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The MES Code: Chemical-Equilibrium Detonation-Product States of Condensed Explosives

by

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Units and Energy Zero

The primary units are centimeters, grams, microseconds, K (pressure in Mbar, specific energy in Mbar - cm^3/g), but the mole and the system mass M_0 (specified by the user) are also used as the mass unit. The energy unit kcal, prevalent in the literature at the time the code was made, is used for a few input and output quantities.

Energies are relative to elements in their standard states (as defined by the NBS) at $T = 0$. For elements which are gaseous under ordinary conditions, such as oxygen, the typical standard state is the molecular form (O_2) in the hypothetical ideal gas state at a pressure of one atmosphere. For elements which are solid under ordinary conditions, such as carbon, the typical standard state is the most common crystalline form (graphite) at zero pressure.

Terms

Contour - Locus of constant T, e, v, or s

CJ - Chapman-Jouguet

CS - Conformal-solution mixture rule

EOS - Equation of state

Ideal (part) - Translation plus internal part of the EOS (Secs. III.B and IV.C)

Imperfection (part) - Configurational part of the EOS (Secs. III.B and IV.C)

KW - Kistiakowsky-Wilson (EOS)

LJD - Lennard-Jones-Devonshire (EOS)

LH - Longuet-Higgins mixture rule

Lattice (in LJD) - The cold ($T = 0$) state with all molecules fixed on their lattice sites

NBS - National Bureau of Standards

Pure-Fluid - Pure species (gas EOS)

Unreacted Material - The unreacted (in general metastable, as in an explosive) material in the initial state (p_0, T_0)

Symbols

Intensive thermodynamic functions

p, T, μ - pressure, temperature, chemical potential

Extensive thermodynamic functions

V, E, H, A, F, S, C_p, C_v - molar volume, internal energy, enthalpy, Helmholtz free energy, Gibbs free energy, entropy, constant-pressure and constant-volume heat capacities

v, e, h, a, f, s, c_p, c_v - corresponding specific quantities (per unit mass)[equal to (n/M_0) times molar]

Composition

n - total number of moles per M_0 grams of system

n_g - number of moles of gas per M_0 grams of system

n_s - number of moles of solid per M_0 grams of system

n_i - number of moles of species i per M_0 grams of system

x_i - mole fraction of species i in the gas phase = n_i/n_g

x_s - n_s/n

Intermolecular potential

r^*, T^* - minimum-energy radius and well depth

$V^* = (N/\sqrt{2})(r^*)^3$ - molar volume of fcc lattice with molecules at distance r^*

n, m - repulsive and attractive indices

Chemical equilibrium calculation

c - number of elements

s - number of species

$\underset{\sim}{Q}$ - empirical-formula coefficients

$\underset{\approx}{\alpha}$ - species-formulae coefficients

$\underset{\sim}{a}$ - renumberings

$\hat{s}$ - supersaturation index

Other

D - detonation velocity

Δ - ΔH_f (NBS)

Symbols (cont)

Other (cont)

$\tilde{F}$ - "free energy" for equilibrium constants; solid: $\tilde{F}_s = F_s$;
gas: $F_i = \mu_i - RT \ln x_i$ (Sec. IV.E)

γ - $(-\partial \ln p/\partial \ln v)_s$ - adiabatic exponent

Γ - $v(\partial p/\partial e)_v$ - Grüneisen coefficient

$\hat{H}$ - $\left[H^o(T) - H^o_o\right]$ (NBS)

M_o - system mass

N - Avogadro's number

q - heat of reaction, Sec. IV.F

R - molar gas constant

ρ - density

Σ - sum over all species

Σ_g - sum over gas species

u - particle velocity

z - pV/RT

Superscript or over

i - ideal

' - imperfection

* - NBS tabular function (translation plus internal)

$\bar{\ }$ - average

$\tilde{\ }$ - (1) function (as distinguished from a variable) e.g. $\tilde{p}(T,v)$, used only when needed to make this distinction
(2) decoration, as in $\tilde{F}$

Subscript or under

i - species index

o - unreacted material in the initial state

g - gas

s - solid

ℓ - lattice (cold curve) function for the LJD EOS

H - Hugoniot

other subscripts - partial derivative

$\underset{\sim}{\ }$ - vector

$\underset{\approx}{\ }$ - matrix

THE MES CODE: CHEMICAL-EQUILIBRIUM DETONATION-PRODUCT STATES OF CONDENSED EXPLOSIVES

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ABSTRACT

The MES code calculates states of the reaction products of detonation in gaseous or condensed explosives under the assumption of thermal and chemical equilibrium. The products may consist of any number of gaseous species and one solid species. The condition of equilibrium includes the number of phases: the solid may or may not be present depending on the current state. In addition to the primary calculation of the Chapman-Jouguet state at a specified set of initial densities, the detonation Hugoniot, and contours of constant temperature, density, energy, or entropy, each at a specified set of pressures may be obtained. All of the first derivatives (e.g., sound speed and heat capacity) are calculated at each point.

The solid equation of state is one constructed from a given shock Hugoniot under the assumption of constant Gruneisen coefficient. For the gas, either the ideal gas, the Kistiakowsky-Wilson, or the LJD (Lennard-Jones-Devonshire cell theory) equation of state may be used. Several choices of "mixture rules" for extending the last one, a pure-fluid equation of state, to mixtures are offered. For LJD, the input data are the parameters defining the intermolecular potentials of the species.

I. INTRODUCTION

The MES code, which performs the calculations described in Refs. 1 and 2, was made some years ago, became dormant when the IBM 7094 became obsolete, and has just been reactivated "as is" in response to a request. I make no apology for things I would now do differently. The only significant changes made in the code are: (1) the replacement of the original machine-language equilibrium routine with an equivalent FORTRAN version, (2) the replacement of several relatively small machine-language I/O routines by approximately equivalent FORTRAN versions, and (3) a new scheme of diagnostic printing.

II. INPUT

The data are entered in packs, each pack preceeded by a CON card. The CON cards have 2A6 format; only the first two fields are data; the user may enter comments on the rest of the card. The first two fields, each left justified, are the word CON and the pack name. Each pack consists of one or more strings, numbered sequentially in the write-up; each string consists of one or more cards. Strings are described by listing their fields; alphameric items are underlined. A few strings, such as the table of initial densities for the CJ locus, and initial pressures for the Hugoniot and contours, are of indefinite length; these must be terminated by a zero. Most of the formats are 6E12.7. A few are 12I6 or 12A6; these are marked (I) or (A).

Data for a job (a batch-type submission) are divided into runs. Each run begins with a CON, PAS card and ends with a CON, REND card. The job ends with a CON, JEND card following the last CON, REND. Each run has two parts. Part 1 (preliminary), beginning with CON, PAS, generally enters parameters of the constitutive relations. In Part 2, beginning with the first CON, SAM card, the packs CJ, TED, and PV each specify a complete calculation to be performed immediately after the pack is read; the user may often want to have more than one of these packs within a run, as well as additional SAM packs. With a few obvious exceptions, the packs of either part may be entered in any order.

The input program reads one pack at a time. It expects to find a fixed number of strings in each pack (even though, under some options, not all of them are used). If the first card of a pack is not a CON card (usually because the user has gotten the wrong number of strings in the previous pack), the program reports an error and skips to the next CON, PAS card and begins reading there. In describing the input data, the phrase "not used" means that the data of the field or string in question is not used by the program under the specified conditions. It will, nevertheless, be read by the program; the user may enter anything, but a blank field(s) is suggested. The only exception is that if an entire pack is not used, it may be omitted.

•Remarks

1. Alphameric constants in the input are given in caps, underlined.
2. Except for the equilibrium calculation, which has its own special order, the first slot of all composition arrays is the number of moles of solid.
3. There are no prestored defaults. Many standard values must be supplied by the user under CON, FOB; the standard pack is given in the sample input,

Sec. VI. CON, SWIT, q.v., does have a mechanism for preserving previously entered items when it reappears.

A. Part 1

•CON, PAS, run label - begin Part 1. The run label becomes part of the standard output header.

•CON, blank, comment.

•CON, SWIT - switches.

(I) diff, fix diff, gas, solid, mix, eq, CJ, PV, PVC.

diff - 0 - no action
1 - calculate equilibrium-composition derivatives at each point
fix diff - 0 - no action
1 - fixed-composition derivatives similarly
gas - 0 - ideal-gas EOS
1 - LJD EOS
9 - KW EOS
solid - 0 - incompressible
1 - Grüneisen EOS
mix - 0 - none (pure fluid); omit XIP pack
1 - ideal mixing
2 - LH mixing
3 - CS (conformal solution) mixing
4 - One-Fluid mixing
eq - 0 - fixed composition
1 - equilibrium composition
CJ - 0 - equilibrium CJ condition
1 - frozen CJ condition
PV - 1, 2, 3, 4 for T, v, s, e constant on contours (see CON, PV)
PVC - 0 - no action
1 - under CON, PV, use last T, p from previous calculation instead of input T_c, p_c

Two of the switches are set (or reset) elsewhere: the mix switch under CON, XIP and the PVC switch under CON, PV.

This pack may also be entered one or more times in Part 2 to change switch settings between calculations. A negative item means: "don't store this item" [use currently stored (last previously entered)] value.

•CON, TIP - ideal thermodynamic functions

1. (I) number of species, degree of fit n.
2. T_{min}, T_{max}.
3. $a_0, a_1, a_2, \ldots, a_n, d, \Delta H_f^o, \Delta H_f(T_0), [H_0(T_0)-H_0^o]/RT_0$.

Polynomial fit coefficients for $[H^o(T)-H_0^o]/RT$, enthalpy integration constant d, heats of formation, and enthalpy at T_0. One such string for each species.

•CON, SEP - solid EOS

1. Γ, Cp/R, α, V_0, T_0, E_0/RT_0.
   Grüneisen coefficient, heat capacity, thermal-expansion coefficient (K^{-1}), initial volume (cm^3/mole), initial temperature (K), initial energy. For incompressible solid, only V_0 is used.
2. blank, c_0, c_1, c_2, c_3, c_4.
   Hugoniot fit coefficients: $P_H(v) = \sum_{i=0}^{4} c_i(v/v_0)^i$

•CON, GEP - gas EOS (omit pack for ideal gas), LJD EOS

1. (I) potential index (1, 2, 3 for LJ, MCM, MR).
2. n, m, A_n, A_m, r^*, T^*.
   repulsive/attractive exponents, multipliers, well radius r^* (Å = 10^{-10}m), well depth T^* (K); r^* and T^* not used for a mixture.

•KW EOS

1. (I) 9.
2. α, β, θ.

•CON, XIP - Mixture (omit if SWIT mix = 0), LJD EOS

1. (I) number of (gas) species, type.
   type - 1, 2, 3, 4 for ideal, LH, CS, One-Fluid;
2. s_r, s_T, r_r^*, T_r^*, n, m.
   s_r, s_T - scale factors: multiply all input r^* by s_r and all input T^* by s_T.
   r_r^*, T_r^* - reference r^*, T^* (LH only).
   n, m - potential n and m (One-Fluid only); ordinarily same as n, m in
   CON, GEP [omit if SWIT gas = 0 (ideal gas)]
3. $\underset{\sim}{r}^*$ - one for each (gas) species.
4. $\underset{\sim}{T}^*$ - one for each (gas) species.

•KW EOS

1. (I) 9.
2. s_r^*, -, κ.
3. $\underset{\sim}{k}$.

   Here $k_i \equiv [r_i^*/(N/\sqrt{2})]^{1/3}$, where k_i is the usual KW covolume and N is Avogadro's number.
4. blank.

•CON, EQP - equilibrium (omit pack for fixed composition)

1. (I) c, s, p, -, p', ϕ.

   c - number of elements

   s - number of species

   p - number of phases minus 1; used only if $\phi = 0$

   p'- first guess for p when $\phi = 1$

   ϕ - 0: fixed number of phases (p + 1)

   1: equilibrium number of phases (one or two);
2. $\underset{\sim}{Q}$ - system empirical-formula coefficients (number of gram-atoms of each element).
3. (A) blank, element symbols, A1, A0.

   A print label; all fields right-justified.
4. $\underset{\sim}{\alpha}$ - species-formulae coefficients.

   This consists of s strings, one for each species, so that each string is a row of $\underset{\sim}{\alpha}$. The first field, format A6, is the right-justified element symbol, and the remaining fields, format I6, are the coefficients. (For example, with elements C, H, O, and N, the string for carbon dioxide is: CO2, 1, 0, 2, 0).
5. (I) $\underset{\sim}{a}^1$ - species renumbering for two-phase system (ϕ=1) or given system (ϕ=0).
6. (I) $\underset{\sim}{a}^0$ - species renumbering for one-phase system (ϕ=1); not used for ϕ=0.

   Dimensions are all fixed once c and s are given:

$$\underset{\sim}{Q}(c),\ \underset{\sim}{\alpha}(s \times c),\ \underset{\sim}{a}^1(c),\ \underset{\sim}{a}^0(c)\ .$$

In $\underset{\sim}{\alpha}$ the species may be listed in any order. The $\underset{\sim}{a}$'s specify renumberings. If k is the number of a species as originally entered in $\underset{\sim}{\alpha}$, then its new number is a_k. The a_k must be chosen so that after renumbering the following conditions are satisfied: the formula coefficients of the first c species must be linearly independent; the danger of convergence failure will be minimized by choosing for them those species expected to be present in largest amounts. Two special requirements simplify the program: For $\phi=0$, $p=1$ (two phases), the solid species must be number c. For $\phi=1$, the user must supply two possible systems: Two phase (solid present) and one phase (solid absent); the program chooses the correct one at each T and p. For the two-phase system the solid must be number c. For the one-phase system it must be (nominally) present as number s; here the program assigns it a large free energy so that its calculated mole fraction is negligibly small.

For details and examples see Secs. IV.E and VI, and Appendix A.

•CON, FOB - knobs

1. FROOT ε's.
2. FROOT r's.
3. $1/2\ \Delta\ \ell n\ p$, $1/2\ \Delta T$, ε_{outer}, ε_{inner}.
4. FROOT bounds.

The FROOT items are in the order given in Sec. V.B, Table III; the bounds are in pairs (min, max). The Δ's are the displacements for the numerical differentiation, Sec. II.B. The ε's in string 3 are for the outer and inner equilibrium iterations, Sec. V.A.

•CON, DBUG - print store

Do the standard error print (mainly the entire common store) at this point.

B. Part 2

•CON, SAM, material label - initial state and begin Part 2

1. ρ_0(g/cm), p_0(Mbar), T_0(K), M_0(g), $\Delta H_f(T_0)$ (kcal/mol).

   M_0 - system mass; must agree with empirical formula under CON, EQP.

   $\Delta H_f(T_0)$ - enthalpy of formation of unreacted material at p_0, T_0 relative to elements in standard states at T_0.

2. $\underset{\sim}{n}$ - number of moles of each species (for system of M_0 grams). First field is for solid. For equilibrium composition, these are guesses for the first iteration.

We have picked T_0 for the heat of formation because $\Delta H_f(T_0)$ is the quantity usually listed for explosives, and because it is needed for the calculation of the heat of reaction q as usually defined (Sec. IV.F). An alternative, which may be more convenient for some cryogenic materials, is to enter in place of $\Delta H_f(T_0)$ the enthalpy of formation at T_0 from elements at T=0. If this is done, the CON, TIP input must also be changed by entering ΔH_f^o in place of $\Delta H_f(T_0)$ and setting

$[H^o(T_o) - H^o_o]/RT_o$ for each species to zero. This has the advantage of making the TIP input simpler and independent of T_o. The disadvantage is that the value of q printed out will have a small error (which does not affect on any other calculated quantity).

•CON, TED - detonation Hugoniot at given $\underset{\sim}{p}$

$\underset{\sim}{p}$ - pressure table.

•CON, PV - contour of constant T, v, s, or e at given p

1. (I) k, PVC.
   k - 1, 2, 3, 4 for constant - T, v, s, e
   PVC - PVC switch (see CON, SWIT)
2. T_c, p_c - initial point (not used if PVC $\neq$ 0).
3. $\underset{\sim}{p}$ - pressure table.

First calculate the point (T_c, p_c), then use the value of T, v, s, or e from this point as the constant value for the locus. Use T and p from last previously calculated point for T_c, p_c instead of input values if PVC $\neq$ 0.

•CON, CJ - CJ locus at given $\underset{\sim}{\rho}_o$

$\underset{\sim}{\rho}_o$ - initial-density table.

•CON, REND - end of run

•CON, JEND - end of job

III. OVERVIEW

In this section we give an overview of the problem and program, including the principal equations. Some of these equations are schematic or just serve as definitions; Sec. IV gives the detailed equations implemented by the program. Section V, together with comments in the program, provides a more detailed description of the program itself.

We define the term state point and some related symbols in Sec. A, the main components of the state-point calculation in Sec. B, and the higher level part of the program which uses the state-point calculation in Sec. C. Principal routine names are given in parentheses with some of the section headings.

A. State Point (MES)

A state point is the usual set of thermodynamic variables V, E, H, A, F, S, and some of their derivatives, the chemical potentials μ_i, the mole fractions x_i, and the total number of moles n (per system mass M_o) at given T and p. Recall that we have at most one solid species, and the convention that it is the first listed.

The mole numbers and mole fractions are given by (see symbol sheet)

$$n = \sum n_i = n_s + n_g$$

$$n_g = \sum_g n_i$$

$$x_1 \equiv x_s = n_s/n$$

$$x_g = n_g/n$$

$$x_i = n_i/n_g, \; i>1(\text{gas}) \quad .$$

Note that x_i, $i>1$ is the mole fraction <u>in the gas phase</u>. The composition may be either fixed (specified) or equilibrium (recalculated at each state point).

Because the equations defining the equilibrium state are implicit and complicated, we obtain derivatives by numerical centered differencing over carefully chosen intervals, rather than attempting to use the very lengthy analytic expressions.

Routine MES calculates a state point at given T and p, using the five packages whose generic names are given in the subheadings of the next section. These packages constitute the bulk of the program.

B. Components of the State-Point Calculation

An extensive quantity for the system is the linear mole fraction sum of those for the two phases, e.g.,

$$E = x_s E_s + x_g E_g \quad .$$

It is convenient to separate functions like E_g and E_s into <u>ideal</u> and <u>imperfection</u> parts. The ideal part, superscript i, represents translation plus the internal partition function; the imperfection part, denoted by a prime, represents the configuration integral.

Descriptions of the five main components of the EOS calculation follow.

1. Ideal Thermodynamic Functions (TIM). We use superscript * to denote the portion of the ideal part that represents the internal partition function; most of the work is in getting this number (for the solid it is the whole value). These functions are tabulated by the NBS and others; they are represented to the program by polynomial fits. The tabulations refer each species to itself at T = 0. The program adds the heats of formation at T = 0 to refer all to the same reference, namely elements in their standard states at T = 0. The physical state corresponding to the tabulation is the given T and $p = p^*$ (1 atm for a gas and zero for a solid), with the stipulation that a gaseous species is in the hypothetical ideal-gas state at T and p^*. For the gas phase, we define the ideal part as that for an ideal gas at the same T, p, and x, so that

$$E^i\,(T, p, x) = \sum\nolimits_g x_i\, E_i^*(T) \;,$$

$$S^i\,(T, p, x) = \sum\nolimits_g x_i\, S_i^*(T) - R\,\ln p/p^* + R \sum\nolimits_g x_i\,\ln x_i \;, \text{ and}$$

$$\mu_i^i\,(T, p, x_i) = F_i^*(T) + RT\,\ln p/p^* + RT\,\ln x_i \;.$$

2. Solid Equation of State (SEM). For the extensive thermodynamic functions we have

$$E\,(T, p) = E^i\,(T, p = 0) + E'\,(T, p) \;, \text{ etc.}$$

With the equation of state in the often-used form p(T, V), the imperfection quantities may be defined as the integrals along the isotherm:

$$E'\,(T, p) = \int_{V(T,\, p\,=\,0)}^{V(T,\, p)} (T\,p_T - p)\,dV \;,$$

$$S'\,(T, p) = \int_{V(T,\, p\,=\,0)}^{V(T,\, p)} p_T\,dV \;, \text{ and}$$

$$\mu' (T, p) \equiv F' = E' + pV - TS' \quad .$$

The EOS used takes the form of equations for T and p along an isentrope through an unknown point T_1, V_1 on $p = 0$, and incorporates simple approximations to the ideal functions on $p = 0$. The equations can be put into a form such that for given T and p the point T_1, V_1 at the foot of the isentrope can be eliminated and the complete EOS at T, p can be obtained by iterative solution of one equation in one unknown. After this is done, the approximate ideal part is subtracted to give the imperfection part (with the correct ideal part, calculated by TIM, added later).

3. Gas Equation of State (GEM). Here we have

$$E (T, p, x) = E^i (T, p, x) + E' (T, p, x) \quad , \text{etc.}$$

For the usual form p(T, V) the imperfection functions are given by the integrals along the constant-composition isotherm

$$E' (T, p, x) = \int_{RT/p^*}^{V(p, T)} (T p_T - p) \, dV \quad \text{and}$$

$$S' (T, p, x) = \int_{RT/p^*}^{V(p, T)} (p_T - R/V) \, dV \quad ,$$

in which the term R/V in the second integral subtracts off the ideal gas part. Also

$$H' = E' + (z-1) \quad ,$$

$$A' = E' - T S' \quad , \text{and}$$

$$F' = H' - T S' \quad ,$$

For the chemical potentials we have

$$\mu_i' = (n\ F')_{n_i}\Big|_{n=1} \quad ,$$

where the partial derivative is at constant T, p, and n_j, $j \neq i$, of the gas phase.

Both of our imperfect-gas equations of state, the LJD and the KW, have the form p (T, V, x), and are not explicitly invertible to V (T, p, x). At given T, p, x we must then first solve the equation

$$\tilde{p}\ (T,\ V,\ x) \ = \ p$$

(where $\tilde{p}$ on the left distinguishes the pressure function from the given value of pressure on the right) for V and then calculate the imperfection functions at the given T and this V.

