBROUTINE CMOL(X1, X2, X3)

C ENERGY ZERO IS ATOMIZED CARBON (ENERGY=5.98566E11 ERGS/G.)

C LAST COMPILED DECEMBER 12, 1965

C X1 IS TAU IN G/CC

C X2 IS THETA IN EV

C X3 .LT. 0. FORCES TRANSLATIONAL-ONLY COMPUTATION

C X3 .GT. 0. FORCES CUTOFF AT 1500. DEGREES KELVIN

C

COMMON/LMS/EION(20)

COMMON /LMSG/CARBENZ(10)

REAL NBAR

REAL NBARO

EQUIVALENCE(OLDNRG,EION(15)), (NBAR,EION(17))

DIMENSION A(10),B(10),C(10),D(10),E(10),FK(10),DELH(10),FRENRG(10),ESPECZ(10),XSET(10),COEF(11)

EQUIVALENCE(COEF(11),CONST)

DIMENSION HSPECZ(10),A2(10),R2(10),C2(10),D2(10),E2(10),FK2(10)

DIMENSION TGGDT(10),DEDT(10),DXDT(10),DXDTAU(10),DREACT(10)

DATA A/2.6167394,4.6083,4.5770171,6.0773535,7.57738,9.0772684,10.5178120,12.07925,13.579007,15.07952/

DATA B/-1.0759307E-4,-4.3094741E-4,1.1354603E-3,1.7218871E-3,2.30817653E-3,2.8958363E-3,3.4815191E-3,4.0668009E-3,4.6540713E-3,5.24022472E-3/

DATA C/3.8601044E-8,2.5534049E-7,-2.0837176E-7,-3.1599548E-7,-4.23185044E-7,-5.3180008E-7,-6.3904472E-7,-7.4600642E-7,-8.5414254E-7,-29.6164066E-7/

DATA D/-4.5084646E-12,-5.0605532E-11,1.7096995E-11,2.3369207E-11,2.1.9691251E-11,3.6032875E-11,4.2223928E-11,4.8371722E-11,5.4737111E-211,6.0982872E-11/

DATA E/1.8258099E-16,3.4887751E-15,-4.9578196E-16,-3.5P33503E-16,-12.2472492E-16,-9.2566753E-17,5.1094666E-17,1.9305455E-16,3.28327212E-16,4.677693E-16/

DATA FK/4.1144,-1.8514979,-.99026691,-5.8835212,-14.367287,-19.2621383,-27.746115,-32.647187,-41.125658,-46.023767/

DATA DELH/1.6958E5,1.97E5,1.88104E5,2.405E5,2.40298E5,2.87E5,2.87E15,3.39E5,3.34E5,3.93E5/

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DATA A2/2.6167394,4.6083,4.0611273,5.6700722,7.2790966,8.8871007,10.496602,12.105599,13.714116,15.322981/

DATA B2/-1.0759307E-4,-4.3094741E-4,2.5016562E-3,2.9414906E-3,3.38110092E-3,3.8217876E-3,

2 4.2621570E-3,4.7017969E-3,5.1433051E-3,5.5834718E-3/

DATA C2/3.8601044E-8,2.5534049E-7,-1.491669E-6,-1.5837991E-6,1-1.6755E-6,-1.7689104E-6,

2 -1.8617521E-6,-1.9536149E-6,-2.0480045E-6,-2.1406085E-6/

DATA D2/-4.5084646E-12,-5.0605532E-11,5.3389410E-10,5.8735896E-10,16.4058152E-10,6.9476531E-10,7.4862238E-10,8.0193467E-10,8.5666328E-2-10,9.1040577E-10/

DATA E2/1.8258099E-16,3.4887751E-15,-7.6824207E-14,-9.2963380E-14,1-1.0905419E-13,-1.2533614E-13,-1.4155192E-13,-1.5766034E-13,-1.74024966E-13,-1.9024594E-13/

DATA FK2/4.1144,-1.8514979,1.0152922,-4.2521956,-13.103985,-18.370156,-27.221515,-32.489186,-41.339045,-46.606231/

C

C

EQUIVALENCE

(PRESHR,CARBENZ(2)),(DEDTAU,CARBENZ(3)),

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1(DEDTHT,CARBENZ(4)),(OPDTAU,CARBENZ(5)),(OPDTHT,CARBENZ(6)),
2(ENERGY,CARBENZ(1))