The KW EOS is a simple one, and includes the composition dependence. The LJD EOS is much more complicated, requiring for its calculation the numerical evaluation of several definite integrals. In its original form it applies to only a single, pure species. Here it is extended to apply to the gas mixture through one of several mixture rules, described next.

4. Mixture (XIM). The program offers several options for describing the gas mixture. The first is the general one of ideal mixing, for which each mixture property is a linear mole-fraction sum of those of the individual species

$$E'\ (T,\ p,\ x) \ = \ \sum\nolimits_g x_i\ E_i'\ (T,\ p) \quad , \text{etc.}$$

This may, of course, be applied to any (pure-species) EOS.

The other mixture rules assume that the pure-species EOS is based on an intermolecular potential function and express the mixture properties as expansions in the potential functions or potential-function parameters of the individual species. In some cases the outcome of this expansion is that the mixture is represented by a fictitious fluid with a certain mean potential whose parameters depend on the composition.

5. Chemical Equilibrium (EQM). The composition of the system can be expressed in terms of the progress variables of J independent reactions (ordinarily

J is the number of species minus the number of elements). We symbolize these reactions by

$$\sum_i \nu_{ij} X_i = 0, \quad j = 1, \ldots, J \quad ,$$

where X_i represents one mole of species i, so that ν_{ij} is the (molar) stoichiometric coefficient of species i in reaction j. The equilibrium composition is the solution of

$$\sum_i x_i \alpha_{ik} = Q_k \qquad k = 1, \ldots, k$$

$$\sum_i \nu_{ij} \mu_i (T, p, n_j) = 0 \quad j = 1, \ldots, J$$

with the α_{ik}, the chemical formula coefficients (number of moles of element k in one mole of species i), and the Q_k, the empirical-formula coefficients of the system (total number of moles of element k in the system; total of k elements). The first set of equations represents mass conservation, one equation for each element; the second represents the usual "equilibrium-constant" relations for the reactions. The second equations are put in the form

$$\sum_{i}{}_{g} \nu_{ij} \ln x_i = -\sum \nu_{ij} \tilde{F}_i (T, p, \underset{\sim}{x})/RT, \quad j = 1, \ldots, J$$

with $\tilde{F}_i$ defined as

$$\tilde{F}_i = \mu_i - RT \ln x_i \qquad \text{for a gas species and}$$

$$\tilde{F}_i = \mu_i = F_s \qquad \text{for the solid.}$$

The advantage of this procedure is that, for the ideal gas, the $\tilde{F}_i$ are independent of x, so the x-dependence is confined to the $\ln x_i$ terms. For the real gas the $\tilde{F}_i$

do depend on $\underset{\sim}{x}$, but this dependence is small enough so that the equations can be solved by a direct iteration method based on a procedure that solves the ideal-gas problem: Guess x, calculate $\tilde{F}_i$ for this $\underset{\sim}{x}$, find the ideal gas x for the $\tilde{F}_i$ fixed at this value, recalculate the $\tilde{F}_i$ from the new $\underset{\sim}{x}$, and repeat to convergence.

6. Derivatives (GAMM). The first partial derivatives (for the complete system) are calculated by centered difference from symmetrical displacements in $\ell n\ p$ and T of carefully chosen size. Three derivatives are approximated by centered differences

$$c_p \equiv (\partial h/\partial T)_p = \Delta h/\Delta T \quad ,$$

$$(\partial\ \ell n\ p/\partial\ \ell n\ v)_T = \Delta\ \ell n\ p/\Delta\ \ell n\ v \quad ,$$

$$(\partial\ \ell n\ v/\partial T)_p = \Delta\ \ell n\ v/\Delta T \quad ,$$

where Δ denotes a difference between the two symmetrically displaced points in p or T. The remaining derivatives are then obtained from these

$$c_p/c_v = 1 + (pv/c_pT)\ (-\partial\ \ell n\ p/\partial\ \ell n\ v)_T\ [T(\partial\ \ell n\ v/\partial T)p]^2 \quad ,$$

$$\gamma = (c_p/c_v)\ (-\partial\ \ell n\ p/\partial\ \ell n\ v)_T \quad \text{, and}$$

$$\Gamma = \gamma\ (pv/c_pT)\ T\ (\partial\ \ell n\ v/\partial T)_p \quad .$$

C. Controls for Particular Loci

The rest of the program uses the (T, p) state-point routine (MES) to calculate points on various thermodynamic loci. The routines are given in the section titles.

1. Contours of Constant T, v, s, or e (PV, MESC). The locus is specified by a given value of the desired variable. Thus for constant e, for example, it is the solution of

$$\tilde{e}\ (T,\ p) = e_c \quad ,$$

with e_c the given value of e, specified either as the values of T_c and p_c at which the program is to calculate e_c, or taken from a previously calculated point. Under control of PV, the program calculates points on the locus for each of the set of specified values of p, using MESC to calculate each point.

2. Detonation Hugoniot (TED, HUG). This procedure works the same way, with TED the control and HUG the Hugoniot-point calculator. In this case the equation solved is the Hugoniot equation

$$h - h_0 = \frac{1}{2} (p-p_0)(v_0-v) \quad .$$

3. Chapman-Jouget Locus (CJ). A CJ point is located by iterative solution of a form of the CJ condition

$$u + c = D \quad ,$$

with u and D given by the shock conservation relations, over a set of points on the Hugoniot, with each Hugoniot point calculated by HUG. The CJ points are determined for the specified set of initial densities.

IV. EQUATIONS

In this section we give the remaining equations in essentially the form used by the program.

A. Ideal Thermodynamic Functions (TIM)

The system is defined by a matrix of constants, one row for each species. Each row contains

$$a_0, a_1, \ldots, a_h, d, \Delta^0, \Delta(T_0), \hat{H}(T_0)/RT_0 \quad .$$

Here we have defined, in terms of the NBS notation

$$\Delta^0 \quad = \quad \Delta H_f^0 = \Delta H_f(0), \quad \Delta(T_0) = \Delta H_f(T_0) \quad ,$$

$$\hat{H}(T) \quad = \quad H^0(T) - H_0^0 \quad ,$$

where ΔH_f^o and $\Delta H_f(T)$ are the heats of formation from the elements in their standard states at T = 0 and T = T. The standard state is defined as the standard form at the temperature of interest and pressure p^* (1 atm for a gas, 0 atm for a solid), with a gaseous form in the hypothetical ideal gas state. For elements carbon, hydrogen, oxygen, and nitrogen (CHON), the standard forms are solid graphite, and gaseous H_2, O_2, and N_2, respectively. The symbol $H^o(T) - H_o^o$ denotes the enthalpy at T relative to that of the same substance at T = 0. The constants a_o through a_n are the coefficients of a polynomial fit of degree n to $\hat{H}(T)/RT$, and d is the integration constant for the entropy. Recalling our convention that the solid always be species 1, we define

$$\delta_{i1} = 0 \quad \text{if } i \neq 1 \text{ and}$$

$$\delta_{i1} = 1 \quad \text{if } i = 1 \quad .$$

With i the row (species) index, and j the column index, we have

$$H_i^*/RT = \sum_{j=0}^{n} a_{ij}T^j + \Delta_i^o/RT \quad ,$$

$$G_i^*/RT = \sum_{j=0}^{n} (j + 1)\, a_{ij}T^j \quad ,$$

$$S_i^*/R = a_{io}\, \ell n\, T + \sum_{j=1}^{n} [(j + 1)/j]\, a_{ij}T^j + d_i - (\delta_{i1} - 1)\, \ell n\, p/p^* \quad , \text{and}$$

$$F_i^*/RT = H_i^*/RT - S_i^*/R \quad .$$

All these quantities are relative to elements at $T = 0^{\dagger}$ (entropy at this temperature is zero for all species).

The ideal functions for the gas mixture are then

$$H_g^i/RT = \sum_g x_i\, H_i^*/RT$$

$$S_g^i/R = \sum_g x_i\, S_i^*/R - \sum_g x_i \ln x_i, \text{ etc.}$$

The mixture heat of formation from elements at T_0 is

$$\Delta_g(T_0) = \sum_g x_i\, \Delta_i(T_0) \quad .$$

The total free energy of the gas is not needed, but the F_i^* of the individual species are used in calculating those F_i that determine the equilibrium composition.

The program uses the fits only over the range of T_{min} to T_{max} from the input. Outside this range, the results are an extrapolation using the assumption that the heat capacity is constant at its boundary value.

B. Solid Equation of State (SEM)

The solid EOS is constructed from a reference curve and the assumption of a constant Grüneisen coefficient to get off the curve. Defining $y = V/V_0$ (with V_0 here the normal volume of the solid at $p = 0$), the reference curve (see Fig. 1) is the shock Hugoniot $p_H(y)$ for $y \leqslant 1$ and the $p = 0$ line for $y > 1$. We assume a simple form for the ideal functions on $p = 0$, use it to calculate the complete

---

[†] The Hugoniot calculation uses the enthalpy relative to elements at T ; with this reference state indicated by explicit inclusion of the reference temperature T_0 as a parameter (together with argument T), the quantity supplied by TIM for this calculation is

$$H_i^*(T;T_0)/RT = \sum_{j=0}^{n} a_{ij}T^j - (T_0/T)\,[\hat{H}_i(T_0)/RT_0] + \Delta_i(T_0)/RT_0 \quad .$$

Note that for the alternate SAM input (Sec.II.B), this becomes identical to H_i^*/RT above, i.e., the reference temperature becomes zero.

EOS, and then subtract it to get the imperfection part. Using superscript I to denote the isentrope through point y_1 on $p = 0$ and superscript o to denote functions on $p = 0$, we have for this isentrope

$$p^I = p^I(y; y_1) \text{ and}$$

$$T^I = T^I\left[y; y_1, T^o(y_1)\right] .$$

On the reference curve $p = 0$ we take

$$T^o = T^o(y) = (y - 1)/\alpha$$

$$E^o = E^o(T^o) = C_p(T^o - T_o)$$

with constant heat capacity C_p and thermal expansion coefficient α. With constant Grüneisen coefficient Γ we find

$$E/V_o = (y/\Gamma)\, p + g(y) ,$$

$$g(y) = p_H(y)\,[1/2(1 - y) - y/\Gamma] + E_o \quad \text{for } y \leqslant 1, \text{ and}$$

$$g(y) = \alpha^{-1} C_p (y - 1) \quad \text{for } y > 1 .$$

For p^I and T^I we find

$$p^I(y; y_1) = \Gamma y^{-(\Gamma + 1)} \int_{y_1}^{y} y^{(\Gamma + 1)} g'(y)\, dy \quad \text{and}$$

$$T^I(y; y_1) = T^o(y_1)\,(y_1/y)^\Gamma .$$

If we represent the reference Hugoniot by a power series

$$p_H(y) = \sum_{i=0}^{n} a_i\, y^i$$

with coefficients chosen such that

$$p_H(1) = \sum_{i=0}^{n} a_i = 0$$

(to make the result simpler), the integral can be done analytically and we find

$$p^I = p_1(y) = (C_p/\alpha V_0) \left[\Gamma/(\Gamma-1)\right] \left[(y_1/y)^{\Gamma+1} - 1\right] \quad \text{for } y > 1 \text{ ,}$$

$$p^I = p_2(y) + p_1(1) \quad \text{for } y \leqslant 1 \text{ ,}$$

$$p_2(y) = -(\Gamma/y)g(y) + (\Gamma^2/y^{\Gamma+1}) \left[I(y) - I(1)\right] \text{ , and}$$

$$I(y) = \int y^{\Gamma-1} g(y)\, dy$$

$$= \sum_{i=o}^{n} \left[\frac{1}{2}\left(\frac{a_i}{\Gamma+i}\right)(y^{\Gamma+i}-1) - \left(\frac{1}{2}+\frac{1}{\Gamma}\right)\left(\frac{a_i}{\Gamma+i+1}\right)(y^{\Gamma+i+1}-1)\right] \quad .$$

To get the EOS for given p and T, we must eliminate (by iterative solution) y_1 from $p^I = p$ and $T^I = T$.

•Computation

Given p, T, the function defining y is

$$T^I(y)/T - 1 = 0 \quad .$$

$T^I(y)$ is calculated (for $y < 1$) by first calculating $p_2(y)$, then solving $p^I(y) = p$ for y_1 to get

$$y_1 = \left[1 + \left(p - p_2(y)\right)\Big/A\right]^{1/(\Gamma+1)}, \; A = (Cp/\alpha\, V_o) \left[\Gamma/(\Gamma+1)\right]$$

and then calculating T^I from the equation above. When y_1 is close to 1 (the usual case) the RHS is expanded in a binomial expansion

$$y_1 = 1 + k\,x + \frac{1}{2}\,k\,(k-1)\,x^2 + \ldots$$

$$k \equiv 1/(\Gamma+1)$$

$$x \equiv \left[p - p_2(y)\right]/A \quad .$$

For $y > 1$, y_1 is

$$y_1 = y\,(1 + p/A)^{1/(\Gamma+1)} \quad ,$$

with expansion

$$y_1 = y\left[1 + k\,x + \frac{1}{2}\,k\,(k-1)\,x^2 + \ldots\right]$$

$$x = p/A \quad .$$

C. Gas Equation of State (GES)

1. Ideal Gas.

The EOS is

$$V = RT/p \quad ,$$

and the imperfection quantities are all zero.

2. LJD (Lennard-Jones-Devonshire Cell Theory). This EOS is based on an intermolecular potential $u(r)$ (see Fig. 2) with well depth kT^* (k is Boltzmann's constant) and radius r^*. We define a reduced temperature and volume

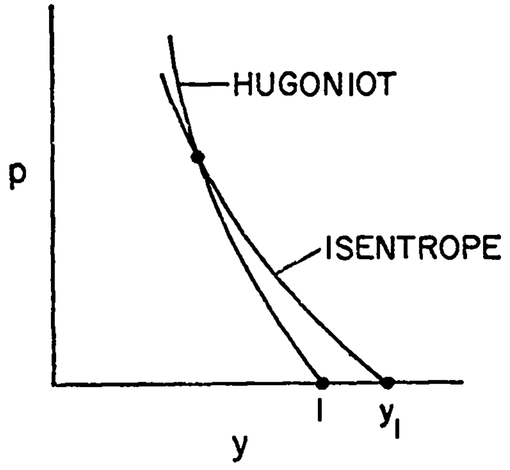


Fig. 1. Solid Hugoniot and isentrope.

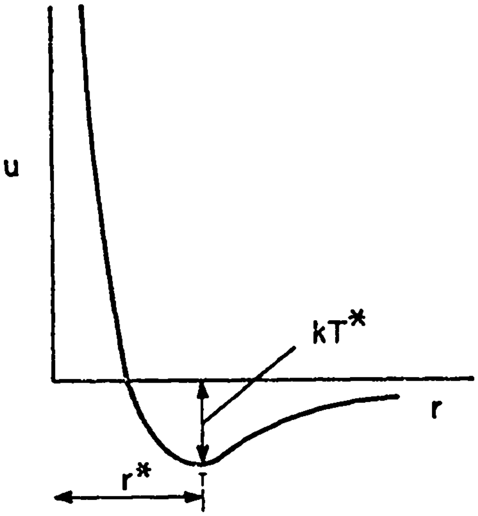


Fig. 2. Intermolecular potential for LJD EOS.

$$\theta = T/T^*, \ \tau = V/V^*, \ V^* = 2^{-1/2} N(r^*)^3 \quad ,$$

with V^* the volume of an fcc lattice with intermolecular separation r^* (N is Avogadro's number). The EOS is a sum of two parts: A lattice ($T = 0$) part, with all molecules fixed on the sites of a regular fcc lattice, and a thermal part, for which the partition function is approximated by a cell integral, in which one molecule moves while all its neighbors remain fixed on their lattice sites.

We first define the lattice and cell-integral functions. We define χ as minus the reduced lattice energy

$$\chi = -\frac{1}{2} Z \, u \, (\tau^{1/3} r^*)$$

with Z the coordination number of the lattice for which we use 12, the fcc value. The cell-integral function G(y) is defined as

$$g(y) = \int_0^{b^*} y \, x^2 \, e^{-W(\tau,x)/\theta} \, dx, \quad b^* = 0.55267$$

$$G(y) = g(y)/g(1) \quad .$$

Here the integration variable x is the distance from the cell center in units of the nearest neighbor distance at the given τ, b^* is the distance of the cell boundary from the center, and W is the <u>cell potential</u> relative to its value at the cell center, the potential of a molecule at a given distance from the cell center, in the field of its 12 nearest neighbors smeared into a uniform spherical shell (at the nearest neighbor distance). The cell potential is given by the spherical-smoothing integral

$$W(x,\tau) = \int_{1-x}^{1+x} x' \left[u\left(\tau^{1/3} r^* x'\right) - u\left(\tau^{1/3} r^*\right)\right] dx' \quad .$$

For the two types of potential-function terms we consider (power and exponential) the smoothing integral can be done analytically, but the cell integral cannot.

The cell integrals come from the canonical ensemble, with independent variables T and V. The natural imperfection quantities are thus those relative to ideal gas at the same T and V. Elsewhere, we have used imperfection quantities relative to the ideal gas at the same T and p. The two are the same for all except the entropy and free energies, which are related by

$$S'(T,p)/R = S'(T,V) + \ln z \quad ,$$

$$A'(T,p)/RT = A'(T,V)/RT - \ln z, \text{ and}$$

$$F'(T,p)/RT = F'(T,V)/RT - \ln z \quad ,$$

with the argument p or V denoting imperfection with respect to ideal gas at the same p or V, respectively. In the following, we mark A' with respect to V by argument V (we will refer to it later); all quantities without an argument are with respect to p.

The imperfection thermodynamic functions are

$$z \equiv pV/RT = 1 + \theta^{-1} \left[\tau\chi_\tau - G\left(\tau W_\tau\right)\right] \quad ,$$

$$E'/RT = \theta^{-1} \left[-\chi + G(W)\right] \quad ,$$

$$H'/RT = E'/RT + (z-1) \quad ,$$

$$A'(T,V)/RT = 1 - \chi/\theta - \log \; 2\pi 2^{1/2} \; g(1) \quad ,$$

$$A'/RT = A'(T,V)/RT - \ell n \; z \quad ,$$

$$F'/RT = A'/RT + z-1 \quad , \text{ and}$$

$$S'/R = E'/RT - A'/RT \quad .$$

The derivatives, with partials written for $p(T,V)$, $E'(T,V)$ [and $z(\tau,\theta)$, $E'(\tau,\theta)$] are

$$(V/R)p_T = (z\theta)_\theta = 1-\theta^{-2}\left[G\left(W\tau W_\tau\right) - G(W)\;G\left(\tau W_\tau\right)\right] \quad ,$$

$$(V^2/RT)p_V = \tau z_\tau - z = \tau(\tau\chi_\tau)_\tau/\theta$$

$$+ \; \theta^{-2}\left[G^2\left(\tau W_\tau\right) g(1) - G^2\left(\tau W_\tau\right) - G\left(\left(\tau W_\tau\right)_\tau\right)\right] \quad , \text{ and}$$

$$C_V'/R \equiv R^{-1}\,E_T' = (E'/RT)_\theta = \theta^{-2}\left[G\left(W^2\right) - G^2(W)\right] \quad .$$

The potential functions may be written in the form

$$u(r)/kT^* = (n-m)^{-1}\left[mf(r,n) + nf(r,m)\right]$$

$$f(r,q) = (r^*/r)^q \text{ or } e^{q(1-r/r^*)}, \quad (q = n \text{ or } m) \quad .$$

The three potential forms are

Potential	Repulsive Term	Attractive Term
LJ	power	power
MCM	exponential	exponential
MR	exponential	power

(The symbols α and β have been previously used instead of n and m for the exponential form). To write χ and W, define coefficients a for χ, and b for W for repulsive and attractive terms as follows:

Coefficients		Repulsive	Attractive
a	=	$-1/2\ A_nZn/(n-m)$	$-1/2\ A_mZm/(n-m)$
b	=	$Zn/(n-m)$	$\delta Zm/(n-m)$
			$\delta = 0,\ 1$ for $A_m = 0,\ A_m \neq 0$

Here the constants A_n and A_m are the Madelung lattice constants for a power-law term and may be regarded as an empirical multiplier for an exponential term. They may also be regarded as switches: $A_n \neq 0$, $A_m = 0$ gives a one-term (repulsive-only) potential. For a power-law term, the proper value of A_n or A_m takes into exact account the contributions of all neighbors for the lattice contribution; to do this for the exponential form a volume-dependent function would be required. For the b-coefficients, used in the cell integrals, only nearest neighbors are considered, so that the A's do not appear.

The functions χ and W and their derivatives, are, like the potential, a sum of a repulsive and an attractive term. Using the coefficients a and b defined above, we write the expressions for one term for each of the two forms.

a. Power Form.

$$t \equiv \tau^{1/3}$$

$$\chi = at^{-q}$$

$$\tau\chi_\tau = -(q/3)\ \chi$$

$$\tau(\tau\chi_\tau)_\tau = (q^2/9)\chi$$

$$W = bt^{-q}\ \ell(x,q)$$

$$\tau W_\tau = -(q/3)\ W$$

$$\tau(\tau W_\tau)_\tau = (q^2/9)\, W$$

$$\ell(x,q) = \Big[2(q-2)\ x\Big]^{-1} \Big[(1-x)^{-(q-2)} - (1+x)^{-(q-2)}\Big] -1$$

$$= \sum_{i=1}^{\infty} c_i\ x^{2i}$$

$$c_i = (q-2+2i)!\,/[(q-2)!\,(2i+1)!\,]$$

$$c_{i+1} = c_i[(q+2i)(q+2i-1)]/[(2i+3)(2i+2)]$$

The series is used for computation.

b. Exponential Form.

$$s \equiv q\tau^{1/3}$$

$$\chi = a\ e^{q-s}$$

$$\tau\chi_\tau = -(s/3)\ \chi$$

$$\tau(\tau\chi_\tau)_\tau = \Big[\big(s^2-s\big)\big/9\Big]\ \chi$$

$$W = be^{q-s}\ f_1(s,x)$$

$$\tau W_\tau = (b/3)e^{q-s}\ f_2(s,x)$$

$$\tau(\tau W_\tau) = (b/9)\ e^{q-s}\ f_3(s,x)$$

where the functions f_1, f_2, and f_3 all have the form

$$f_i(s,x) = \alpha_i(s)\ (sx)^{-1}\ \sinh(sx) + \beta_i(s)\ sx\ \sinh(sx) + \gamma_i(s,x)\ \cosh(sx) + \delta_i(s)$$

with the coefficients α_i, β_i, γ_i, δ_i given in Table I.