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TAU=      X1
EZERO=    5.98566E11
      IF(X3 .LT. 0. .AND. A(1) .NE.2.5) GO TO 10

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11 CONTINUE
      IF( TAU.LT.1.E-1) GO TO 900
      T=      -1.
      UPPERT=  J.
      CONST=  -1./(12.*TAU)
      TKEL=   11605.4 * X2
      IF(TKEL.GT.7.E3) GO TO 550

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551 CONTINUE

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      TKELN=  ALOG(TKEL)
      RTKEL=  1.98726*TKEL
      R2TKEL= 82.06*TKEL

```

C

1.98726 IS THE GAS CONSTANT IN CALORIES/MOLE/DEGREE KELVIN

C

82.06 IS THE GAS CONSTANT IN CC.-ATMOSPHERES/MOLE/DEGREE KELVIN

DO 201 I=1,10

IF (TKEL.LT.1750.) GO TO 400

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      FRENRG(I)= A(I)*(1.- TKELN ) -(FK(I)+TKEL*(B(I)+TKEL*(C(I)'2.+
1      TKEL*(D(I)/3.+TKEL*(E(I)/4. ))) +DELH(I)/RTKEL

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      DEDT(I)= 1.98726*( A(I)-1.+TKEL*(2.*B(I)+TKEL*(3.*C(I)+TKEL*
1      (4.*D(I)+TKEL*5.*E(I) )))

```

401 CONTINUE

FI=

I

COEF(I)= FI*EXP(-FRENRG(I))/R2TKEL

201 CONTINUE

IF(TKEL.LT.1.E3) GO TO 650

IF(X3 .GT. 0. .AND. TKEL .LT. 1.5E3) GO TO 650

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THE LOWER BOUND ON X IS 0.

Y= 0.

C

DEVELOP UPPER BOUND TO X

Z= -CONST/COEF(1)

IF (Z.LE. 1.) GO TO 604

602 CONTINUE

DO 221 I=1,9

J= 10-I

IF(COEF(J).NE.0.) GO TO 222

221 CONTINUE

222 CONTINUE

IF(COEF(1).EQ.0.) CALL UNCLE

Z= 1.+((-CONST/COEF(J))**(1./FLOAT(J)))

IF (Z.LT. 2.) Z= Z-1.

604 CONTINUE

X= Z

BACK1= 0.

XTRY= -1.E-38

F OF XM1=0.

211 CONTINUE

DO 203 J= 1,25

F OF X = COEF(10)

DO 204 I=1,9

III= 10-I

```

      F OF X      F OF X * X + COEF(III)
204 CONTINUE
      F OF X =    F OF X * X + CONST
      FJ=        J
      IF (F OF X .GT. 0.) Z= X
      IF (F OF X .LT. 0.) Y= X
      IF (J.EQ.1.AND.FOFX.GT.(-2.*CONST)) GO TO 212
      IF (ABS(F OF X) .LT. (1.E- 6*(- CONST )) ) GO TO 205
      IF (ABS(FOFX).GE.(-.1*CONST)) GO TO 206
      IF ( FOFX.EQ.FOFXM1) GO TO 206
209 CONTINUE
      IF (J.GT.1) XTRY =  X - (X-BACK1)/(FOFX-FOFXM1)*F OF X
206 CONTINUE
      BACK1=      X
      X=          (Z+Y)*.5
      IF ( F OF X .EQ. FOFXM1 ) GO TO 208
      IF (XTRY.GE.Y.AND.XTRY.LE.Z.AND.ABS(FOFX).LT.(-.1*CONST)) X=XTRY
208 CONTINUE
      FOFXM1=F OF X
203 CONTINUE
      J=          J-1
297 CONTINUE
      CARBNZ(8)= 97.0297
      RETURN
205 CONTINUE
      FJ=        J
C      PRESSURE
      SUMCON=    0.
      DO 301 I=1,10
      XSET(I)=    0.
      IF (COEF(I).EQ.0.) GO TO 301
      FI=        I
      XSET(I)= (COEF(I)/FI*X**(FI/2.))*X**(FI/2.)
      SUMCON=    SUMCON + XSET(I)
301 CONTINUE
      NBAR=      -CONST /SUMCON
      PRESHR=    1.01325E6*R2TKEL*SUMCON
C      ENERGY
      INITAL=    1
      LAST=      10
      4 CONTINUE
      SUMNRG=    0.
      DO 302 I=INITAL, LAST
      IF (TKEL.LT.1750.)GO TO 402
      HSPECZ(I)= RTKEL*(A(I)+TKEL*(B(I)+TKEL*(C(I)+TKEL*(D(I)+TKEL*(E(I)
1          )))))+DELH(I)
403 CONTINUE
      ESPECZ(I)= HSPECZ(I) - RTKEL
      SUMNRG=    SUMNRG + XSET(I)*ESPECZ(I)
302 CONTINUE
      ENERGY=   TAU*SUMNRG*4.185E7
      IF (TKEL.LT.1.E3) GO TO 601
      SUM1DX=    0.
      SUM2DX=    0.
      DO 500 I=1,10
      FI=        I
      TDGDT(I)=  -HSPECZ(I)/RTKEL

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DREACT(I)= F1*TDGDT(1)-TDGDT(I)
SUM1DX= SUM1DX+XSET(I)*F1*DREACT(I)
SUM2DX= SUM2DX + F1*F1*XSET(I)
500 CONTINUE
DXDT(1)= -XSET(1)*(( CONST +SUM1DX)/SUM2DX+1.)/TKEL
DXDTAU(1)= -XSET(1)/(12.*TAU*TAU*SUM2DX)
DO 501 I=2,10
FI=1
DXDT(I)= XSET(I)*(FI/XSET(1)*DXDT(1)+(DREACT(I)+FI-1.)/TKEL)
DXDTAU(I)= FI*DXDTAU(1)/XSET(1)*XSET(I)
501 CONTINUE
DCONDT= 0.
SUM3DX= 0.
SUM4DX= 0.
SUM5DX= 0.
SUM6DX= 0.
SUM7DX= 0.
SUM8DX= 0.
DO 502 I=1,10
FI=I
DCONDT= DCONDT + DXDT(I)
SUM3DX= SUM3DX+DXDTAU(I)
SUM4DX= SUM4DX+DXDTAU(I)*ESPECZ(I)
SUM5DX= SUM5DX+ESPECZ(I)*DXDT(I)
SUM6DX= SUM6DX+DEDT(I)*XSET(I)
SUM7DX= SUM7DX+FI*DXDT(I)
SUM8DX= SUM8DX+FI*DXDTAU(I)
502 CONTINUE
DNDT= SUM7DX/SUMCON+DCONDT* CONST /SUMCON/SUMCON
DNDAU= SUM8DX/SUMCON+SUM3DX* CONST /SUMCON/SUMCON
DPDN= -PRESHR/NBAR
DPDTAU= DPN * DNDAU
DPDHT= DPN * DNDT * 11605.4
DEDTAU= 4.185E7*TAU*(SUM4DX+SUMNRG*SUM8DX/CONST)
DEDTHT= 4.85686E11*TAU*(SUM5DX+SUM6DX+SUMNRG*SUM7DX/COEF(11))
IF(T.NE.(-1.)) GO TO 503
GO TO 901
650 CONTINUE
PRESHR= -1.125833E5*R2TKEL*CONST
INITAL= 9
LAST= 9
NBAR= 9.
XSET(9)= -CONST/9.
GO TO 4
601 CONTINUE
DPDTAU= 0.
DPDHT= 0.
DEDTAU= 0.
DEDTHT= 4.4971E9*DEDT(9)
GO TO 901
212 CONTINUE
X= .1*X
GO TO 211
400 CONTINUE
FRENRG(I)= A2(I)*(1.-TKELN)-(FK2(I)+TKEL*(B2(I)+TKEL*(C2(I)*.5+TKE
1 L*(B2(I)/3.+TKEL*E2(I)*.25))))+DELH(I)/RTKEL
DEDT(I)= 1.98726*( A2(I)-1.+TKEL*(2.*B2(I)+TKEL*(3.*C2(I)+TKEL*

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1          (4.*D2(1)+TKEL*5.*E2(1) )))
GO TO 401