- Computation of the g-integral

The 16-point Gauss method is used:

$$\int_0^{b^*} f(x)\ dx \cong \frac{1}{2}\, b^* \sum_{i=1}^{16} a_i\ f(x_i)$$

$$x_i = \frac{1}{2}\, b^*\ (1-y_i) \quad ,$$

where the a_i and y_i are the weights and arguments of the method. These are symmetric about the center of the interval $(0,b^*)$

$$y_1 = y_{16} \cong 0.99$$

$$\vdots$$

$$y_8 = y_9 \cong 0.1$$

$$a_1 = a_{16} \cong 0.03$$

$$\vdots$$

$$a_8 = a_9 \cong 0.19 \quad .$$

TABLE I

COEFFICIENTS FOR THE EXPONENTIAL FORM

i	$\alpha_i(s)$	$\beta_i(s)$	$\gamma_i(s,x)$	$\delta_i(s)$
1	$1+s^{-1}$	0	$-s^{-1}$	-1
2	$-(s+2+2s^{-1})$	-1	$2(1+s^{-1})$	s
3	$s^2+2s+4+4s^{-1}$	$2+3s$	$-(3s+4+4s^{-1}+sx^2)$	$s-s^2$

In the region of interest, the integrands often effectively vanish for x significantly less than b^*. The program allows for this by, in effect, choosing the numerically appropriate upper limit each time, as described in Sec. V.C.

3. KW (Kistiakowsky-Wilson). The KW EOS has its own built-in mixture rule in the form of a linear mole-fraction sum of covolumes k_i

$$k = \kappa \sum_g x_i k_i \quad .$$

Its reduced variable x:

$$x = k/V(T+\theta)^\alpha$$

for $\theta = 0$, would be that corresponding to a repulsive-only potential with

$$k \propto (r^*)^3 (T^*)^\alpha \quad .$$

(actually θ is fixed at 400 K). The equations are

$$z \equiv pV/RT = 1+xe^{\beta x} \quad ,$$

$$E'/RT = [\alpha T/(T+\theta)](z-1) \quad ,$$

$$F'/RT = (e^{\beta x}-1)/\beta + z - 1 - \ell n\, z \quad , \text{ and}$$

$$\mu_i'/RT = (e^{\beta x}-1)/\beta - \ell n\, z + (\kappa k_i/k)(z-1) \quad .$$

The derivatives are, with partials of p (T,V) and E' (T,V)

$$(V/R)p_T = z - (1+\beta x)E'/RT \quad ,$$

$$(V^2/RT)p_V = -(1+\beta x)(z-1) - z \quad , \text{ and}$$

$$C_V'/R = \{2 - [1+\alpha(1+\beta x)]T/(T+\theta)\}E'/RT \quad .$$

D. Mixture (XIM)

All the following forms except ideal mixing require the intermolecular potential functions for all binary interactions. To get these from the given potentials for each species, we use the combining rules for r^* and T^*

$$r^*_{ij} = \frac{1}{2}(r^*_i + r^*_j) \text{ and}$$

$$T^*_{ij} = (T^*_i \, T^*_j)^{1/2} \quad ,$$

and assume the same functional form for all (including common values of the repulsive and attractive exponents n and m).

All of the sums in this section, of course, extend only over the gas species.

1. Ideal Mixing. The properties of the mixture are just linear mole fraction sums of the properties of the components, each calculated as a pure fluid at the given T and p. Thus

$$V(T,p) = \sum x_i \, V_i(T,p) \quad ,$$

and similarly for the other extensive variables. The chemical potential of each component is just equal to its Gibbs free energy at the given T and p

$$\mu'_i(T,p)/RT = F'_i(T,p)/RT \; .$$

2. LH Mixing. This is based on an expansion about the properties of a fixed specified reference fluid (subscript r) in powers of $r^*_i - r^*_r$ and $T^*_i - T^*_r$. All the pure species are assumed to be described by the same reduced EOS p (τ_i, θ_i), $\tau_i = V/V^*_i$, $\theta = T/T^*_i$. The partial derivatives are those of the reference-fluid functions with T and V as independent variables: p (T,V), E' (T,V). The equations are

$$f = \sum_{j,k} x_j \, x_k \, f_{jk}$$

$$g = \sum_{j,k} x_j \, x_k \, g_{jk}$$

$$f_{jk} = r^*_{jk}/r^*_r$$

$$g_{jk} = T^*_{jk}/T^*_r$$

$$z = z_r \left\{1 - \left[T/V\left(-p_T/p_V\right) + \left(p/V\right)/p_V\right](f-1) + 3\left[1 + \left(p/V\right)/p_V\right](g-1)\right\}_r$$

$$H'/RT = \left\{H'/RT + \left[E'/RT - C'_V/R - R^{-1}\left(Tp_T - p\right)\left(-p_T/p_V\right)\right](f-1)\right\}_r$$

$$F'/RT = \left[F'/RT + (E'/RT)(f-1) + 3(z-1)(g-1)\right]_r$$

$$\mu'_i/RT = \left\{F'/RT + E'/RT\left[2\left(\sum_j x_j \, T^*_j/T^*_r - 1\right) + \left(f-1\right)\right]\right.$$

$$\left. + \; 3(z-1)\left[2\left(\sum_j x_j \, r^*_j/r^*_r - 1\right) + \left(g-1\right)\right]\right\}_r ,$$

with all of the thermodynamic functions and their derivatives on the right evaluated for the reference fluid at the given T and V.

3. CS Mixing. This is an improvement over the LH form, with a composition-dependent reference fluid chosen to make $f = g = 1$. The same assumptions apply. The reference fluid is defined by

$$r^*_r = \bar{r}^* = \sum_{i,j} x_i \, x_j \, r^*_{ij} \quad \text{and}$$

$$T^*_r = \bar{T}^* = \sum_{i,j} x_i \, x_j \, T^*_{ij} \; .$$

The thermodynamic functions are all just those of this reference fluid except for the chemical potentials, which are the same as those for LH but with r_r^* and T_r^* as defined here and f = g = 1:

$$\mu_i'/RT = \left\{ F'/RT + E'/RT \left[\left(n/\bar{T}^*\right) \partial\bar{T}^*/\partial n_i\right] + 3(z-1) \left[\left(n/\bar{r}^*\right)\partial n_i\right]\right\}_r ,$$

$$n/\bar{T}^* \quad \partial\bar{T}^*/\partial n_i = 2\left(\sum_j x_j T_{ij}^*/\bar{T}^* - 1\right) , \text{ and}$$

$$n/\bar{r}^* \quad \partial\bar{r}^*/\partial n_i = 2\left(\sum_j x_j r_{ij}^*/\bar{r}^* - 1\right)$$

These partials are at constant n_j, $j \neq i$.

4. One-Fluid Mixing. This is similar to the CS form, except that the expansion variable is taken to be the potential function itself instead of its parameters r_i^* and T_i^*. It yields a tractable result only for a power-law potential. The reference fluid is defined by the mean parameters

$$s_q = \sum_{i,j} x_i x_j T_{ij}^* (r_{ij}^*)^q, \quad q = n \text{ or } m ,$$

$$\bar{r}^* = (s_n/s_m)^{1/(n-m)} , \text{ and}$$

$$\bar{T}^* = s_m^{n/(n-m)}/s_n^{m/(n-m)} .$$

Again the thermodynamic functions are those of the reference fluid. The chemical potentials are those of the CS form but with

$$(n/\bar{T}^*) \quad \partial\bar{T}^*/\partial n_i = \left[2/(n-m)\right] \left(S_{ni}/s_n - S_{mi}/s_m\right) ,$$

$$(n/\bar{r}^*) \quad \partial\bar{r}^*/\partial n_i = \left[2 + 2/(n-m)\right] \left(mS_{ni}/s_n - nS_{mi}/s_m\right) , \text{ and}$$

$$S_{qi} = \sum_j x_j T_{ij}^* (r_{ij}^*)^q , \quad q = n \text{ or } m .$$

E. Chemical Equilibrium

Recall the definitions given in the input description:

c = number of independent species

= number of elements

s = total number of species

$p+1$ = Number of phases ($p=0$: gas only, $p=1$: gas + solid)

$\underset{\sim}{Q}$ = empirical-formula coefficients

$\underset{\approx}{\alpha}$ = species-formulae coefficients ,

and that, for a complete equilibrium calculation, the user supplies two possible systems: a one-phase system with the solid only nominally present as species number s, and a two-phase system with the solid present as species number c.

Symbols newly defined here are

$\underset{\sim}{q}$ = number of moles of each species for a system prepared from independent species only,

$\underset{\approx}{\nu}$ = stoichiometric (chemical reaction) coefficients of the dependent species (independent species have coefficient 1),

$\nu_k = \sum_{j=1}^{c-p} \nu_{kj}$ = change in number of moles of gas in reaction k,

n^s = number of moles of solid,

n^g = number of moles of gas,

x_i = (gas) mole fraction n_i/n^g except $x_c = n^s/n^g$ for solid present, and

K_k = equilibrium constant for reaction k.

We change to superscript s and g here for solid and gas to avoid confusion with indicial subscripts.

1. Initial Calculation. The initial calculation generates constants for the main calculation. Mathematically, it consists of a change of basis from (moles of) elements to (moles of) independent species. In the new basis each dependent species is expressed as a linear combination of independent species, with coefficients that are just the independent-species stoichiometric (chemical reaction) coefficients for the reaction producing one mole of the given dependent species from the independent ones. The system could, of course, be prepared from q_i moles of each independent species i (i = 1 to c) instead of Q_i moles of each element.

We now define some index conventions to simplify writing the equations. Divide the α-matrix into independent (c by c) and dependent (s - c by c) parts. Number the complete columns, and the rows of the independent part, with i or j. Number the rows of the dependent part with k. (See Fig. 3.) The ranges are

i and j: 1 to c

k: c+1 to s,

and denote by Σ_i or Σ_j a sum over i or j from 1 to c and by Σ_k a sum over k from c+1 to s. Then α and ν are solutions of the linear equations

$$\sum_i \alpha_{ij}\, q_i = Q_j, \quad j = 1 \text{ to } c \text{ and}$$

$$\sum_i \alpha_{ij}\, \nu_{ki} = \alpha_{kj}, \quad j = 1 \text{ to } c,\ k = c+1 \text{ to } s.$$

The dimensions of $\underset{\approx}{\nu}$ are the same as the dependent part of $\underset{\approx}{\alpha}$ and we retain the same usage and range of indices for it. (See Fig. 4.)

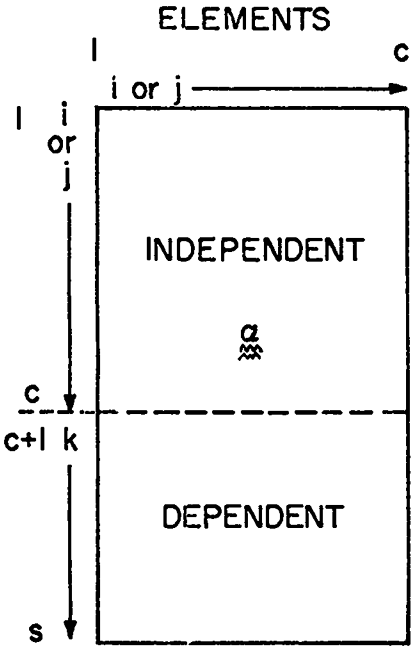


Fig. 3. The α-matrix.

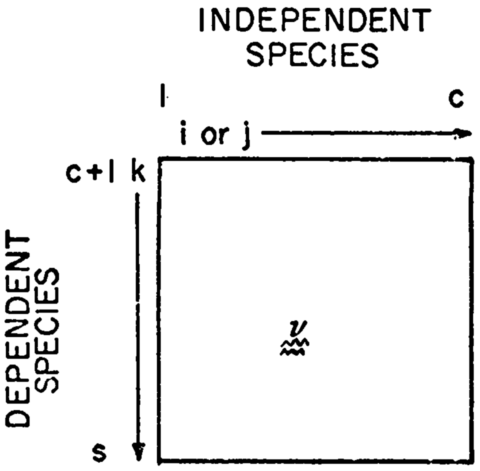


Fig. 4. The ν-matrix.

2. Main Calculation. We retain the above index conventions except that now in all sums except that in the definition of K_k the ranges of i and j are

$$i \text{ and } j: \ 1 \text{ to } c-p \ ,$$

and we use primes to denote sums or products over this range.

The equations can be reduced to a set of c-p equations in c-p unknowns; the remaining mole fractions are determined in the process of solving these or are calculated afterward. The equations are obtained by expressing the dependent species in terms of the independent ones, writing out the first derivatives, and applying the Newton-Raphson method of iteration. Letting superscript (n) number the iteration step, the result is

$$x_i^{(n+1)} = (1 + h_i^{(n)})\, x_i^{(n)}, \quad i = 1 \text{ to } c - p$$

(with super (n) understood in the following equations). The increments $h_j^{(n)}$ are the solutions of the linear set

$$\sum_j{}' A_{ij}\, h_j = \tilde{F}_i, \quad i = 1 \text{ to } c - p$$

$$A_{ij} = x_i\, \delta_{ij} + \sum_k x_k\, \nu_{kj}\, G_{ki}$$

$$F_i = -\bar{q}_i + x_i + \sum_k x_k\, G_{ki}$$

$$G_{ki} = \nu_{ki} - (\nu_k - 1)\, \bar{q}_i$$

$$\nu_k = \sum_j{}' \nu_{kj}$$

$$\bar{q}_i = q_i / \sum_j{}' q_j$$

$$x_k = K_k \Pi_j' x_i^{\nu_{ki}}$$

$$-\ln K_k = \tilde{F}_k - \sum_j \nu_{kj} \tilde{F}_j \quad .$$

The first equation is a linear system for the h_j. In the second equation δ_{ij} is the Kronecker delta, the x_i's are the independent-species mole fractions, and the x_k's are the dependent-species mole fractions, expressed in terms of the mole fractions of the first c - p species through the next-to-the-last equation, which is just the set of equilibrium-constant relations for the reactions. Finally $\bar{q}_i$ is the normalized q_i and ν_k the (gas) mole change in reaction k. The K_k and $\bar{q}_i$ are independent of the x's and are calculated at the beginning.

The x_k's, k = c+1 to s, are found in the process of solving this system. The number of moles of gas is

$$n^g = \left(\sum_j' q_j\right) \Big/ \left[1 + \sum_k \left(\nu_k - 1\right) x_k\right] \quad .$$

When the solid is present (p = 1) the c th equation is decoupled from the first c - p equations because, although each of the first c - p equations contains in general all of the first c - p x_i (by virtue of the presence of the x_i in the equilibrium-constant relations), none contain x_c (by virtue of its absence from the same). Thus, in this case, only the first c - p equations are solved iteratively, and then x_c is determined from the c th equation evaluated for this solution.

As mentioned earlier, in the complete equilibrium case, when a solid may or may not be present, the program carries two possible systems, one with and one without the solid. It begins by solving the case found to be correct on the previous entry, then tests to see if it has the correct one and switches to the other if necessary. If the two-phase system is solved, the test is the sign of the number of moles of solid; if it is positive, the choice was the correct one. If the one-phase system is solved, the test is as follows. Find the first reaction in the two-phase system that involves the solid. Call this the test reaction. In the two-phase system the mole fractions involved in it would have to satisfy

$$K_k = x_k / \Pi_j^{'} x_i^{\nu_{ki}} \quad .$$

(with K and the ν's, of course, from the two-phase system). Define a saturation index $\hat{s}$ for the test reaction as

$$\hat{s} = (x_k / \Pi_j^{'} x_i^{\nu_{ki}}) / K_k$$

and evaluate $\hat{s}$ for the x's (of the species involved) from the one-phase solution. If $\hat{s} < 1$ the system is unsaturated with respect to deposition of solid, and the one-phase choice was the correct one.

F. Miscellaneous

The actual Hugoniot and CJ iteration functions are given in Sec. V.B. (Table III). Note that the Hugoniot function uses enthalpy relative to T_0 and that h_0 is for the unreacted material.[†]

The "heat of reaction" q is defined, for products at given T, p, as the energy released by reaction of the unreacted material in the initial state (T_0, p_0) to products at the same temperature and pressure (but having the composition calculated at the given T, p)

$$Q = \left[x_g \Delta_g(T_0) + x_s \Delta_s(T_0)\right]_{\text{products}} - \left[\Delta(T_0)\right]_{\text{unreacted}} - RT_0$$

$$q = (n/M_0)Q \quad .$$

The particle velocity u and detonation velocity D are given by

$$u^2 = (p-p_0)(v_0-v)$$

[†] If the alternative procedure (heat of formation at T = 0 entered under CON, SAM, Sec. II) is followed, then the Hugoniot energies will be relative to T = 0. The value of Q will be that at T = 0, with the term ($-RT_0$) incorrectly subtracted.

$$\rho_0^2 D^2 = (p-p_0)/(v_0-v) \quad .$$

On the isentrope, the particle velocity u, which would require evaluation of the Riemann integral, is not calculated. For the isentrope whose initial point is a CJ point, the quasi-static work done by the explosive in expansion of the products to the given pressure, described in Appendix B,

$$W(p) = e_j - \frac{1}{2} u_j^2 - e_i(p)$$

is printed in the u-slot.

V. PROGRAM

The program listing, Appendix C, contains a list of all routines and common data blocks, with a one-line description of each. It also contains, with each routine, comments giving the routine's specifications. In most cases, the logic is simple enough that suitably placed internal comments suffice to describe it. The exceptions are collected here, in order of decreasing logical level in the program. A detailed list of the contents of all common data blocks is given in Appendix D.

A. Equilibrium Iteration - EQM

To calculate a state point at given T and p, MES calls TIM for the ideal free energies (F_i^i at the given T), and then SEM for the solid free energy $\mu_s' \equiv F_s'(T, p)$. It then calls EQM, which calls XIM for the gas mixture EOS in the process of finding the equilibrium compositon. Finally it calls TIM for the complete set of ideal functions at the new composition, and then COUT for the complete state.

Because of the multiplicity of EOS and mixture-rule options, EQM and XIM are the most complex routines of the program. EQM is outlined in Table II. Subscript i means all species; for example, $\hat{x}_i \leftarrow x_i$ means save all gas mole fractions. Also, only the most important input and output items of routines XIM and EQMS are indicated. In words, the solid $\tilde{F}$ is calculated once at the start because it depends only on T and p, which are here fixed. First, the mixture routine XIM(1) is called for the imperfection chemical potentials. These are then added to the ideal ones (calculated earlier by TIM) to get the $\tilde{F}_i$ which are the input to the (ideal, i.e., constant-$\tilde{F}_i$) equilibrium routine EQMS. The current

TABLE II

THE EQUILIBRIUM-EOS ROUTINE EQM

```
     $\tilde{F}_s \leftarrow F_s^i + F_s'$                        solid $\tilde{F}$, depends on T, p only
α    $\mu_i', r^* \leftarrow$ XIM(1)                       gas $\mu_i'$ ($r^*$ for LH & One-Fluid only)
β    $\tilde{F}_i \leftarrow F_i^i + \mu_i'$                        ($F_i^i$ from TIM earlier)
     $\hat{x}_i \leftarrow x_i$                                 save old $x_i$
     $x_i \leftarrow$ EQMS($\tilde{F}_i$, $\tilde{F}_s$)                    new $x_i$ at constant $F_i$
     if ($\Sigma|x_i - \hat{x}_i| < \varepsilon$): go to γ       done?
     $x_i \leftarrow 1/2\ (x_i + \hat{x}_i)$                      next guess: mean of new and old
     $\tilde{F}_i$, $\bar{r}^* \leftarrow$ XIM(2); go to β            (CS or One-Fluid only)
γ    if [(CS or One-Fluid) and
        ($|r^*-\bar{r}^*| < \varepsilon$)]: go to α             outer done?
     (gas state) ← XIM(3)                        final state
```

composition is saved for later use in the convergence test and in getting the next guess, and then EQMS is called to calculate the composition implied by the current $\tilde{F}_i$ and $\tilde{F}_s$. If the resulting composition change is small enough, this finishes the iteration for other than the CS or One-Fluid mixture rules (used only with LJD EOS). If not, the next guess for the composition is taken as the mean of the new and old values, new $\tilde{F}_i$ are computed by XIM(2), and the cycle is repeated starting at β. For the CS and One-Fluid mixture rules the completion of the above (inner) iteration is one step of an outer iteration whose convergence test is that the value of $\bar{r}^*$ from XIM(2) after the inner iteration is complete be close enough to its value furnished by XIM(1) at the start at α. This is discussed in more detail below.

We next describe the action of XIM, which is different for the different equations of state and mixture rules. Here GEP is the gas EOS routine, which gives the ideal-gas, LJD, or KW equations of state (according to the gas switch from CON, SWIT) and XIM chooses the mixture rule from this switch and the mix switch, which we here call k, from CON, SWIT or CON, XIP. For the LH, CS, and One-Fluid mixture rules, XIM calls XIMS for the detailed computations. The notation XMT ← GM indicates that the pure-fluid state in the GM array is moved to the mixture state in the XMT array. Also, T^* and V^* are to be understood in addition wherever r^* is indicated. The numbers (1), (2), and (3) refer to action taken at the XIM(i) calls, i = 1, 2, 3. The options are as follows:

- KW EOS

Recall that GEP calls HKW, which calculates the complete (mixture) EOS.

(1), (2), (3) HKW via GEP supplies the state, including the μ'_i.

- k=0: No-mix [normally used only for a pure fluid (single species)]

(1) GEP supplies the pure-fluid EOS for the input r^*. The μ'_i are all set to the pure-fluid F'_g, and XMT ← GM.

(2) No action.

(3) XMT ← GM.

- k=1: Ideal mix

(1) For each species, set r^* to r^*_i, call GEP for the pure-fluid EOS, and set μ'_i to F'_g.

(2) No action.

(3) Calculate all mixture imperfection quantities as linear mole-fraction sums of those for the individual species.

- k=2: LH mix

(1) Set r^* to the input reference-fluid value, then call GEP for the pure-fluid EOS, and call XIMS for the μ'_i.

(2) Call XIMS for the μ'_i.

(3) Call GEP for the final state, then XMT ← GM. (Why any action is needed here is no longer clear to me.)

- k=3: CS mix, and k=4: One-Fluid mix

(1) Call XIMS to get $\bar{r}^*$, set r^* to $\bar{r}^*$ and call GEP for the EOS, then XIMS for the μ'_i. (XIMS calculates both $\bar{r}^*$ and the μ'_i, using the reference-fluid state. Here two calls on it are necessary, the first gets r^*, which is needed for the reference-fluid state. There are actually two entries to XIMS that are not distinguished here; the first calculates only $\bar{r}^*$, the second both $\bar{r}^*$ and the μ_i.)

(2) Call XIMS for the μ_i' and $\bar{r}^*$.

(3) No action.

The outer iteration described earlier is necessitated by a time-saving device introduced in GEP. A second entry GEP(2) calculates the approximate gas EOS (for LJD) by the quick route of the LH expansion from the reference state currently stored. This time-saving entry is used by XIMS to get the gas state required for the calculation of the μ_i. Where the mean r^* depends on composition as for the CS and One-Fluid mixture rules, the validity of this expansion is ensured by the outer iteration.

B. Iterations

The iterations are tabulated in Table III. All except that for the equilibrium composition described above can be written as a function of a single variable and are controlled by FROOT. Note that the gas and solid EOS iterations, independent and on the same level, must both be completed as part of the equilibrium iteration, which must in turn be completed as part of the calculation of the function for the Hugoniot or constant-v, s, or e iterations. Finally the Hugoniot iteration must be completed as part of the calculation of the function for the CJ iteration. This stacking requires careful adjustment of the convergence criteria for a reliable system. The functions chosen are not too nonlinear and their magnitudes and slopes are reasonable size (the factor of 20 in the Hugoniot function is introduced for this reason). In general there are slots in CON, FOB for several constants for each FROOT iteration: (1) The convergence criterion ε, (2) The "guess-constant" r, in most cases the ratio of the second to first guess, and (3) upper and lower bounds for the iteration variable or the related physical quantity. Not all of (2) and (3) are used in every case. Under "Bounds", subscripts min and max denote (3), other bounds are computed as indicated. Finally, we use subscripts 1 and 2 in the "Guesses" column to denote iteration steps 1 and 2. Remarks on some of the iterations follow.

- CJ

For the second guess, a constant-γ isentrope is a sufficiently good approximation to the CJ locus. For the lower bound, we use the constant-γ approximation to the constant-volume detonation pressure. In the function, γ is evaluated for either fixed or equilibrium composition according to the setting of the input switches; thus either a frozen or equilibrium CJ point may be obtained.

TABLE III

ITERATIONS

Iteration for[a]	FROOT C-array	In Routine	Guesses	Bounds	Independent Variable x	Function f(x)
Chapman-Jouguet	CC	CJ	p_1 = previous (0.3) [b] $p_2 = p_1\,(v_1/v_2)^{\gamma_1}$ $v_2 = g\,(p_1)$	$p > \frac{1}{2}(\gamma-1)\rho_0 q \cong p_H(\rho_0)$	p	$j(p) - 1$ $j(p) = \left[\frac{v/v_0}{\gamma\left(\gamma+1 - p_0/p\right)}\right]^{-\gamma}$
Hugoniot	CH	HUG	T_1 = previous (3000) $x_2 = x_1 - f_1/f_1'$ [c]	$T > T_{min}$ $T < T_{max}$	T/1000	$20\left[\frac{h\left(T;T_0\right) - h_0\left(T_0:T_0\right)}{\left(p-p_0\right)v_0} - \frac{1}{2}\left(1 + \frac{v}{v_0}\right)\right]$ [d]
Contour (constant-v, s, or e)	CM	MESC	T_1 = previous $T_2 = r\,T_1$	none	T	v: $v-v_c$ s: $e^{s/s_c} - 1$ e: $e-e_c$
Gas EOS	CG	GEP	x_1 = previous (ℓn 10) $x_2 = x_1 - f_1/f_1'$	$V_g > V_{g\ min}$ $V_g < V_{g\ max}$	$\ell n\ V_g$	$\ell n\left[\tilde{p}\left(V_g,T\right)/p\right]$
Solid EOS	CS	SEMS	x_1 = previous (0.8) $x_2 = rx_1$	$x > x_{min}$ $x < 1+\alpha(T-T_0)$	V_s/V_{so}	see Sec. IV
Equilibrium composition	See Sec. V.A.					

---

[a] The order given is that of the CON, FOB input corresponding to that of the C-arrays in store. Logically, the equilibrium-composition iteration be just above that for the gas EOS, and the gas and solid EOS are on the same level as are the Hugoniot and the contour.

[b] The value in parentheses is used on first entry.

[c] On first entry, $f' = r$.

[d] The energy zero for h is T_0; see Sec. IV.A.

•Hugoniot

The value of f' for the second guess is that calculated by numerical difference on the last step of the iteration for the previous point. On the first time through it is the input guess-constant r.

•Gas

The derivative f_1' for the second guess is calculated from the derivative $(\partial p/\partial V_g)_T$ furnished by the gas EOS routine GEM.

•Solid

The function, given in Sec. IV.B, is based on the isentrope relation. The quantity α in the upper bound is the thermal-expansion coefficient.

C. LJD Gas EOS Integration (In GES)

As shown in Fig. 5 the problem is to evaluate to prescribed accuracy for any α an integral

$$\int_0^{b^*} f(x;\alpha)dx \quad ,$$

with the integrand depending on α in such a way that for some α it effectively vanishes at some x appreciably less than b^*. We use the 16-point Gauss approximation (Sec. IV.C); its straightforward application to this case would waste those points lying in the region of $f(x) \cong 0$. (Actually all seven integrals are done at the same time; for simplicity the description here is for one.)

The method is to check for the vanishing of the integrand and to perform the integration in segments if necessary. Because α changes little between most of the entries, this turns out to be reasonably efficient. The part of GES that does the integration consists of a control code, which chooses and adds the segments, and a procedure that integrates over a segment and reports how soon the integrand becomes negligible, if at all. All segment lengths are $b^*/2^n$, n integral.

The segment integration procedure $\mathcal{I}(b_1, b_2)$ evaluates $\int_{b_1}^{b_2} f(x;\alpha)\,dx$ by the 16-point Gauss method and reports three conditions for the size of the integrand near the end of the interval. Let i (i = 1 to 16) be the Gauss point at which the integrand first becomes negligibly small. Then I reports that the upper limit b_2 is

"too small" for no such i (LD = 1),

"just right" for $14 \leqslant i \leqslant 16$ (LD = 3), or

"too large" for $i < 14$ (LD = 2),

LD being the Fortran variable that reports the condition. (The actual test is that the condition $|f(x_i)/\sum_{j=1}^{i} a_j\, f(x_j)| < \varepsilon$ be satisfied for each of the seven integrals). The algorithm which evaluates the complete integral using the segment procedure $\tilde{I}\,(b_1, b_2)$ is given in Table IV.

D. FROOT-Solve f(x) = 0 by Iteration

Number the successive steps in the iteration 1, 2, 3, ..., n, ... with <u>n</u>th (function) argument x^n and function $f^n \equiv f(x^n)$. The complete current state of the iteration is contained in FROOT's argument array $\underset{\sim}{c}$

$\underset{\sim}{c}$ 1 ε - convergence: $|f^n| < \varepsilon$

2 x^n

3 f^n

4 x^{n-1}

5 f^{n-1}

6 x^{n-2}

7 f^{n-2}

8 n - step number

9 k - branch index:

- 1 - finished ($|f^n| < \varepsilon$)
- 2 - continue
- 3 - error 1: $\tilde{x}^n = x^n$ (see below)
- 4 - error 2: $f^n = f^{n-1}$.

Each time it is called, FROOT bumps n by 1, finds the new x^n and returns to the user, who calculates $f^n = f(x^n)$ and calls FROOT again. The user exits from this loop on convergence via the branch number k. The prototype program is (ε prestored)

$$n \leftarrow 0, \quad x^n \leftarrow x_g^2, \quad x^{n-1} \leftarrow x_g^1$$

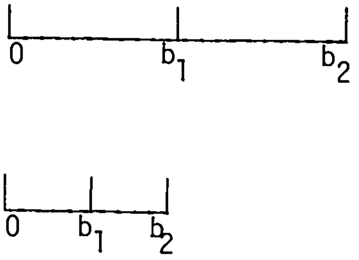
TABLE IV

ALGORITHM FOR THE CELL INTEGRAL

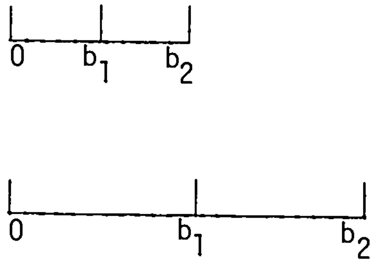
```
$\alpha$ $b_2 \leftarrow b'$, $b_1 \leftarrow b'/2$                    b' is upper limit from
                                                   last entry
  $I \leftarrow \tilde{I}(0,b_1)$                               first segment
  if ($b_1$ just right):  done
  if ($b_1$ too large):  <$b' \leftarrow b^*/2$, go to $\alpha$>        halve and start again
  if ($b_1$ too small):
     <$\beta$ $I \leftarrow I \pm \tilde{I}(b_1, b_2)$                    add 2nd segment
     if ($b_2$ too large or right):  done
     if ($b_2$ too small):  < $b' \leftarrow 2b'$,                double
            $b_2 \leftarrow b'$, $b_1 \leftarrow b'/2$, go to $\beta$ >>
```

The upper limit b' (not shown is that b' is bounded $\leqslant b^*$) is saved each time and used as the first guess on the next entry. The successive segments look like

b_1 too large



b_1 too small



```
$\alpha$  CALL FROOT
    GO TO ($\beta$, $\gamma$, $\delta_1$, $\delta_2$) k
$\gamma$  calculate $f^n \equiv f\ (x^n)$
    GO TO $\alpha$
$\delta_1$, $\delta_2$  error handling
$\beta$  done, proceed
```

Here n, x^n, etc., refer to slots in $\underset{\sim}{c}$ as indicated above. The user starts the iteration by setting the step index n to zero and supplying x_g and x_g^2, the first two guesses for x. The iteration then proceeds through the α-γ loop to convergence. Because all the current state is in $\underset{\sim}{c}$ (and none of it is stored in FROOT), one copy of FROOT can simultaneously control any number of interdependent iterations (i.e., the calculation of f(x) for some iteration may itself require an iterative solution involving FROOT).

The algorithm is the secant method

$$x^1 = x_g^1 \quad ,$$

$$x^2 = x_g^2 \quad ,$$

$$x_n = x^{n-1} - f^{n-1}\ (x^n - x^{n-1})/(f^n - f^{n-1}) \quad ,$$

with a refinement wherein $\tilde{x}^n$ is a provisional value of x^n subject to modification. In the normal case it is accepted and the store is stepped down as follows:

$$(x,f)^{n-2} \leftarrow (x,f)^{n-1} \quad ,$$

$$(x,f)^{n-1} \leftarrow (x,f)^{n} \quad ,$$

$$x^n \leftarrow \tilde{x}^n \quad .$$

The modification replaces $\tilde{x}^n$ if, roughly, it does not lie in the range of previous x's and if two f's of opposite sign are on hand. Precisely, if

(1) $\tilde{x}^n$ is not between x^n and x^{n+2}, and

(2) (sign f^n = sign f^{n-1}) and (sign $f^n \neq$ sign f^{n-2})

then $\tilde{x}^n$ is recalculated (before the step-down) with point (n-2) instead of (n-1)

$$\tilde{x}^n = x^n - f^n (x^n-x^{n-2})/(f^n-f^{n-2}) \quad .$$

Also, saving of old points is done in such a way that once two f's of different sign are on hand, the step-down will never result in three f's of the same sign. Precisely, if condition (2) is satisfied, then the step-down is preceded by

$$(x,f)^{n-1} \leftarrow (x,f)^{n-2} \quad .$$

We remark that, because $\underset{\sim}{c}$ specifies the state completely, the user, knowing the program's algorithm, may wish to change it in flight. A common case is that a lower bound x^* is known for x, and FROOT at some step supplies $x^n < x^*$. The user might replace x^n by x^* whenever this happens.

As an example (see Fig. 6), we write the code to solve $f(x) = x^{1/2} - A = 0$. The secant recipe can easily give a negative x as the next guess; we prevent this by introducing a fixed lower bound $x = x^*$, x^* small.

```
     DATA  C(1)/1.0 E-8/
     DIMENSION C(9), KC(2)
     EQUIVALENCE (KC, C(8))
     KC(1) = 0
     C(4) = 1.
     C(2) = 1.2
  α  CALL FROOT (C)
     GO TO (β, γ, δ, δ) KC(2)
```

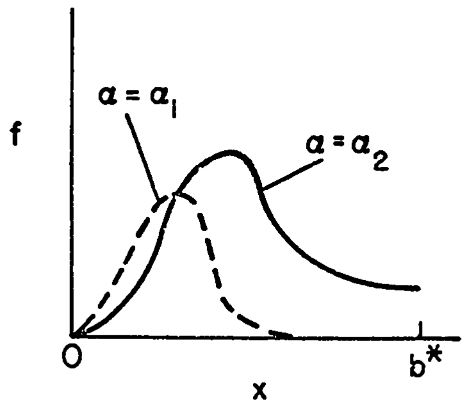


Fig. 5. Integrands for the LJD cell integral.

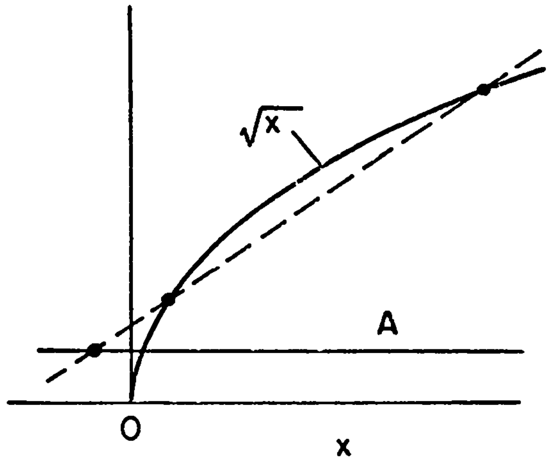


Fig. 6. Iterative solution of $f(x) = x^{1/2} - A = 0$ by FROOT.

```
γ  IF (C(3) < $x^*$) C(3) = $x^*$
   C(3) = SQRT (C(2)) - A
   GO TO α
δ  CALL ERR
β  CONTINUE
```

VI. SAMPLE INPUT/OUTPUT AND TEST

Tables V and VI are a key to the output labels and a sample calculation, which also serves as a fairly complete test of the program. The calculation is a chemical equilibrium calculation for the explosive RDX with the LJD EOS and the CS mixture rule. Part 2 of the input defines the following:

(1) A state point at $T = 2000$, $p = 0.3$.

(2) Detonation Hugoniot points at $p = 0.3$ and 0.2.

(3) CJ points for $\rho_0 = 1.6$ and 1.8.

(4) CJ isentrope points at $p = p_{CJ}$, 0.3, and 0.2.

A CON, DBUG print follows item (1). The point printed here is the last slightly displaced one used in the finite-difference calculation of the derivatives.

TABLE V

OUTPUT KEY

Line							
1	p	v/v_0	T	u or W	D	ρ_0	q
2	v	e	s	n_g	n_s	n	$(\ln \hat{s}$ or $- \hat{n}_s)$
3	V	E/RT	S/R	z	n_1	n_2	n_3
4	V_g	E'_g/RT	S'_g/R	z'_g	n_4	n_5	n_6
5	V_r	E'_r/RT	S'_r/R	z'_r	n_7	n_8	n_9
6	V_s	E'_s/RT	S'_s/R	z_s	n_{10}	n_{11}	n_{12}
7	$\bar{r}^*$	$\bar{T}^*$	$\bar{V}^*$	γ	α	β	c

Notes

1. Lines 1-3 are for the complete system. For lines 4-6 the first four items are for the gas phase, the gas-phase reference fluid, and the solid phase, respectively. The reference fluid differs from the gas phase only for the LH mixing rule (Sec. IV.D.2).

2. The last item in line 2 gives the state of super- or undersaturation of the system with respect to the solid phase; $\ln \hat{s}$ (the saturation index, Sec. IV.E) is printed if a single-phase system was specified and it wants to precipitate solid, and $-\hat{n}_s$ (the number of added moles of solid which would just saturate the system) is printed if a two-phase system was specified and no solid is present.

3. All mole numbers are moles per mole of system (one mole of system = M_0 grams, with M_0 from the SAM input pack).

4. The "u or W" slot in line 1 is the particle velocity for the Hugoniot or CJ point, the quasi-static expansion work (Sec. IV.F and Appendix B) for the CJ isentrope, and meaningless otherwise.

5. All other symbols are defined in the symbol list. Recall that $z \equiv pV/RT$ (and $z' = pV/RT - 1$) and that a prime denotes an imperfection quantity (Secs. III.B.1-3). Molar quantities for the system are per mole of system and for the phases are per mole of phase. All quantities divided by RT are dimensionless.

TABLE VI

SAMPLE CALCULATION

Input Data

```
CON   PAS   MES1 - SHORT TEST - CJ, HUG, ISENTROPE
CON   SWIT  DIFF
        1
CON   F08
 5.0    E-05  2.0    E-06  1.2    E-05  7.0    E-07  1.0    E-07  0.0
 0.0          1.0          1.1          0.0          9.7    E-01  0.0
 1.01         1.01   E-02  1.0    E-05  2.0    E-06  0.0           0.0
 1.0    E-03  1.0    E+06  5.0    E+02  8.0    E+03  4.3    E-01  0.0
 0.0          0.0          0.0          0.0          0.0           0.0
CON   GEP
      2     1
 1.0    E-01 6.0    E+00 1.0    E+00 1.0    E+00 4.4365 E+00 7.54837E+01
CON   SEP
 1.656  E-01  2.5          8.03  E-06  5.333       2.9816E+02  4.246 E-01
 0.0          3.2751       -7.9015     6.6656      -2.0392     0.0
CON   TIP
      8     4
 1.6    E+03 6.0    E-03
 4.8761 E-01 1.4949 E-03 -4.2896E-07 6.2644 E-11 -3.4991E-15 -2.81   E+00
 0.0    E+00 0.0    E+00 4.2457 E-01
3.1499  E+00 5.8718 E-24 -1.3665E-07 1.6756 E-11 -8.2278E-16 4.673  E-00
 0.0    E+00 0.0    E+00 3.4975 E-00
 3.1318 E-00 5.9459 E-04 -1.4065E-07 1.7307 E-11 -8.47   E-16 5.2157 E+00
 -2.7272E+01 -2.6416E+01 3.4979 E-00
 3.28222E+00 1.18370E-03 -2.1492E-07 2.28480E-11 -1.0874E-15 3.19230E+00
 -5.7107E+01 -5.7798E+01 3.99610E-00
 3.327  E+00 5.80470E-04 -1.5608E-07 2.04140E-11 -1.0944E-15 5.93   E+00
 2.1477 E-01 2.16   E+01 3.7032 E-00
 3.2375 E-00 2.3187 E-24 5.0938 E-09 -3.9631E-12 2.931  E-16 -2.8804E+00
 0.0    E+00 0.0    E+00 3.4157 E-00
 3.7308 E-00 1.9444 E-03 -5.121  E-07 6.8031 E-11 -3.5368E-15 3.4656 E-00
 -9.3969E-01 -9.4052E+01 3.7772 E-00
 3.4234 E+00 4.55   E-04 -8.0583E-08 9.4557 E-12 -4.8556E-16 4.862  E+00
 0.0    E+00 0.0    E+00 3.4934 E-00
CON   XIP    H2 - BEST MCM SET FROM OTHER SOURCES ,GMX-10-54,P43
      7     2
 1.0    E+00 1.0    E+00 3.80012E-00 1.41744E+02 6.0    E-00 1.2    E+01
 4.05   E+00 4.05   E+00 3.35   E-00 3.56   E+00 3.34   E+00 4.2    E+00
 3.73   E-00
 1.2    E+02 1.2    E+02 1.38   E+02 1.31   E+02 3.7    E+01 2.0    E+02
 1.32   E+02
CON   EQP
    4       8       1       0       1       1
   3.0           6.0             6.0             6.0
            C       H       O       N      A1      A0
   C(S)     1       0       0       0
     N2     0       0       0       2
     CO     1       0       1       0
    H2O     0       2       1       0
     NO     0       0       1       1
     H2     0       2       0       0
```

```
   CO2      1      0      2      0
    O2      0      0      2      0
     4      1      6      3      7      5      2      8
     8      1      2      3      5      4      6      7
CON   3AM   RDX, RHO=1.8, CO2=ARBITRARY COMPOSITION GUESS
     8
 1.8     E+00 0.0     E+00 2.9816 E+02 2.2213 E+02 1.471  E+01
 1.5     E+00 3.0     E+00 0.0    E+00 3.0    E+00 0.0    E+00 0.0    E+00
 1.5     E+00 0.0     E+00
CON   PV
     1      0
 2.0     E+03  3.0    E+01
 0.0     E+00  0.0    E+00
CON   DBUG
CON   TED   OETCNATION HUGDNIOT
   0.3          0.2          0.0
CON   CJ    CJ LOCUS
  1.6           1.8
CON   PV    CJ ISENTROPE
     3      1
     3.0          0.0
     0.3          0.2
CON   REND
CON   JEND
```