402 HSPCZ(1)= RTKEL*(A2(1)+TKEL*(B2(1)+TKEL*(C2(1)+TKEL*(D2(1)+TKEL*E
1          2(1) ))) +DELH(1)
GO TO 403
550 CONTINUE
T=
      TKEL
      IF (T.GE.8.5E3 .AND. TAU.GE.1.E3 ) GO TO 504
      IF (T.GT.1.05E4 .AND. TAU.GE. 1. ) GO TO 504
      IF ( T .GE. 1.3E4 ) GO TO 504
TKEL= 7.E3
GO TO 551

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503 CONTINUE
NBARO= NBAR
UPPERT= 7.E3-(NBARO-1.)/DNDT
      IF(T.GT.UPPERT) GO TO 504
TUPM7= UPPERT-7.E3
TDIF= T-7.E3
NBAR= NBAR+TDIF*DNDT
EO= ENERGY
E1= 1.0392445E7*UPPERT+5.98566E11
EONBAR= EO*NBARO
EDIF= EONBAR-E1
ENERGY= (EONBAR-TDIF/TUPM7*EDIF)/NBAR
DEDTHT= -11605.4*(ENERGY*DNDT+EDIF/TUPM7)/NBAR
DEDTAU= (-ENERGY*DNDAU +((UPPERT-T)/TUPM7)*(EO*DNDAU+NBARO*
1      DEDTAU) - EDIF/TUPM7 * DNDAU/DNDT * TDIF/TUPM7)/NBAR
PRESHR= - CONST /NBAR*T*8.3139564E7
UPDTAU= -PRESHR/NBAR*DNDAU
UPDTHT= -PRESHR*11605.4*DNDT/NBAR
TKEL= T
901 CONTINUE
ENERGY= ENERGY-1.0392445E7*TKEL/NBAR- EZERO
DEDTHT= DEDTHT-1.2060848E11/NBAR
902 CONTINUE
CARBNZ(8)= 0.
CARBNZ(7)= NBAR
RETURN
504 CONTINUE
ENERGY= 5.98566E11 - EZERO
TKEL= T
PRESHR= - CONST *TKEL*8.3139564E7
UPDTAU= 0.
UPDTHT= 0.
DEDTAU=0.
DEDTHT= 0.
NBAR= 1.
XSET(1)= -CONST
GO TO 902
900 CONTINUE
197 CONTINUE
CARBNZ(8)= 97.0197
RETURN
10 CONTINUE
DO 15 I=1,10
A(1) = 2.5

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B(1) = 0.  
C(1) = 0.  
D(1) = 0.  
E(1) = 0.  
FK(1) = 0.  
A2(1) = 2.5  
B2(1) = 0.  
C2(1) = 0.  
D2(1) = 0.  
E2(1) = 0.  
FK2(1) = 0.  
15 CONTINUE  
GO TO 11  
END
```

REFERENCE

1. Duff, Russell E., and S. H. Bauer, "Equilibrium Composition of the C/H System at Elevated Temperatures," J. Chem. Phys. **36**, 1754 (1962).

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13. ABSTRACT Various analytic and numerical methods are described for the phenomena which take place when a high-energy-density source interacts with matter. The interaction usually begins with the transient heating of a solid surface for which analytical methods of study have been developed (Section I). The second phase of the interaction process is vaporization. Recent developments in numerical techniques for simulating vaporization are discussed in the context of the two-dimensional interaction code HECTIC (Section II). The third phase normally involves the nonsteady flow of ionized vapor, for which equations of state are required. A general numerical technique (EIONX) for evaluating internal energy and pressure for a given temperature and density has been developed and incorporated in the SPUTTER program (Section III). For computer programs, e.g., HECTIC, which use internal energy and density as the independent variables, numerical methods were developed to invert the equations of state generated by EIONX (Section IV). For relatively low energy-density sources, the vapor may be in a molecular phase for a significant part of the interaction process, thus requiring the development of special techniques for evaluating the molecular dissociation energy as a function of temperature and density. The calculations for one particular material--carbon--are discussed in detail (Section V). (Distribution Limitation Statement No. 2)			

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