Calculation

```
FESI - 744:620                          MESI - SHORT TEST - CJ. HUG. ISENTHOPE
YFICKET13".      .004 SEC ON RUN.      .056 SEC ON JOB

CON   SWIT  DIFF
DIFF. FX DIFF. GAS. SOLID. MIX. EO. CJ. PV
    1    -0    -0    .0    .0    .0    .0    .0    .0    .0    .0    .0

CON   FOR
   FROOT FPSI(CC.CH.CM.CG.C5.C)/ RATIOS/ DP.OT.EPSIN.OUT/ FROOT  ROUNOS
      5.00000E-05  2.00000E.06  1.20000E-05  7.00000E.07  1.00000E.07
      0.           0.           1.00000E.00  1.10000E.00  0.
      9.70000E-01  0.           1.01000E.00  1.01000E.02  1.00000E.05
      2.00000E.06  0.           0.           1.00000E.03  1.00000E.06
      5.00000E.02  8.00000E.03  4.30000E.01  0.           0.
      0.           0.           0.           0.           0.

CON   GEP
0      POT (1=LJ/2-MCM,3=MRI .W (NOW 1)  / N.M.AN.AN.R*.T*
   2       1
      1.00000E.01  6.00000F.00  1.00000E.00  1.00000E.00  4.43650E.00
      7.54837E.01
V*        37.2000300

CON   SEP
CX     G. CPH. AL. V0. T0. FOR / C0. C1. C2. C3. C4
      1.65600E-01  2.50000E.00  8.03000E-06  5.33300E.00  2.98160E.02
      4.24600E-01  0.           3.27510E.00 -7.90150F.00  6.66560E.00
     -2.03920E.00  0.
```

```
CON   T1P
    KS,KN/ T BOUNDS/ FIT COEFFS.-A1 TO AN,Q,DEL,HF,HR...
    8      4
      1.50000E•03  6.00000E•03
      4.87610E-01  1.49490E•03 -4.28960E•07  6.26440E•11 •3.49910E•15
     •2.81000E•00  0.            0.            4.24570E•01
      3.14990E•00  5.87180E•04 •1.36650E•07  1.67560E•11 •8.22780E•16
      4.67300E•00  0.            0.            3.49750E•00
      3.18180E•00  5.94590E•04 -1.40650E•07  1.73070E•11 •8.47000E•16
      5.21570E•00 -2.72020E•01 •2.64160E•01  3.49790E•00
      3.29220E-00  1.18370E-03 •2.14920E•07  2.28490E•11 •1.08740E•15
      3.19230E•00 •5.71070E•01 -5.77980E•01  3.99610E•00
      3.32700E•00  5.80470E-04 •1.50080E•07  2.04140E•11 •1.09440E•15
      5.93800E•00  2.14770E•01  2.16000E•01  3.70320E•00
      3.23750E•00  2.31870E•04  5.09380E•09 •3.96310E•12  2.93100E•16
     •2.88040E•00  0.            0.            3.41570E•00
      3.73080E•00  1.94440E-03 •5.12100E•07  6.80310E•11 •3.53680E•15
      3.46550E•00 •9.39690E•01 •9.40520E•01  3.77720E•00
      3.42340E•00  4.56000E•04 •8.05830E•08  9.45570E•12 •4.85560E•16
      4.86200E•00  0.            0.            3.49340E•00

CON   AIR     M2 - BEST MCM SET FROM OTHER SOURCES .GMX-10-54.P43
   KR,KAL/ SCR,SCT,R*EFF,T*EFF,N,M/ (R*)/ (T*)
    7      2
      1.00000E•00  1.00000E•00  3.80012E•00  1.41744E•02  6.00000E•00
      1.20000E•01
      4.05000E•00  4.05000E•00  3.35000E•00  3.56000E•00  3.34000E•00
      4.20000E•00  3.73000E•00
      1.20000E•02  1.20000E•02  1.38000E•02  1.31000E•02  3.70000E•01
      2.00000E•02  1.32000E•02

CON   EQP
     C,S,P,-,PP,PHI / CAP Q
    4      8  .  1      0      1      1

      3.00000E•00  6.00000E•00  6.00000E•00  6.00000E•00

                  C      H      O      N     A1     A0
        C(S)      1      0      0      0      4      8
          N2      0      0      0      2      1      1
          CO      1      0      1      0      6      2
         H2O      0      2      1      0      3      3
          NO      0      0      1      1      7      5
          H2      0      2      0      0      5      4
         CO2      1      0      2      0      2      6
          O2      0      0      2      0      8      7

     QBAR         .3333333E•00   .3333333E•00   .3333333E•00  0.

     NU MAT       .5000000E•00  0.              .1000000E•01  -.1000000E•01
           2    0.               .1000000E•01   .1000000E•01  -.1000000E•01
           3    0.              0.              .2000000E•01  -.2000000E•01
           4    0.               .1000000E•01  -.1000000E•01   .1000000E•01

     QBAR         .4000000E•00   .2000000E•00   .4000000E•00

     NU MAT     0.              -.5000000E•00   .1000000E•01   .5000000E•00
           2    0.               .5000000E•00  0.              .5000000E•00
           3     .5000000E•00    .5000000E•00  0.             -.5000000E•00
           4    0.               .1000000E•01  0.             -.1000000E•01

CON   SAM   RDX. RHO=1.8, CO2-ARBITRARY COMPOSITION GUESS
```

```
MES1 - 76AUG20                     MES1 - SHORT TEST - CJ. HUG. ISENTROPE                                               09/02/76
TFICKETIGN.     .055 SEC ON RUN.     .107 SEC ON JOB                                                              SAM - INPUT PART 2
  KS/ RHO. PO, TO. MO. HFE/ NI
    8
       1.80000E+00  0.             2.98160E+02  2.22130E+02  1.47100E+01
       1.50000E+00  3.00000E+00  0.             3.00000E+00  0.
       0.           1.50000E+00  0.

CON   PV

MES1 - 76AUG20                     MES1 - SHORT TEST - CJ. HUG, ISENTROPE                                               09/02/76
TFICKETIGN.     .063 SEC ON RUN.     .115 SEC ON JOB                                                                       LOCUS
  BRANCH (1-T,2-V,3-S,4-E) / TC.PC/ P-TABLE
    1     0
       2.00000E-03  3.00000E-01
       0.

        OUTPUT LABELS

              1     P              V/V0           T              U              D              RHO            QCAL
              2     V              E              S              NG             NS             N              SUPSAT
              3     V              E/RT           S/R            PV/RT          N1             N2             N3
              4     NO. FOR GAS                                                 N4.N5.N6
              5     NO. FOR REF.                                                N7.N8.N9
              6     NO. FOR SOLID                                               N10.N11.N12
              7     RBAR*          TBAR*          VBAR*          GAMMA          ALPHA          BETA           C

POINT   1     1   3.0000000E-01  6.2501147E-01  2.0000000E-03  0.             0.             1.8000000E+00  1.5056345E+00
              2   3.4722859E-01 -6.5145242E-03  5.6504530E-05  7.5019585E+00  1.4980495E+00  9.0000080E+00  1.9968779E+01
              3   8.5699799E+00 -9.6691129E-01  1.6773249E+01  1.5461110E+01  1.4980495E+00  2.9999918E+00  2.5002893E-03
              4   9.5186840E+00  4.8978060E+00 -1.5675174E+00  1.6172668E+01  2.9985825E+00  1.6077797E-05  1.4173827E-03
              5   9.5182069E+00  4.8980736E+00 -1.5673720E+00  1.6171806E+01  1.4994504E+00  6.9640955E-11  0.
              6   3.8190426E+00  1.1026119E+00 -1.4349374E-01  6.8899389E+00  0.             0.             0.
              7   3.9000514E+00  1.4179073E+02  2.3377078E-01  3.1776524E+00  4.7999481E+00  1.8252305E+00  5.7533602E-01

CON   OBUG


        OUTPUT LABELS

              1     P              V/V0           T              U              D              RHO            QCAL
              2     V              E              S              NG             NS             N              SUPSAT
              3     V              E/RT           S/R            PV/RT          N1             N2             N3
              4     NO. FOR GAS                                                 N4.N5.N6
              5     NO. FOR REF.                                                N7.N8.N9
              6     NO. FOR SOLID                                               N10.N11.N12
              7     RBAR*          TBAR*          VBAR*          GAMMA          ALPHA          BETA           C

POINT   2     1   3.0000000E-01  6.2460797E-01  2.0000000E-03  0.             0.             1.8000000E+00  1.5056645E+00
              2   3.4722859E-01 -6.8373056E-03  5.6308524E-05  7.5017720E+00  1.4982350E+00  9.0000070E+00  1.9971748E+01
              3   8.5644482E+00 -1.0251742E+00  1.6715067E+01  1.5608779E+01  1.4982350E+00  2.9999930E+00  2.2461195E-03
              4   9.5123182E+00  4.9430188E+00 -1.5737043E+00  1.6336280E+01  2.9987042E+00  1.4021508E-05  1.2958093E-03
              5   9.5116041E+00  4.9433074E+00 -1.5735481E+00  1.6335343E+01  1.4995168E+00  5.4543140E-11  0.
              6   3.8183935E+00  1.1149935E+00 -1.4354516E-01  6.9590543E+00  0.             0.             0.
              7   3.8000467E+00  1.4179416E+02  2.3376903E-01  3.1776524E+00  4.7999481E+00  1.8252305E+00  5.7533602E-01
```

```
CAR - CC/CH/CB/CG/ES/CE
              5.0000E-05             0             0             0             0             0             0             0             0             0
        11    2.0000E-06             0             0             0             0             0             0             0             0             0
        21    1.2000E-05             0             0             0             0             0             0             0             0             0
        31    7.0000E-07     2.2525336    1.4990E-08     2.2536794   -4.0977E-03     2.2538794    1.3987E-07             2             1             0
        41    1.0000E-07      .7159935   -6.9344E-08      .6947497   -7.0571E-03      .7162368    8.0800E-05             3             1             0
        51             0             0             0             0             0             0             0             0             0             0
DER             .3000000      .3472286    2.0000E-03    15.4611100      .3474532      .3470044    2.6194E-05    2.5985E-05             0             0
CCNT           1.9871900    8.3144E-05    1.0133E-06      .0418400      .4260120    OUTvvvvvvv             0             0             0             0
EMG            5.5463507    11.5144119     3.8396325   -1.1803E-01     8.6697400     5.7635820   -1.2483E-01     6.0081464             0             0
EMN            7.5017720     1.4982350     9.0000070      .8335296      .1664704      .0405168      .1997175             0             0             0
EMX             .1997175      .3999046    2.9968E-04      .3997328    1.8631E-06    1.7273E-04      .1998884    7.2707E-12             0             0
FMU            5.5463507    10.5983826    -4.2731680   -1.2720E-01    -4.5203174    -2.9001771   -1.4093E-01   -1.9639E-01             0             0
FN             1.4982350     2.9999930    2.2481E-03     2.9987042    1.4022E-05    1.2958E-03     1.4995168    5.4543E-11             0             0
FOB           5.0000E-05    2.0000E-06    1.2000E-05    7.0000E-07    1.0000E-07             0             0     1.0000800     1.1000000             0
        11      .9700000             0     1.0100000      .0101000    1.0000E-05    2.0000E-06             0             0    1.0000E-03    1.0000E-06
        21   500.0000000    8.0000E-03      .4300000             0             0             0             0             0             0             0
        31             0             0             0             0             0             0             0             0             0             0
GM              .4068639    13.9674342    17.3353432     4.9433074    22.8521988     3.4805650   -3.5445E-01     1.3783533     8.9631098    16.3353432
        11    -1.5735481     -.0960282    3.0424E-05    3.1682E-04     9.5118041      .3000000    21.2786506    13.6869471     3.5092382     6.5168555
        21    7.7477E-03      .2137223             0             0     3.1614524     4.4353851     1.7192683     3.0446711     6.2135484    3.3309E-05
GP            10.0000000     6.0000000     1.0000000     1.0000000     3.8001200   141.7440000    23.3783451             0             0             0
HE             1.8000000             0   298.1600000   222.1300000    14.7100000      .5555556    2.7707E-03             0             0             0
BS            ^^^^^^^^^^    PAS^^^^^^^    SWIT^^^^^^    FOB^^^^^^^    ^^^^^^^^^^    DIP^^^^^^^    DIS^^^^^^^    DIG^^^^^^^    ^^^^^^^^^^    GEP^^^^^^^
        11    SEP^^^^^^^    TIP^^^^^^^    XIP^^^^^^^    EOP^^^^^^^    ^^^^^^^^^^    SAM^^^^^^^    YEO^^^^^^^    PV^^^^^^^^    CJ^^^^^^^^    TEST^^^^^^
        21    CHEC^^^^^^    ^^^^^^^^^^    SPEC^^^^^^    SPECI^^^^^    ^^^^^^^^^^    CORE^^^^^^    DBUG^^^^^^    LOAD^^^^^^    ^^^^^^^^^^    ^^^^^^^^^^
        31    ^^^^^^^^^^    ^^^^^^^^^^    ^^^^^^^^^^    FORM^^^^^^    REND^^^^^^    JEND^^^^^^    ^^^^^^^^^^    ^^^^^^^^^^    CON^^^^^^^    ^^^^^^^^^^
        41             0             0             0             0             0             0             0             0             0             0
EA             3.0384415     4.3249603     4.3544083     6.0676472     4.4102504     4.1150092     7.2481605     4.5376236             0             0
        21     2.1982201     3.8941711     3.9289667     4.9438824     4.0295596     3.6902711     6.0466781     4.0762518             0             0
        41    -7.7289125    17.6638773    18.4597811    19.1471831    20.1923019    10.0089666    24.5109752    19.6701102             0             0
        61    -6.8346448    -5.8346448     5.6058558    20.6832141   -4.1912E-01    -6.4741709     2.1982201     3.0384415     4.8694622    -2.6712422
        71             0     2.1342794             0             0             0             0             0             0             0             0
EV            6.6694E-03   -1.9277E-05    8.0466E-04    5.1418E-04    1.5617E-04             0             0             0             0             0
FLAB          MESIA-ASHO    RTATESTA-A    CJ.AHUG.AI    SENTROPEAA    ^^^^^^^^^^    ^^^^^^^^^^    ^^^^^^^^^^             0             0             0
GMT                    0             0             0             0             0             0             0             0             0             0
KEV                    1             0             0             0             0             0             0             0             0             0
SPC            -.0124245             0             0    19.7771739    -6.7789121     3.0779461     -.6441749             0             0     2.8097975
KAL                    1             0             1             1             2             1             0             1             0             0
        11             0             0
KON                    0             0             0             0             0             0             0             0             0             0
        51             0             0             0             0             0             0             0             0             0             0
KEN                   11             5            10            15             5             5             0             0             2             0
        11             2             0             2             5             0             0             0             0            11             0
KIM                    7             8             4             4             0             0             0             0             0             0
PT                     0             0            -0            -0            -0            -0             0             0             0             0
RHOT                   0             0             0             0             0             0    FIOvvvvvvE    DVVCSvvvvv    BEWAHMIGIP    MIBAR3+I]X
SM             3.8183935     1.1149935     8.0740477     1.2585386     8.2175929     -.1435452     6.9590543             0      .7159935     1.0126165
        11    1.9794E+03    1.8693E-03      .2862833             0    -1.1971305      .2850152      .0126165      .0147211     1.0135036             0
SP              .1656000     2.5000000    8.0300E-06     5.3730000   298.1600000      .4246000             0     3.2751000    -7.9015000     6.6656000
        11    -2.0392000             0      .6895949      .8579272     6.5386473     2.6338046             0      .8579272     -.0609440      .0232009
SUC           2.0000E-03      .3000000      .3472286    5.6505E-05   -6.5145E-03             0             0             0             0             0
SUCG           3.1776524     -.7999481     1.8252305      .5753360      .8664209     3.0700306     5.7377295    3.1992E-05             0             0
THER            .3300000      .6246080    2.0000E+03             0             0      .0629970     1.5056645      .3472286   -6.8373E-03      .0572649
        11     -.1163169     -.0152156    5.6309E-05      .0936378     8.5444482    -1.0251742    14.5836047   -1.7740E-01    -2.1314622    16.7150670
        21    15.6087789     3.1776524     4.7999481     1.8252305      .5753360             0      .8664209             0             0             0
TMG           -2.6712422   -1.3770E-01   -2.1445E-01   -2.8719E-01   -1.0704E-01    -6.3186955   -4.2349E-01   -1.5594E-01             0             0
TMS           -6.8346448    -5.8346445     5.6058558    20.6832141   -4.1912E-01    -6.4741709     2.1982201     3.0384415     4.8694622    -2.6712422
        11             0     2.1342794             0             0             0             0             0             0             0             0
TP              .4876100     3.1499000     3.1818000     3.2822000     3.3270000     3.2375000     3.7308000     3.4234000             0             0
        21    1.4949E-03    5.8718E-04    5.9459E-04    1.1837E-03    5.8047E-04    2.3187E-04    1.9444E-03    4.5600E-04             0             0
        41   -4.2896E-07   -1.3665E-07   -1.4065E-07   -2.1492E-07   -1.5008E-07    5.0938E-09   -5.1210E-07   -8.0583E-08             0             0
        61    6.2644E-11    1.6756E-11    1.7307E-11    2.2848E-11    2.0414E-11   -3.9631E-12    6.8031E-11    9.4557E-12             0             0
        71             0             0             0             0             0             0             0             0             0             0
XMT            9.5123182     4.9430188    21.2792989     6.5167234    22.8530034    -1.5737043    16.3362801     8.9636239             0             0
        11     3.8001200   141.7440000     6.0000000    12.0000000             0     3.8000467   141.7941606    23.3769932             0             0
```

```
XMU       25.2846190  25.2846180  16.9160201  19.3734848  12.0822775  29.8665753  21.6020048          0          0          0
XPF      120.0000000 120.0000000 128.6656635 125.3794241  66.6333250 154.9193338 125.8570618          0          0          0
XPG        4.0500000   4.0500000   3.7000000   3.8050000   3.6950000   4.1250000   3.8900000          0          0          0
XPR        4.0500000   4.0500000   3.3500000   3.5400000   3.3400000   4.2000000   3.7300000          0          0          0
XPT      120.0000000 120.0000000 138.0000000 131.0000000  37.0000000 200.0000000 132.0000000          0          0          0

CON   TEO   OETONATION HUGONIOT

MES1 - 76AUG20                      MES1 - SHORT TEST - CJ. HUG. ISENTROPE                                    09/02/76
TFICKETIGN.    .255 SEC ON RUN.     .306 SEC ON JOB                                                     TEO - HUGONIOT
  P-TABLE
     3.00000E-01  2.00000E-01  0.

       OUTPUT LABFLS

          1     P               V/V0            T               U               O               RHO             QCAL
          2     V               E               S               NG              NS              N               SUPSAT
          3     V               E/RT            S/R             PV/RT           N1              N2              N3
          4     DO. FOR GAS                                                     N4.N5.N6
          5     DO. FOR REF.                                                    N7.N8.N9
          6     DO. FOR SOLID                                                   N10.N11.N12
          7     RBAR*           TBAR*           VBAR*           GAMMA           ALPHA           BETA            C

POINT  3  1   3.0000000E-01  6.8209108E-01  4.1800622E-03  2.3018432E-01  7.2405743E-01  1.8000000E-00  1.4490847E-00
          2   3.7893949E-01  3.2889369E-02  7.2737497E-05  7.8132457E-00  1.1953025E-00  9.0085483E-00  1.5298412E-01
          3   9.3437728E-00  2.3334302E-00  2.1571501E-01  8.0654831E-00  1.1953025E-00  2.9914696E-00  4.7909272E-01
          4   1.0178271E-01  2.5983520E-00 -1.0676278E-00  7.7858160E-00  2.8526013E-00  1.7060806E-02  1.4739874E-01
          5   1.0239780E-01  2.5880818E-00 -1.0832547E-00  7.8389102E-00  1.3256048E-00  1.7850473E-05  0.
          6   3.8889734E-00  4.6778127E-01 -1.4269480E-01  3.3569362E-00  0.             0.             0.
          7   3.8054155E-00  1.3674799E-02  2.3476215E-01  2.7005031E-00  3.4377594E-00  1.6433084E-00  5.5407417E-01

POINT  4  1   2.0000000E-01  7.9305378E-01  3.8045213E-03  1.5163781E-01  7.3274016E-01  1.8000000E-00  1.4282619E-00
          2   4.4058553E-01  1.7894021E-02  7.2769569E-05  7.9598912E-00  1.0428837E-00  9.0027748E-00  1.3101733E-01
          3   1.0870786E-01  1.3957523E-00  2.1594852E-01  6.8732248E-00  1.0428837E-00  2.9972308E+00  7.0824972E-01
          4   1.1733924E-01  2.0083885E-00 -1.0222304E-00  6.4189573E-00  2.7884647E-00  5.5375631E-03  2.1153484E-01
          5   1.1814529E-01  1.9896563E-00 -1.0439009E-00  6.4699210E-00  1.2488675E-00  6.0617958E-06  0.
          6   4.2828177E-00  2.4792361E-01 -1.0179689E-01  2.7078785E-00  0.             0.             0.
          7   3.8091047E-00  1.3463469E-02  2.3544560E-01  2.6846183E-00  3.0978413E-00  1.5264149E-00  4.8637510E-01

CON   CJ    CJ LOCUS

MES1 - 76AUG20                      MES1 - SHORT TEST - CJ. HUG. ISENTROPE                                    09/02/76
TFICKETIGN.    .583 SEC ON RUN.     .634 SEC ON JOB                                                                 CJ
  CJ RHO-TABLE
     1.60000E-00  1.80000E-00  0.

       OUTPUT LABELS

          1     P               V/V0            T               U               D               RHO             QCAL
          2     V               E               S               NG              NS              N               SUPSAT
          3     V               E/RT            S/R             PV/RT           N1              N2              N3
          4     DO. FOR GAS                                                     N4.N5.N6
          5     DO. FOR REF.                                                    N7.N8.N9
          6     DO. FOR SOLID                                                   N10.N11.N12
          7     RBAR*           TBAR*           VBAR*           GAMMA           ALPHA           BETA            C

POINT  5  1   1.9888975E-01  7.2232555E-01  4.0809243E-03  1.8578651E-01  6.6908030E-01  1.6000000E-00  1.4015000E-00
          2   4.5145347E-01  2.3655305E-02  7.4780944E-05  8.1163490E-00  8.8812807E-01  9.0044771E-00  1.0942458E-01
          3   1.1136833E-01  1.7198412E-00  2.2187546E-01  6.5280756E-00  8.8812807E-01  2.9955360E-00  9.4626716E-01
          4   1.1885171E-01  1.9013426E-00 -9.5906179E-01  5.9667285E-00  2.7135671E-00  8.9273000E-03  2.8643254E-01
          5   1.1991605E-01  1.8784533E-00 -9.8744023E-01  6.0291173E-00  1.1656054E-00  1.3430422E-05  0.
          6   4.2979901E-00  2.2279628E-01 -1.0119332E-01  2.5193522E-00  0.             0.             0.
          7   3.8119124E-00  1.3238677E-02  2.3596662E-01  2.6013401E-00  2.9184306E-00  1.5063123E-00  4.8329384E-01
```

```
POINT  6   1     2.4894704F-01  7.2997845E.01  3.9844666E.03  1.9324864E.01  7.1567857E.01  1.8000000E.00  1.4418736E.00
           2     4.0554358F.01  2.5069501E.02  7.2603669E.05  7.8696632E.00  1.1353011F.00  9.0049643E.00  1.4426299F.01
           3     1.0003748F.01  1.8666819E.00  2.1540388E.01  7.5174255E.00  1.1353011E.00  2.9950458E.00  5.6811003F.01
           4     1.0858513F.01  2.3172328E.00 -1.0528061E.00  7.1597479E.00  2.8287812E.00  9.9076675E.03  1.7121838E.01
           5     1.0926612F.01  2.3031322E.00 -1.0707144E.00  7.2109219E.00  1.2965897E.00  1.0485669E.05  0.
           6     4.0787016E.00  3.5453600E.01 -1.2246953E.01  3.0649847E.00  0.             0.             0.
           7     3.8070314F.00  1.3593882E.02  2.3506133E.01  2.7034071E.00  3.2774684E.00  1.5822509E.00  5.2242984E.01

CON   PV    CJ ISENTROPE
MES1 - 76AUG20                       MES1 - SHORT TEST - CJ. HUG. ISENTROPE                                      09/02/76
TFICKETIGN.    1.632 SEC ON RUN.    1.684 SEC ON JOB                                                                LOCUS
  BRANCH (1-T.2-V.3-S.4-E) / TC.PC/ P-TABLE
    3      1
      0.           0.
      3.00000E-01  2.00000E-01  0.

     OUTPUT LABELS

           1      P              V/V0           T              U              D              RHO            QCAL
           2      V              E              S              NG             NS             N              SUPSAT
           3      V              E/RT           S/R            PV/RT          N1             N2             N3
           4      NO. FOR GAS                                                N4.N5.N6
           5      NO. FOR REF.                                               N7.N8.N9
           6      NO. FOR SOLID                                              N10.N11.N12
           7      RBAR.          TBAR.          VBAR.          GAMMA          ALPHA          BETA           C

POINT  7   1     2.4894704F-01  7.2997845E-01  3.9844666E.03  1.9324864E-01  7.1567857E-01  1.8000000E.00  1.4418736E.00
           2     4.0554358F.01  2.5069501E.02  7.2603680E.05  7.8696632F.00  1.1353011F.00  9.0049643F.00  1.4426299F.01
           3     1.0003748F.01  1.8666819E.00  2.1540388E.01  7.5174255E.00  1.1353011E.00  2.9950458E.00  5.6811003F.01
           4     1.0858513F.01  2.3172328E.00 -1.0528061E.00  7.1597479E.00  2.8287812F.00  9.9076675E-03  1.7121838F.01
           5     1.0926612F.01  2.3031322E.00 -1.0707144F.00  7.2109219E.00  1.2965897F.00  1.0485669F.05  0.
           6     4.0787016F.00  3.5453600E.01 -1.2246953E-01  3.0649847E.00  0.             0.             0.
           7     3.8070314F.00  1.3593882E.02  2.3506133F.01  2.7034071E.00  3.2774684E.00  1.5822509F.00  5.2242984E.01

POINT  8   1     3.0000000F-01  6.8133790E-01  4.1506194E.03 -6.2285136E-01  7.1567857F-01  1.8000000E.00  1.4504140F.00
           2     3.7852106F.01  3.2457083E.02  7.2603704E.05  7.8061860F.00  1.2020925F.00  9.0082785E.00  1.5399230F.01
           3     9.3357347F.00  2.3147033E.00  2.1532467E.01  8.0983612F.00  1.2020925E.00  2.9917379F.00  4.6627416F.01
           4     1.0172292F.01  2.6091067E.00 -1.0716390F.00  7.8259305F.00  2.8558995F.00  1.6523390F.02  1.4410009F-01
           5     1.0232402F.01  2.5989927E.00 -1.0869242E.00  7.8780844F.00  1.3296342E.00  1.6865346E.05  0.
           6     3.8882459F.00  4.7078891E-01 -1.4269568E.01  3.3736489E.00  0.             0.             0.
           7     3.8053098F.00  1.3685726E.02  2.3474259E.01  2.7056370E.00  3.4509657E.00  1.6450713E.00  5.5429430F-01

POINT  9   1     2.0000000F-01  7.9167471E.01  3.7817053E.03 -2.6341168E.01  7.1567857E.01  1.8000000E.00  1.4302499F.00
           2     4.3981928F.01  1.7418127E.02  7.2603722F.05  7.9482801F.00  1.0543765E.00  9.0026566F.00  1.3265467F.01
           3     1.0852025F.01  1.3668470E.00  2.1545919E.01  6.9027591E.00  1.0543765F.00  2.9973496E.00  6.9044635F.01
           4     1.1723572F.01  2.0172005E.00 -1.0273858E.00  6.4571326E.00  2.7938894E.00  5.3018977F.03  2.0611114F-01
           5     1.1802219E.01  1.9967990E.00 -1.0485454E.00  6.5071586F.00  1.2551761E.00  5.6424670F.06  0.
           6     4.2819856F.00  2.4994174E.01 -1.0180381E.01  2.7236865E.00  0.             0.             0.
           7     3.8088931F.00  1.3480486E.02  2.3540636E.01  2.6914850E.00  3.1134498E.00  1.5283198E.00  4.8657312F.01

CON   REND

CON   JEND

MES1 - 76AUG20                       MES1 - SHORT TEST - CJ. HUG. ISENTROPE                                      09/02/76
TFICKETIGN.    2.112 SEC ON RUN.    2.164 SEC ON JOB                                                               JOBEND

DAY-TIME START 21.00.59  . END 21.01.01


  COMPLETE TFICKETIGN
```

ACKNOWLEDGMENTS

James D. Kershner, T-4, and Jack D. Jacobson, T-4, helped with the programming required to reactivate the code. The equilibrium routine was redone earlier in FORTRAN by Paul Bird, L-3.

APPENDIX A

CHEMICAL EQUILIBRIUM EXAMPLE

We give in Table A-I an example of a system with an equilibrium number of phases (solid carbon may be present or absent). The user must specify two systems, a two-phase system and a one-phase system, and make an appropriate choice of independent species for each. He does this, after defining the species and empirical formula via $\underset{\approx}{\alpha}$ and $\underset{\sim}{Q}$, by giving the two renumberings $\underset{\sim}{a}^1$ and $\underset{\sim}{a}^0$. Recall the definition of a_i: the (original) *ith* species becomes the a_i*th*. Take, for example, $i = 4$, $a_4^1 = 1$; CO, originally the fourth species, becomes the first in this the two-phase system. Recall that the solid must be number *c* in the two-phase system, and number *s* in the one-phase (where the program assigns it a large F to make its mole fraction negligibly small). The horizontal dashed lines divide the α matrices into independent and dependent parts. The corresponding $\underset{\approx}{\nu}$ and $\underset{\sim}{q}$ are given below each $\underset{\approx}{\alpha}$, and the reactions are written out in full below the $\underset{\approx}{\nu}$'s. The saturation test for the one-phase system is made on the two-phase system reaction

$$CO + H_2 - C(S) \rightarrow H_2O$$

with the saturation index $\hat{s}$,

$$\hat{s} = \left(x_{H_2O} / x_C x_{H_2}\right) \Big/ K_4 \quad ,$$

evaluated for the mole fractions from the one-phase solution. If $\hat{s} < 1$ the system is unsaturated with respect to deposition of solid carbon, and the one-phase system is the correct choice.

TABLE A-I

EQUILIBRIUM EXAMPLE CH_2O_2, c=3, s=6

$\underset{\sim}{a}$, $\underset{\approx}{\alpha}$, and $\underset{\sim}{Q}$:

		Entry			Two-Phase(p=1)					One-Phase(p=0)				
i		C	H	O	a_i^1		C	H	O	a_i^0		C	H	O
1	C(s)	1	0	0	3	CO	1	0	1	6	CO_2	1	0	2
2	H_2	0	2	0	2	H_2	0	2	0	3	H_2O	0	2	1
3	O_2	0	0	2	6	C(s)	1	0	0	4	H_2	0	2	0
4	CO	1	0	1	1	H_2O	0	2	1	5	O_2	0	0	2
5	CO_2	1	0	2	5	CO_2	1	0	2	1	CO	1	0	1
6	H_2O	0	2	1	4	O_2	0	0	2	2	C(s)	1	0	0
	$\underset{\sim}{Q}$	1	2	2										

$\underset{\approx}{\nu}$ and $\underset{\sim}{q}$:

k		CO	H_2	C(s)		CO_2	H_2O	H_2
4	H_2O	1	1	-1	O_2	0	2	-2
5	CO_2	2	0	-1	CO	1	-1	+7
6	O_2	2	0	-2	C(s)	1	-2	+2
	$\underset{\sim}{q}$	2	1	-1	$\underset{\sim}{q}$	1	0	1

Reactions:

Two-Phase(p=1)	One-Phase(p=0)
$CO + H_2 - C(s) \rightarrow H_2O$	$CO_2 + 2H_2O - 2H_2 \rightarrow O_2$
$2CO - C(s) \rightarrow CO_2$	$CO_2 - H_2O + H_2 \rightarrow CO$
$2CO - 2C(s) \rightarrow O_2$	$CO_2 - 2H_2O + 2H_2 \rightarrow C(s)$

APPENDIX B

QUASI-STATIC WORK

Summarized here is what might be loosely termed the Carnot cycle for explosives; plus a numerical example. The object is to calculate the maximum energy that can be extracted quasi-statically from an explosive by detonating it. The quasi-static process is that given by Jacobs.[3]

Confine the explosive in an upright cylinder of unit length and cross section, closed at the top by a rigid cap and at the bottom by a movable piston. Assume that all confining materials including the piston are rigid massless nonconductors of heat. Move the piston into the cylinder with constant velocity u_1 greater than or equal to the Chapman-Jouguet (CJ) particle velocity. As the piston begins to move, instantaneously initiate the detonation at the piston surface. The detonation front will then move upward with complete-reaction wave velocity D_1 determined by u_1. The detonation products (reacted material) will be in a uniform state with pressure p_1 and particle velocity u_1. When the detonation wave reaches the upper end of the cylinder, attach the piston to the cylinder at its position at that instant of time and remove the driving force on the piston. Allow the cylinder to move upward under gravity deceleration until its velocity is reduced to zero. Extract work reversibly from the cylinder of product gases in this position by first lowering it slowly to its original position, and then releasing the piston and allowing the products to expand adiabatically and reversibly to some final pressure.

Calculate the net work done on the surroundings in this process. The cylinder has unit volume and contains ρ_0 grams of material. Take work and energy per unit mass of material. The piston moves a distance u_1/D_1 with force p_1, so the work W_p done by it is

$$W_p = p_1 u_1/\rho_0 D_1 \quad ,$$

or, using the conservation relation $p = \rho_0 u_1 D_1$ (neglecting p_0),

$$W_p = u_1^2 \quad .$$

The kinetic energy K of the reaction products is

$$K = u_1^2/2 \quad .$$

The work done by the system in expanding to pressure p is

$$I(p) = \int_{v_1}^{v_i(p)} p_i(v)\, dv \quad ,$$

where $p_i(v)$ is the isentrope through the product state (p_1, v_1). Summing the contributions gives for the net work W(p) on the surroundings for expansion to pressure p

$$W(p) = -W_p + K + I(p)$$

$$= I(p) - \frac{1}{2} u_1^2$$

$$= e_1 - \frac{1}{2} u_1^2 - e_i(p) \quad .$$

We remark that $W(p_o)$ differs little from the heat of reaction q as conventionally defined -- the energy change in the surroundings for reaction to products at T_o, p_o. To see this and show how the various energy changes enter, we have prepared Fig. B-1, which shows the closed cycle in the p-v plane, and Table B-I, which lists the steps in clockwise traversal beginning at point 0, the unreacted explosive. The numerical example consists of the calculated values for Comp. B from Ref. 2, and is for $T_c = 300$ K, $p_o = 1$ atm. For state 2, the calculated temperature is 518 K and the mean γ is 1.25.

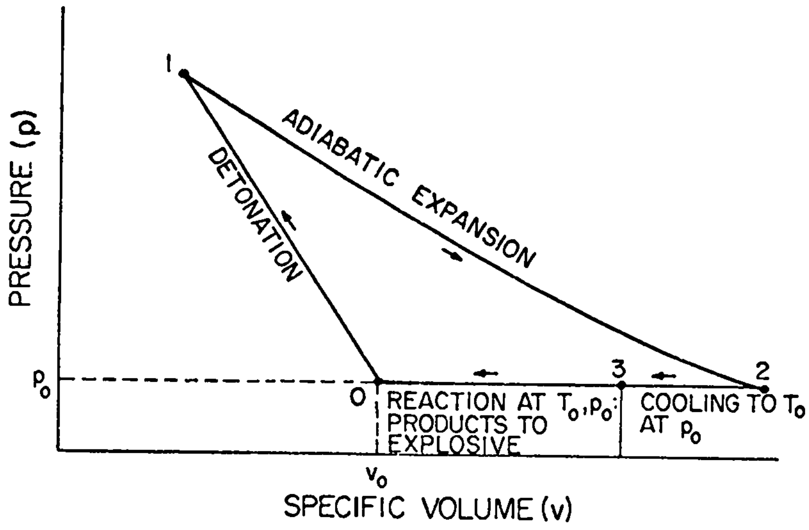


Fig. B-1. Closed cycle of energy changes in the p-v plane.

TABLE B-I

ENERGY STEPS IN CLOCKWISE TRAVERSAL OF FIG. B-1

Process	Energy Change	Comp. B $(mm/\ s)^2$ = Mj/kg
Detonation	$e_1 - e_o = \frac{1}{2} p_1 (v_o - v_1) = \frac{1}{2} u_1^2$	1.80
Adiabatic expansion	$e_2 - e_1 = - I(p_o)$	-7.56
Cooling at p_o	$e_3 - e_2 = C_p\ (T_o - T_2)$	-0.28
Reverse reaction	$e_o - e_3 = q$	6.04
Thus	$W(p_o) = e_o - e_2 = q - C_p\ (T_2 - T_o)$	5.76

APPENDIX C

PROGRAM

I.D. LP-0730

```
     C      AAA                                                                 AAA
     C      CAA                                                                 CAA
     C  MES CODE - WFC-58-1, DET. PROD. LJD EOS   / W. FICKETT, T4              MESO
     C********************************************************************** MESO
     C      CONTENTS                                                            MESO
     C        1. MAIN PROGRAM MESO                                              MESO
     C        2. UTILITY                                                        MESO
     C        3. CALCULATION SECTIONS AND PRINT                                 MESO
     C        4, CALCULATION CONTROLS                                           MESO
     C        5, READ CONTROL (CON)                                             MESO
     C        6. OUT OF PLACE                                                   MESO
     C           EQOS PACKAGE (SEC. 3)                                          MESO
     C           HEAP (SEC.2                                                    MESO
     C        7. DUMMIES                                                        MESO
     C                                                                          MESO
     C********************************************************************** MESO
     C*     1. MAIN PROGRAM                                                  * MESO
     C********************************************************************** MESO
            PROGRAM MESO(INP, OUT, FSET9=OUT, FSET10=INP                        MESO
           1, JOHIN                                                             MESO
           X)                                                                   MESO
     C****************************** COMMON ********************************** MESO
2           COMMON Z(4000)                                                      MESO
2           DIMENSION                                                           MESO
           1 BS     (    60) ,CONT   (    20)                                   MESO
           2, KON (60)                                                          MESO
2           EQUIVALENCE                                                         MESO
           1 (Z(  400),BS     ) ,(Z(  460),CONT   )                             MESO
           2, ( Z(1600) , KON )                                                 MESO
     C********************************** LOCAL ****************************** MESO
2           DIMENSION EBS(40),ECONT(10)                                         MESO
            DATA EBS/                                                           MESO
           1  1H , 3HPAS, 4HSAIT, 3HFUB, 1H                                     MESO
           2, 3HMIP, 3HDIS, 3HUTG, 1H , 3HGEP                                   MESO
           3, 3HSEP, 3HTIP, 3HAIP, 3HEOP, 1H                                    MESO
           4, 3HSAM, 3HTED, 2HPV, 2HCJ, 4HTEST                                  MESO
           5, 4HCHEC, 1H , 4HSPEC, 5HSPEC1, 1H                                  MESO
           6, 4HCORE, 4HDBUG, 4HLOAD, 1H ,1H                                    MESO
           7, 1H , 1H ,1H , 4HFORM, 4HRENU                                      MESO
           8, 4HJEND, 1H , 1H , 3HCON, 1H                                       MESO
           */                                                                   MESO
     C                                                                          MESO
            DATA ECONT/                                                         MESO
           1 1.98719, 8.31439E-5, 1.01325E-6, 4.184E-2, 0.426012                MESO
           2 ,3LOUT                                                             MESO
           */                                                                   MESO
            DATA JOHIN /5LJOHIN/,OUT /3LOUT/                                    MESO
2           INTEGER OUT                                                         MESO
     C********************************** EXECUTE **************************** MESO
2           CALL SERR                                                           MESO
3           CALL HEADI (                                                        MESO
           1 9L*MES1 - 76AUG20* )                                               MESO
5           CALL MOVE (EBS,BS,40)                                               MESO
10          CALL MOVE (ECONT,CONT,10)                                           MESO
     C          --- DATA STATEMENT CANT LOAD BLANK COMMON                       MESO
     C---------------------------------- PRINT DECK ------------------------- MESO
13          CALL HEAD (5LINPUT)                                                 MESO
     C---------------------------------- READ CONTROL ----------------------- MESO
15          CALL CON(0.)                                                        MESO
```

```
17          END                                                                  MESO
      C******************************************************************** MESO
      C*      2. UTILITY                                                  * MESO
      C******************************************************************** MESO


            SUBROUTINE DBUG(A,B)                                              DBUG
      C       OLD ERR ROUTINE                                                 DBUG
      C         CHANGE DBUG CALLS TO ERR CALLS AS NEEDED                      DBUG
 6            CALL ERR(A,B,4LDBUG)                                            DBUG
 7          RETURN                                                            DBUG
10          END                                                               DBUG


            SUBROUTINE ERR(ISUB,IMES,ERRD)                                    ERR
      C******************************************************************** ERR
      C     ERROR CONTROL                                                     ERR
      C     ARGS - ROUTINE, MESSAGE, DATA (10 WORDS)                          ERR
      C++++++++++++++++++++++++++++++++++ COMMONS ++++++++++++++++++++++++++ ERR
10          COMMON Z(4000)                                                    ERR
10          DIMENSION KON(60), CONT(20)                                       ERR
10          EQUIVALENCE (Z(460),CONT), (Z(1690),KON)                          ERR
10          EQUIVALENCE (CONT(8),OUT),(KON(6),QERRGAT)                        ERR
10          COMMON /SERRC/ SERRCA(16)                                         ERR
      C++++++++++++++++++++++++++++++++++ LOCALS +++++++++++++++++++++++++++ ERR
10          DIMENSION ILAB(5)                                                 ERR
            DATA ILAB/30H/////// ERROR (ERR CALL) IN - ,1H ,1L                ERR
      C++++++++++++++++++++++++++++++++++ EXECUTE ++++++++++++++++++++++++++ ERR
10          ILAB(4)=ISUB                                                      ERR
      C---------------------------------- 1. CHECK GATE - WARN IF CLOSED     ERR
10          IF(QERRGAT.EQ.0.) GOTO 150                                        ERR
12          PRINT 130, ILAB                                                   ERR
        130 FORMAT(/// 30X,4(*/////*),* ERR RE-ENTERED FROM  *,5A10///)       ERR
21     150  QERRGAT = QERRGAT + 1.0                                           ERR
23          IF(QERRGAT .GT. 1.) CALL EXIT                                     ERR
      C---------------------------------- 2. PRINT HEAD ARGS, ERP --------- ERR
26          CALL HEAD (ILAB)                                                  ERR
32          CALL PRIN (IMES, 10, ERRD)                                        ERR
35          IF (ISUB.EQ.4LSERR) CALL UMPPK(OUT,SERRCA)                        ERR
44          CALL TRACE                                                        ERR
47          CALL ERP(3LERR)                                                   ERR
      C---------------------------------- 3. TERMINAL LINE ---------------- ERR
51          PRINT 860                                                         ERR
        860 FORMAT(///21(5H*****),* END OF RUN AFTER ERR* ///)                ERR
61          CALL CON(1.)                                                      ERR
63          END                                                               ERR


            SUBROUTINE ERP(L)                                                 ERP
      C     DIAGNOSTIC COMMON PRINT                                           ERP
 3          COMMON Z(4000)                                                    ERP
 3          EQUIVALENCE                                                       ERP
           1 (Z( 920),CAR ),(Z( 460),CONT),(Z(1000),DER ),(Z(1010),EMG )      ERP
           2,(Z(1030),EPN ),(Z(1170),ENX ),(Z(1370),FMU ),(Z(1390),FN  )      ERP
           3,(Z(1410),FCB ),(Z(1490),GM  ),(Z(1470),GP  ),(Z(1590),HE  )      ERP
           4,(Z(1600),KAL ),(Z(1620),KEN ),(Z(1680),KIM ),(Z(1690),KON )      ERP
           5,(Z(1750),PT  ),(Z(1800),ROT ),(Z(1820),SM  ),(Z(1840),SP  )      ERP
           6,(Z(1880),SUC ),(Z(1900),SUCG),(Z(1920),THER),(Z(1970),IMG )      ERP
           7,(Z(1990),TMS ),(Z(2010),IP  ),(Z(2210),XMT ),(Z(2240),XMU )      ERP
           8,(Z(2260),XPF ),(Z(2660),XPG ),(Z(3060),XPR ),(Z(3980),XPT )      ERP
```

```
          X,(Z( 400),BS  ),(Z( 460),EA  ),(Z( 680),EV  ),(Z(3100),FLAB)
          Y,(Z(1530),GMT ),(Z( 900),KEV),(Z(1860),SPC)
  3        CALL PRTN(1L , 0, 0 )
  6        CALL PRIN ( L, 0, 0)
 11        CALL POUT(1)
 13        CALL POUT(2)
 15        CALL POUT(3)
 17        CALL PRIN (24LCAR - CC/CH/CM/CG/CS/CE  , 60, CAR)
 22        CALL PRTN(3LDER,10,DER)
 25        CALL PRIN(4LCONT,10.CONT)
 30        CALL PRIN(3LEMG,10,EMG)
 33        CALL PRIN(3LEMN,10,EMN)
 36        CALL PRTN(3LEMX,10,EMX)
 41        CALL PRIN(3LFMU,10,FMU)
 44        CALL PRTN(2LFN,10,FN)
 47        CALL PRTN(3LFOB,40,FOB)
 52        CALL PRIN(2LGM,30,GM)
 55        CALL PRTN(2LGP,10,GP)
 60        CALL PRTN(2LHE,10,HE)
 63        CALL PRTN(2LBS,50,BS)
 66        CALL PRIN(2LEA,80,EA)
 71        CALL PRTN(2LEV,10,EV)
 74        CALL PRTN(4LFLAB,10,FLAB)
 77        CALL PRIN(3LGMT,10,GMT)
102        CALL PRIN(3LKEV,10,KEV)
105        CALL PRTN(3LSPC,10,SPC)
110        CALL PRTN(3LKAL,12,KAL)
113        CALL PRTN(3LKON,60,KON)
116        CALL PRIN(3LKEN,20,KEN)
121        CALL PRTN(3LKIM,10,KIM)
124        CALL PRIN(2LPT,10,PT)
127        CALL PRTN(4LRHOT,10,RHOT)
132        CALL PRTN(2LSH,20,SH)
135        CALL PRIN(2LSP,20,SP)
140        CALL PRTN(3LSUC,10,SUC)
143        CALL PRTN(4LSUCG,10,SUCG)
146        CALL PRIN(4LTHER,40.THER)
151        CALL PRIN(3LTMG,10,TMG)
154        CALL PRIN(3LTMS,20,TMS)
157        CALL PRIN(2LTP, 80, TP)
162        CALL PRTN(3LXMT,20,XMT)
165        CALL PRIN(3LXMU,10,XMU)
170        CALL PRIN(3LXPF,10,XPF)
173        CALL PRIN(3LXPG,10,XPG)
176        CALL PRTN(3LXPR,10,XPR)
201        CALL PRIN(3LXPT,10,XPT)
204        RETURN
205        END


           SUBROUTINE FIO (B,FMT,N,A,KL)
      C
      C    B=READ  ,RIT   ,PRINT ,WO!
      C    FMT=FORMAT
      C    N=NUMBER OF WORDS OF ARRAY A FOR I.O.
      C    FOR N=0,FMT IS HOLLERITH ARGUMENT LABEL
      C           ,KL IS THE WORD LENGTH OF THE LABEL.
 14        DIMENSION BS(4),FMT(60), A(10)
 14        INTEGER B,FMT,BS
      C
```

```
     C                                BS(1)=READ   , BS(2)=RIT                      FIO      12
     C                                BS(3)=PRINT  , BS(4)=WOT                      FIO      13
 14             BS(1)=4HREAD                                                        FIO      14
 14             BS(2)=3HRIT                                                         FIO      15
 14             BS(3)=5HPRINT                                                       FIO      16
 14             BS(4)=3HWOT                                                         FIO      17
     C                                                                              FIO      18
 21             DO 24 J=1,4                                                         FIO      19
 23             I=J                                                                 FIO      20
 23             IF(B.EQ.BS(I))GO TO 30                                              FIO      21
 26          24 CONTINUE                                                            FIO      22
 30             WRITE(9,26)B                                                        FIO      23
             26 FORMAT (18H0 FIO    -BAD ARG=   A6)                                 FIO      24
 40             CALL EXIT(3)                                                        FIO      25
 45          30 IF (N)200,100,200                                                   FIO      26
     C                                I.O. WITH NO DATA                             FIO      27
 46         100 GO TO (500,500,130,140),I                                           FIO      28
     C                                                                              FIO      29
     C                                                                              FIO      30
 56         130 WRITE (2,150)(FMT(J),J=1,KL)                                        FIO      31
 67             GO TO 500                                                           FIO      32
     C                                                                              FIO      33
     C                                                                              FIO      34
 73         140   WRITE (9,150)(FMT(J),J=1,KL)                                      FIO      35
104             GO TO 500                                                           FIO      36
            150 FORMAT (12A6)                                                       FIO      37
     C                                I.O. WITH DATA                                FIO      38
110         200 GO TO (210,220,230,240),I                                           FIO      39
     C                                                                              FIO      40
120         210 READ (2,FMT)(A(J),J=1,N)                                            FIO      41
132             GO TO 500                                                           FIO      42
     C                                                                              FIO      43
136         220 READ(10,FMT)(A(J),J=1,N)                                            FIO      44
150             GO TO 500                                                           FIO      45
     C                                                                              FIO      46
154         230 WRITE (2,FMT)(A(J),J=1,N)                                           FIO      47
166             GO TO 500                                                           FIO      48
     C                                                                              FIO      49
172         240 WRITE(9,FMT)(A(J),J=1,N )                                           FIO      50
204             GO TO 500                                                           FIO      51
     C                                                                              FIO      52
210         500 CONTINUE                                                            FIO      53
210         510 CONTINUE                                                            FIO      54
210         520 RETURN                                                              FIO      55
211             END                                                                 FIO      56

                SUBROUTINE FROOTT(C,K)                                              FROOTT    2
     C                                FROOT FUNCTION TABULATOR                      FROOTT    3
     C                                                                              FROOTT    4
     C                                C  -  FROOT ARG ARRAY                         FROOTT    5
     C                                C(5) - X0                                     FROOTT    6
     C                                C(6) - DELTA X                                FROOTT    7
     C                                C(7) - XN                                     FROOTT    8
     C                                                                              FROOTT    9
     C                                FOR K=0,ITERATE                               FROOTT   10
     C                                FOR K=1,TABULATE. PROVIDE FROOT WITH VALUES   FROOTT   11
     C                                          X0,X0+DELTA X,....,XN,THEN EXIT     FROOTT   12
     C                                                                              FROOTT   13
  6             EQUIVALENCE (E1,KC1),(E2,KC2)                                       FROOTT   14
```

```
  6       DIMENSION C(10)                                                    FROOTT   15
  6     8 E1=C(8)                                                            FROOTT   16
 10     9 E2=C(9)                                                            FROOTT   17
 12    10 IF (K)50,20,50                                                     FROOTT   18
 13    20 CALL FROOT (C)                                                     FROOTT   19
 17    30 GO TO 210                                                          FROOTT   20
 20    50 IF(KC1)100,60,100                                                  FROOTT   21
 21    60 C(2)=C(5)                                                          FROOTT   22
 23    70 GO TO 102                                                          FROOTT   23
 24   100 C(2)=C(2)+C(6)                                                     FROOTT   24
 26   102 KC1=KC1+1                                                          FROOTT   25
 30   110 IF ((C(2)-C(7))*C(6)) 150,150,120                                  FROOTT   26
 34   120 KC2=1                                                              FROOTT   27
 35   130 GO TO 200                                                          FROOTT   28
 36   150 KC2=2                                                              FROOTT   29
 37   200 C(8)=E1                                                            FROOTT   30
 41   202 C(9)=E2                                                            FROOTT   31
 43   210 RETURN                                                             FROOTT   32
 44       END                                                                FROOTT   33
    C*********************************************************************** GEP       2
    C*    3. CALCULATION SECTIONS                                          * GEP       3
    C*********************************************************************** GEP       4

          SUBROUTINE GEP(K)                                                  GEP       5
    C K=1 - CALCULATE PURE GAS EOS AT GIVEN T,P                              GEP       6
    C  K=2 - APPROXIMATE SAME BY LH EXPANSION                                GEP       7
    C     CALLED BY XIM                                                      GEP       8
    C------------------------------------- SPECS      ---------------------- GEP       9
    C K=1                                                                    GEP      10
    C     REGULAR CALCULATION OF GAS EOS FOR PURE                            GEP      11
    C     SPECIES AT GIVEN T,P BY ITERATIVE SOLUTION                         GEP      12
    C     OF P(T,V)=P, WITH P(T,V) GIVEN BY GEM.                             GEP      13
    C     FOR CS OR 1-FLUID MIX, THIS CAN BE A MIXTURE                       GEP      14
    C     EOS VIA COMPOSITION DEPENDENCE OF THE                              GEP      15
    C     MEAN RSTAR AND TSTAR.                                              GEP      16
    C   INPUT                                                                GEP      17
    C     P=THER(1)                                                          GEP      18
    C     IMPLICIT FOR GEM -                                                 GEP      19
    C       T=THER(3)                                                        GEP      20
    C       MEAN RSTAR, TSTAR = RSTA=GP(5), TSTA=GP(6)                       GEP      21
    C       KAL(5) - 1,2,3 FOR IDEAL,LJD, KW                                 GEP      22
    C   OUTPUT                                                               GEP      23
    C     V=VR=GM(15) - VOLUME                                               GEP      24
    C     IMPLICIT FROM GEM -                                                GEP      25
    C       GM - STATE POINT                                                 GEP      26
    C                                                                        GEP      27
    C   VARIABLES                                                            GEP      28
    C     PG=GM(16) - CALCULATED (GAS) PRESSURE                              GEP      29
    C     VRL, VRU - LOWER AND UPPER LIMITS ON ITERATION V                   GEP      30
    C   ROUTINES                                                             GEP      31
    C     GEM(2) - PURE-FLUID EOS AT T,P                                     GEP      32
    C     FROOTT - ITERATE                                                   GEP      33
    C   PLAN                                                                 GEP      34
    C     SOLVE ITERATIVELY PG(V,T)=P FOR V(=VR) BY                          GEP      35
    C     FROOT ITERATION.                                                   GEP      36
    C     VARIABLE, FUNTION - LOG(V), LOG(P/PG)                              GEP      37
    C     SECOND GUESS - NEWTON-RAPHSON FROM DP/DV=GM(12)                    GEP      38
    C K=2                                                                    GEP      39
    C   INPUT                                                                GEP      40
```

```
      C       T,P=THER(1),(3)                                                     GEP
      C       GM - STATE POINT FROM PREVIOUS K=1 CALCULATION                      GEP
      C            (GEM(2) OUTPUT)                                                GEP
      C       EMX(2...) - (GAS) MOLE FRACTIONS                                    GEP
      C     OUTPUT                                                                GEP
      C       XMT - MIXTURE STATE POINT                                           GEP
      C             (NOTE - CHEMICAL POTENTIALS IN XMU ARE                        GEP
      C              CALCULATED BY CALLER)                                        GEP
      C     VARIABLES                                                             GEP
      C       EV - 1,2 - TSTAR AND RSTAR DISPLACEMENTS                            GEP
      C            3,5 - EXPANSION COEFFICIENTS                                   GEP
      C                                                                           GEP
   3          COMMON Z(4000)                                                      GEP
   3          DIMENSION                                                           GEP
             1 CAR    (    80) ,CONT   (    20) ,EV     (    20)                  GEP
             2,FOB    (    60) ,GM     (    40) ,KEN    (    60)                  GEP
             3,KON    ( 6,10) ,THER   (    50) ,XMT    (    30)                   GEP
             4,GP(20)                                                             GEP
   3          EQUIVALENCE                                                         GEP
             1 (Z(  920),CAR   ) ,(Z(  460),CONT  ) ,(Z(  680),EV    )            GEP
             2,(Z( 1410),FOB   ) ,(Z( 1490),GM    ) ,(Z( 1620),KEN   )            GEP
             3,(Z( 1690),KON   ) ,(Z( 1920),THER  ) ,(Z( 2210),XMT   )            GEP
             4,(Z(1470),GP)                                                       GEP
   3          DIMENSION CG(10),KCG(2)                                             GEP
      C                                                                           GEP
   3          EQUIVALENCE                                                         GEP
             1 (CAR(31),CG),(CG(8),KCG)                                           GEP
             2,(CONT(2),R)                                                        GEP
             3,(FOB(20),VRU),(FOB(19),VRL)                                        GEP
             4,(GM(15),VR),(GM(10),PG)                                            GEP
             5,(THER(1),P),(THER(3),T)                                            GEP
             6,(GP(5),RSTA),(GP(6),TSTA)                                          GEP
             7,(XMT(16),RSTAT),(XMT(17),TSTAT)                                    GEP
      C                                                                           GEP
      C                                                                           GEP
   3        4  GO TO ( 10,300) , K                                                GEP
      C---------------------------------- K=1 - REGULAR ------------------        GEP
  11       10 IF (VR) 20,12,40                                                    GEP
  12       12 VR=10.0                                                             GEP
  14       20 CG(4)=ALOG(VR)                                                      GEP
  20       22 CALL COUT (3HGEP,1)                                                 GEP
  24       40 KCG(1)=0                                                            GEP
      C                                                                           GEP
  25       50 CALL FROOTT (CG,KON(4,8))                                           GEP
  31       52 KEXIT=KCG(2)                                                        GEP
  33       60 GO TO (150,88,80,70),KEXIT                                          GEP
  42       70 CALL DBUG (3HGEP,1)                                                 GEP
  47       72 GO TO 150                                                           GEP
  50       80 CALL DBUG (3HGEP,2)                                                 GEP
  54       82 GO TO 150                                                           GEP
  55       88 IF (KON(4,8)) 92,90,92                                              GEP
  56       90 IF (KCG(1)-2)92,91,92                                               GEP
  60       91 CG(2)=CG(4)-CG(3)*PG/(VR*GM(12))                                    GEP
  65       92 VR= EXP(CG(2))                                                      GEP
  71       93 IF (VRU-VR)94,94,96                                                 GEP
  74       94 VR=VRU                                                              GEP
  76       95 GO TO 98                                                            GEP
  77       96 IF (VR-VRL) 97,97,98                                                GEP
 102       97 VR=VRL                                                              GEP
 104       98 KEN(11)=KEN(11)+1                                                   GEP
```

```
106      100 CALL GEP(2)
111      105 IF (FG)106,110,110
113      106 IF (VRL-VR/3.)107,97,97
117      107 VR=VR/3.
121      108 GO TO 100
122      110 CG(3)=ALOG(PG/P)
130      112 CG(2)=ALOG(VR)
134      120 CALL COUT (3HGEP,2)
140      130 GO TO 500
141      150 CALL COUT (3HGEP,3)
145      160 GO TO 600
       C---------------------------------- K=2 - LH EXPANSION --------------
146      300 EV(1)=TSTAT/TSTA-1.0
151      310 EV(2)=RSTAT/RSTA-1.0
       C 400
       C 410 E                                COMPUTE THERMO OUTPUT
154      412 EV(3)=GM(4)*EV(1)+3.0*GM(10)*EV(2)
161      420             EV(4)=-(T*GM(14)+P/GM(12))*EV(1)
           1                   +3.0*(GM(15)+P/GM(12))*EV(2)
172      430             EV(5)=(GM(8)+(T*GM(13)-P)*(GM(14)/R))*EV(1)
           1                   +3.0*(P*GM(14)/R-1.0)*EV(2)
206      500             XMT(1)=GM(15)+EV(4)
210      510             XMT(2)=GM(4)+EV(3)-(P/(R*T))*EV(4)-EV(5)
217      520             XMT(7)=P*XMT(1)/(R*T)-1.0
224      530             XMT(3)=XMT(2)+XMT(7)
225      540             XMT(5)=GM(5)+EV(3)
231      550             XMT(4)=XMT(5)-XMT(7)
232      560             XMT(6)=GM(11)-EV(5)
234      570             XMT(8)=XMT(1)-R*T/P
       C 580 U
       C
240      590 CALL COUT (3HGEP,4)
       C
244      600             RETURN
       C
       C      SPECS (FOR PART 2)
       C
       C      IN                              OUT                 ERASE
       C
       C      NOTE - Z=PV/RT
       C      T,P
       C      EMX
       C      GM         1                    XMT 1 VG            EV 1  F-1
       C                 2                        2 EGP/RT           2  G-1
       C                 3                        3 HGP/RT           3  FGP
       C                 4 ERP/RT                 4 AGP/RT           4  D F/DP
       C                 5 FRP/RT                 5 FGP/RT           5  D F/D RT
       C                 6                        6 SGP/R
       C                 7                        7 ZGP
       C                 8 D ERP/D RT             8 VGP
       C                10 ZRP
       C                11 SRP/R
       C                12 D P/D VR
       C                13 D P/D T
       C                14 D VR/D T
       C                15 VR
       C                16
       C                17                   XMU   MUGP/RT
       C
       C
```

```
245        END
           SUBROUTINE GEM (K)
      C    PURE GAS EOS AT GIVEN T,V
      C -----------------------------------------------------------------------
      C    K=1 PRELIM. READ INPUT PACKS AND FOR LJD
      C          CALL GES (1,...) FOR PRELIMINARY PROCESSING (SETS UP GP).
      C          CALLED BY CON
      C    K=2: MAIN. CALCULATE STATE POINT: KAL(3)=
      C          0 - IDEAL GAS: LOCAL
      C          9 - KW EOS: CALL HKW
      C          OTHER - LJD EOS: CALL GES(2,...)
      C-----------------------------------------------------------------------
      C                                       MAIN (K=2) SPECS
      C   INPUT
      C     T=THER(3)
      C     V=VR=GM(15)
      C     TSTA,VSTA=GP(6),(7) - TSTAR, VSTAR. THESE ARE
      C            COMPOSITION DEPENDENT FOR LH AND 1-FLUID MIX.
      C     KAL(3) - EOS CHOICE. SEE ABOVE
      C   OUTPUT
      C     GM - STATE POINT. GM IS REARRANGED AND
      C          FILLED OUT HERE.
      C   NOTES
      C     1. NO IDEAL-GAS BRANCH IN PRELIM FOR THIS
      C        CASE: GEP PACK  SHOULD NOT BE ENTERED.
      C     2. POOR LOGICAL ORGANIZATION: HKW WAS ADDED
      C        LATE WITH BRANCH UNDER LJD. IDEAL
      C        GAS, KW, AND LJD SHOULD ALL HAVE SAME LEVEL.
      C     3. I DO NOT NOW (WF 1/75) UNDERSTAND WHY
      C        TMS (IDEAL PART) IS USED IN CPR. IT SEEMS TO
      C        ME IT SHOULD BE AN
      C        IMPERFECTION QUANTITY LIKE THE OTHERS.
      C+++++++++++++++++++++++++++++++++++ COMMONS +++++++++++++++++++++++++
3          COMMON Z(4000)
3          DIMENSION
          1 CONT   (   20) ,GP     (   20) ,GM     (   40)
          2,KAL    (   20) ,KEN    ( 6,10) ,KON    ( 6,10)
          3,THER   (   50) ,TMS    (   20)
3          DIMENSION KE(6)
3          EQUIVALENCE
          1 (Z(  460),CONT   ) ,(Z( 1470),GP     ) ,(Z( 1490),GM     )
          2,(Z( 1600),KAL    ) ,(Z( 1620),KEN    ) ,(Z( 1690),KON    )
          3,(Z( 1920),THER   ) ,(Z( 1990),TMS    )
      C
      C                           LOCAL EQ
      C
3          EQUIVALENCE (GP(6),TSTA),(GP(7),VSTA)
          1            ,(GM(1),TAU),(GM(2),THETA),(GM(16),PG)
          2            ,(THER(3),T),(CONT( ),R)
          3            ,(GM(15),VR)
      C
3          EQUIVALENCE (GM(25),GAM),(GM(26),ALPH),(GM(27),BET)
          1            ,(GM(28),CGAM),(GM(29),CPR),(GM(30),DLVDT)
      C
      C
3       100 GO TO (1000,2000),K
      C 994
      C 996                       PRELIMINARY
```

```
     C 998
 11   1000 CALL READ (
          1   60H0        POT (1-LJ,2-MCM,3-MR) ,W (NOW I)  / N,M,AN,AM,R*,T*$
          1 ,-2,KE)
 14         CALL READ(0,6,GP)
 20   1010 KE(3)=0
 21   1012 KE(4)=0
 22   1020 KE (5)=KON(1,4)
 24   1022 KE (6)=KON(2,4)
 26   1024 IF (KE(1)-9) 1030,1025,1030
 30   1025 KAL(3)=9
 31   1026 VSTA=1.0
 33   1027 TSTA=1.0
 35   1028 GO TO 3000
 36   1030 CALL GES(1,KE,GP,GM)
 43   1040 CALL PRTN(4HV*$ ,1,VSTA)
 47   1050 KAL(3)=1
 50   1060 GO TO 3000
     C1994
     C1996                        MAIN
     C1998
 51   2000 KEN(1)=KEN(1)+1
 53   2002  E1 = VP
     C2004
     C2006                                              IDEAL
 55   2010 IF (KAL(3)) 2200,2050,2200
 56   2050 DO 2060 I=3,15
 63   2060 GM(I)=0.0
 65   2070 GM(3)=1.0
 67   2080 GM(9)=1.0
 71   2090 GM(14)=1.0
 73   2100 GO TO 2300
     C2194
     C2196                                              LJD
 74   2200 TAU=VR/VSTA
 76   2210 THETA=T/TSTA
100   2220 KE(5)=KON(1,4)
102   2230 KE(6)=KON(2,4)
     C                                                          KW
104   2234 IF (KAL(3)-9) 2240,2236,2240
106   2236 CALL HKW(1)
111   2238 GO TO 2300
     C
112   2240 CALL GES (2,KE,GP,GM)
     C                                                  REARRANGE AND FINISH GM
117   2300 GM(22)=GM(15)
121   2310 GM(21)=GM(14)
123   2320 GM(20)=GM(6)
125   2330 GM(19)=GM(13)
127   2340 GM(18)=GM(12)
131   2350 GM(17)=GM(5)
133   2352  VP = E1
135   2360 PG=GM(3)*R*T/VR
141   2370 GM(15)=VR
143   2380 GM(12)=(R*T/VR**2)*(GM(10)-GM(3))
150   2390 GM(13)=(R/VR)*GM(9)
153   2400 GM(14)=-GM(13)/GM(12)
155   2410 E1=GM(11)
157   2412 E2=GM(7)
161   2420 GM(11)=GM(8)
```

```
163    2430 GM(7)=GM(10)                                                              GEM        119
165    2440 GM(6)=GM(9)                                                               GEM        120
167    2450 GM(10)=GM(3)-1.0                                                          GEM        121
172    2460 GM(9)=VR-R*T/PG                                                           GEM        122
176    2470 GM(8)=E1                                                                  GEM        123
200    2490 GM(5)=E2                                                                  GEM        124
      C2496                                                                           GEM        125
202    2500 KEN(1,4)=KE(3)                                                            GEM        126
204    2510 KEN(2,4)=KE(4)                                                            GEM        127
      C                                                                               GEM        128
206    2514 CGAM=-VR*GM(12)/PG                                                        GEM        129
211    2520 CVR=IMS(3)-1.0+GM(8)                                                      GEM        130
215    2524 DLVDT=GM(14)/VR                                                           GEM        131
217    2530 GAM=CGAM*(1.0+CGAM*GM(3)    *(T*DLVDT)**2/CVR)                            GEM        132
225    2534 BET=1.0/(CGAM*GM(3)    *T*DLVDT/CVR)                                      GEM        133
232    2540 ALPH=GAM*BET-1.0                                                          GEM        134
235    2544 CPR=CVR*GAM/CGAM                                                          GEM        135
      C2594                                                                           GEM        136
240    2600 CALL DOUT (3HGEM,1)                                                       GEM        137
      C2994                                                                           GEM        138
244    3000 RETURN                                                                    GEM        139
245         END                                                                       GEM        140


            SUBROUTINE GES (K,L,GP,GM)                                                GES          2
      C                                                                               GES          3
      C     LJD CELL THEORY GAS EQN. STATE SUBROUTINE                                 GES          4
      C                                                                               GES          5
      C                      REVISION 1. CORRECT MINOR ERROR -                        GES          6
      C                               POINTS 14 AND 16 USE A FOR 13 AND 15            GES          7
      C                                      W. F. 1/5/62                             GES          8
      C                                                                               GES          9
      C                     REVISION 2.CHANGE OBS. CALL ON NEG. KAP PRINT             GES         10
      C                              W.F. 2/26/62                                     GES         11
      C                                                                               GES         12
      C                                                                               GES         13
 12      10 DIMENSION A(8),Y(8),S(7),W(5),W1(5),W2(5),                                GES         14
         1                CP(4),GM(15),G(15),GP(7),L(6),E(10)                         GES         15
 12         EQUIVALENCE (G(1),TAU),(G(2),THETA),(G(15),B),(W,X)                       GES         16
      C  96                                                                           GES         17
      C  98                               PREL.-MAIN BRANCH                           GES         18
 12     100 GO TO (200,1000),K                                                        GES         19
 20     200 Y(1)=0.98940093                                                           GES         20
 22     202 Y(2)=0.94457502                                                           GES         21
 24     204 Y(3)=0.86563120                                                           GES         22
 26     206 Y(4)=0.75540441                                                           GES         23
 30     208 Y(5)=0.61787624                                                           GES         24
 32     210 Y(6)=0.45801678                                                           GES         25
 34     212 Y(7)=0.28160355                                                           GES         26
 36     214 Y(8)=0.095012510                                                          GES         27
 40     220 A(1)=0.027152459                                                          GES         28
 42     222 A(2)=0.062253524                                                          GES         29
 44     224 A(3)=0.095158512                                                          GES         30
 46     226 A(4)=0.12462897                                                           GES         31
 50     228 A(5)=0.14959599                                                           GES         32
 52     230 A(6)=0.16915652                                                           GES         33
 54     232 A(7)=0.18260342                                                           GES         34
 56     234 A(8)=0.18945061                                                           GES         35
 60     240 B=0.276335                                                                GES         36
 62     242 BMAX=0.276335                                                             GES         37
```

```
 64      244 BUP=1.0663420
 66      246 BDOWN=0.93778543
 70      248 EPS=18.0
 72      260 GP(7)=0.426012*GP(5)**3
 75      300 CALL WR(1,L,GP)
102      310 GO TO 5000
       C 990
       C 992                               MAIN ENTRY
       C 994                                   INITIAL
103     1000 TAU=GP(1)
104     1010 THETA=GP(2)
106     1012 L(3)=L(3)+1
110     1020 IF(TAU)1040,1040,1030
112     1030 IF(THETA)1040,1040,1050
114     1040 CALL DBUG(3HGES,1)
122     1050 CH(1)=TAU
124     1060 CALL WR (2,L,CH)
132     1070 KE1=0
133     1080 IF (L(5)) 4000,1200,4000
       C1190                                   FIND LIMIT
134     1200 W1=B*(1.0+Y(1))
137     1210 CALL WR (3,L,W1)
145     1220 IF ((W1(3)- ABS(CH(2)))/THETA-EPS) 1400,1400,1250
       C1238
       C1240                                       CHECK AND LOWER
153     1250 W2=B*(1.0+Y(3))
156     1260 CALL WR (3,L,W2)
164     1270 IF ((W2(3)- ABS(CH(2)))/THETA-EPS) 1600,1600,1300
172     1300 KE1=KE1+1
174     1310 DO 1320 I=1,5
201     1320 W1(I)=W2(I)
205     1330 B=B*BDOWN
207     1340 IF (L(5)) 4100,1250,4100
       C1394
       C1396                                       RAISE
211     1400 IF (B-BMAX)1450,1410,1410
214     1410 W2=B*(1.0+Y(3))
217     1420 CALL WR (3,L,W2)
225     1430 GO TO 1600
226     1450 DO 1460 I=1,5
233     1460 W2(I)=W1(I)
237     1470 B=B*BUP
241     1472 IF(L(5))4150,1474,4150
242     1474 KE1=KE1+1
244     1480 IF (B-BMAX) 1520,1520,1490
247     1490  B=BMAX
251     1500 W2=B*(1.0+Y(3))
254     1510 CALL WR (3,L,W2)
262     1520 W1=B*(1.0+Y(1))
265     1530 CALL WR(3,L,W1)
273     1540 IF ((W1(3)- ABS(CH(2)))/THETA-EPS) 1550,1600,1600
301     1550 IF (B-BMAX) 1450,1600,1600
       C1596                                       FINISH
304     1600 KE2=KE1+KE2
306     1610 L(4)=KE2/L(3)
       C1696
       C1698                                   INTEGRATE
312     2000 DO 2010 I=1,7
317     2010 S(I)=0.0
       C2048
```

```
323    2050 DO 2550 IG=1,16
325    2060 IF(IG-14) 2100,2070,2100
327    2070 DO 2080 I=1,5
334    2080 W(I)=W2(I)
340    2082 KE=17-IG
342    2090 GO TO 2400
343    2100 IF(IG-16)2150,2110,2150
345    2110 DO 2120 I=1,5
352    2120 W(I)=W1(I)
356    2122 KE=17-IG
360    2130 GO TO 2400
      C
361    2150 IF(IG-8) 2160,2160,2200
364    2160 X=B*(1.0-Y(IG))
370    2170 KE=IG
372    2180 GO TO 2300
      C2198
373    2200 KE=17-IG
375    2210 X=B*(1.0+Y(KE))
      C2298
401    2300 CALL WR(3,L,W)
      C2398                                           CALC. INTEGRANDS
407    2400 E(1)=A(KE)*W(2)* EXP(-W(3)/THETA)
421    2410 E(2)=W(4)*E(1)
423    2420 E(3)=W(3)*E(1)
425    2430 E(4)=W(4)*E(2)
427    2440 E(5)=W(3)*E(3)
431    2450 E(6)=W(3)*E(2)
433    2460 E(7)=W(5)*E(1)
      C2498
439    2500 DO 2510 I=1,7
442    2510 S(I)=E(I)+S(I)
      C           ---NOTE - SUM S(I) IS 1/2 INTEGRAL
      C2538
447    2540 IF (L(5)) 4200,2550,4200
450    2550 CONTINUE
      C2994
      C2996                                  CALC OUTPUT
      C2998                                       INTEGRALS
452    3000 DO 3010 I=2,7
457    3010 S(I)=S(I)/S(1)
464    3020 TM=1./THETA
466    3030 S(1)= 2.0*B*S(1)
471    3032 G(12)=TM*CH(3)
473    3040 G(3)=1.0+G(12)-TM*S(2)
477    3042 G(13)=-TM*CH(2)
501    3050 G(4)=G(13)+TM*S(3)
504    3052 G(14)=8.8857662*S(1)
506    3060 G(6)=1.0+G(13)-ALOG(G(14))
516    3070 IF(G(3))3080,3080,3100
520    3080 CALL PRIN(14HGES NEG. KAP $,1,G(3))
525         CALL PRIN(4HTAU$,1,TAU)
533    3090 GO TO 3110
534    3100 G(6)=G(6)-ALOG(G(3))
542    3110 E2=TM*TM
544    3120 G(9)=1.0-E2*(S(6)-S(3)*S(2))
551    3130 G(10)=TM*CH(4)+E2*(S(4)-S(2)**2-THETA*S(7))
560    3140 G(11)=E2*(S(5)-S(3)**2)
      C
563    3150 G(5)=G(4)+G(3)-1.0
```

```
567    3160 G(7)=G(6)+G(3)-1.0                                                     GES      158
573    3170 G(8)=G(4)-G(6)                                                         GES      159
      C                                                                            GES      160
575    3200 DO 3210 I=3,15                                                         GES      161
602    3210 GM(I)=G(I)                                                             GES      162
606    3220  IF( L(5)) 4300,5000,4300                                              GES      163
      C3094                                                                        GES      164
      C3096                       DIAGNOSTIC PRINT                                 GES      165
      C3098                                                                        GES      166
610    4000 CALL PRIN (28H GES DIAG. -TAU,THETA,B     $,0,B)                       GES      167
616    4010 E(1)=TAU                                                               GES      168
620    4020 E(2)=THETA                                                             GES      169
622    4030 E(3)=B                                                                 GES      170
624    4040 CALL PRIN (2H $,3,E)                                                   GES      171
632    4050 GO TO 1200                                                             GES      172
633    4100 CALL PRIN (2HB$,1,B)                                                   GES      173
641    4110 GO TO 1250                                                             GES      174
642    4150 CALL PRIN (2HB$,1,B)                                                   GES      175
650    4160 GO TO 1474                                                             GES      176
651    4200 DO 4210 I=1,7                                                          GES      177
661    4210 E(I)=E(I)/A(KE)                                                        GES      178
665    4220 E(8)=1G                                                                GES      179
667    4230 E(9)=X                                                                 GES      180
671    4240 E(10)=W(3)                                                             GES      181
673    4250 CALL PRIN(7HI,X,W $,3,E(8))                                            GES      182
700         CALL PRIN(7HINTS  $,7,E)                                               GES      183
706    4260 GO TO 2550                                                             GES      184
707    4300 CALL PRIN(7HG(OUT)$,15,G)                                              GES      185
712         CALL PRIN(7HS(INT)$,S)                                                 GES      186
      C4990                                                                        GES      187
717    5000 RETURN                                                                 GES      188
720         END                                                                    GES      189


            SUBROUTINE WR(K,L,D)                                                   WR         2
      C                               GES CELL POTENTIAL                           WR         3
 10      20 DIMENSION CC(6),C(6),WN(6),WC(6),W(6)                                  WR         4
          1            ,KFPS(2),NMAX(2),F(6),A(60),AL(30),D(7),L(6)                WR         5
 10      30 EQUIVALENCE (WN,CC(7)),(KONE,ONE),(KY,Y)                               WR         6
          1            ,(A(31),AL)                                                 WR         7
 10     200 GO TO (1000,2000,3000),K                                               WR         8
      C 990                                                                        WR         9
      C 994                           PRELIM. ENTRY                                WR        10
      C 996                                                                        WR        11
      C 998                                    SET POT. AND EQUIV. ARGS            WR        12
 17    1000 DO 1004 I=1,6                                                          WR        13
 21    1002 W(I)=0.0                                                               WR        14
 23    1004 C(I)=0.0                                                               WR        15
 25    1006 M=30                                                                   WR        16
 26    1010 GO TO (1020,1040,1060),L                                               WR        17
 35    1020 KA=1                                                                   WR        18
 36    1022 KR=1                                                                   WR        19
 37    1030 GO TO 1100                                                             WR        20
 40    1040 KA=2                                                                   WR        21
 41    1042 KR=2                                                                   WR        22
 42    1050 GO TO 1100                                                             WR        23
 43    1060 KA=1                                                                   WR        24
 44    1062 KR=2                                                                   WR        25
      C1070                                                                        WR        26
      C                                                                            WR        27
```

```
 45    1100 FN=D(1)
 47    1110 FM=D(2)
 50    1120 AN=D(3)
 52    1130 AM=D(4)
      C1190
      C1194                                      REPULSIVE PART
 54    1200 IF (AN) 1300,1800,1210
      C
 56    1210 G=FN
 60    1212 GB=FM
 62    1220 AG=AN
 64    1230 KB=KR
 66    1240 KQ=1
      C1290
      C1294                                           CALC.
 67    1300 BB= 12.0*GB/(FN-FM)
 73    1310 AA=-AG*BB/2.0
      C1320
 76    1330 GO TO (1350,1650),KB
      C1344
      C1348                                                LJ
104    1350 J=(KQ-1)*M
110    1352 KE1=J+M
112    1360 A(KE1)=G *(G -1.0)/6.0
117    1370 E=A(KE1)/4.0
122    1380 E1=1.0E-7*E
      C1394
124    1400 DO 1480 I=2,M
126    1410 KE=KE1+1-I
131    1420 E2=2*(I-1)
134    1440 E3=(G +E2)*((G +E2)-1.0)/((E2+3.0)*(E2+2.0))
144    1450 A(KE)=E3*A(KE+1)
147    1460 E=E3*E/4.0
152    1470 IF(E1-E)1480,1480,1510
155    1480 CONTINUE
      C1498
160    1500 CALL FIO (3HWOT,
           1  53H (1H0,12X,32H A-DIM. TOO SMALL, A30*1/4**30= 1PE15.7),
           21,A(J+1),0)
      C1508
171    1510 NMAX(KQ)=I
173    1520 KEPS(KQ)=-ALOG(1.0E-7*A(KE1)/A(KE))/0.6931
      C1544
206    1550 J=(KQ-1)*3
211    1560 CC(J+1)=AA
213    1570 CC(J+2)=-AA*G/3.0
217    1580 CC(J+3)=-CC(J+2)*G/3.0
223    1590 WN(J+1)=BB
225    1600 WN(J+2)=-BB*G/3.0
231    1610 WN(J+3)=-WN(J+2)*G/3.0
235    1620 GO TO 1750
      C1644
      C1646                                                EXP
236    1650 J=(KQ-1)*3
241    1660 CC(J+1)=AA
243    1670 CC(J+2)=-AA/3.0
246    1680 CC(J+3)=AA/9.0
251    1690 WN(J+1)=BB
253    1700 WN(J+2)=BB  /3.0
256    1710 WN(J+3)=BB  /9.0
```

```
      C1746                                                                  WR       88
261    1750 GO TO (1800,1900),KQ                                             WR       89
      C1796                                                                  WR       90
      C1798                                   ATTRACTIVE PART                WR       91
267    1800 IF (AM) 5000,5000,1810                                           WR       92
271    1810 G=FM                                                             WR       93
273    1812 GB=FN                                                            WR       94
275    1820 AG=AM                                                            WR       95
277    1830 KB=KA                                                            WR       96
301    1840 KQ=2                                                             WR       97
302    1850 GO TO 1300                                                       WR       98
      C1894                                                                  WR       99
303    1900 IF (L(6))4000,5000,4000                                          WR      100
      C1990                                                                  WR      101
      C1992                                                                  WR      102
      C1994                          MAIN INITIAL ENTRY                      WR      103
      C1996                                                                  WR      104
      C1998                                   REPULSIVE PART                 WR      105
305    2000 IF (AN) 2500,2500,2010                                           WR      106
307    2010 G=FN                                                             WR      107
311    2020 KB=KR                                                            WR      108
313    2030 KQ=1                                                             WR      109
      C2044                                                                  WR      110
      C2046                                        CALC.                     WR      111
314    2050 GO TO (2060,2150),KB                                             WR      112
      C2054                                                                  WR      113
      C2058                                             LJ                   WR      114
322    2060 E=D(1)**(-G/3.0)                                                 WR      115
327    2070 J=(KQ-1)*3                                                       WR      116
332    2080 DO 2110 I=1,3                                                    WR      117
334    2090 KE=J+I                                                           WR      118
336    2100 C(KE)=CC(KE)*E                                                   WR      119
341    2110 WC(KE)=WN(KE)*E                                                  WR      120
344    2120 GO TO 2450                                                       WR      121
      C2144                                                                  WR      122
      C2146                                             EXP                  WR      123
345    2150 T=D(1)**0.33333333                                               WR      124
      C2176                                                                  WR      125
351    2180 S=G*T                                                            WR      126
353    2190 E= EXP(G-S)                                                      WR      127
362    2200 J=(KQ-1)*3                                                       WR      128
365    2210 DO 2240 I=1,3                                                    WR      129
367    2220 KE=I+J                                                           WR      130
371    2230 C(KE)=CC(KE)*E                                                   WR      131
374    2240 WC(KE)=WN(KE)*E                                                  WR      132
377    2250 C(J+2)=C(J+2)*S                                                  WR      133
402    2260 C(J+3)=C(J+3)*(S*S-S)                                            WR      134
      C2296                                                                  WR      135
406    2300 J=(KQ-1)*9                                                       WR      136
412    2310 A(J+1)=S                                                         WR      137
414    2320 S1=1.0/S                                                         WR      138
416    2330 A(J+2)=S1                                                        WR      139
420    2340 A(J+3)=1.0+S1                                                    WR      140
423    2350 A(J+4)=-(S+2.0+2.0*S1)                                           WR      141
430    2360 A(J+5)=2.0*(1.0+S1)                                              WR      142
435    2370 A(J+6)=S*S+2.0*S+4.0+4.0*S1                                      WR      143
444    2380 A(J+7)=2.0+3.0*S                                                 WR      144
450    2390 A(J+8)=-(3.0*S+4.0+4.0*S1)                                       WR      145
456    2400 A(J+9)=S-S*S                                                     WR      146
      C2444                                                                  WR      147
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```
461    2450 GO TO (2500,2600),KQ                                                   WR       148
      C2494                                                                        WR       149
      C2494.                                                                       WR       150
      C2496                              ATTRACTIVE PART                           WR       151
467    2500 IF (AM) 2600,2600,2510                                                 WR       152
471    2510 G=FM                                                                   WR       153
473    2520 KB=KA                                                                  WR       154
475    2530 KQ=2                                                                   WR       155
476    2540 GO TO 2050                                                             WR       156
      C2594                                                                        WR       157
      C2596                              WHOLE                                     WR       158
477    2600 U(2)=C(1)-C(4)                                                         WR       159
502    2610 U(3)=C(2)-C(5)                                                         WR       160
505    2620 U(4)=C(3)-C(6)                                                         WR       161
510    2630 IF(L(6))4100,5000,4100                                                 WR       162
      C2990                                                                        WR       163
      C2992                                                                        WR       164
      C2994                        MAIN ENTRY FOR CELL POTENTIAL                   WR       165
      C2996                                                                        WR       166
      C2998                              REPULSIVE PART                            WR       167
512    3000 X=R(1)                                                                 WR       168
513    3002 U(2)=X**2                                                              WR       169
515    3004 IF (AN) 3600,3600,3010                                                 WR       170
517    3010 KB=KR                                                                  WR       171
521    3020 KQ=1                                                                   WR       172
      C3030                                                                        WR       173
      C3040                                 CALC.                                  WR       174
522    3050 GO TO (3060,3300),KB                                                   WR       175
      C3054                                                                        WR       176
      C3056                                    LJ                                  WR       177
530    3060 UNF=1.0                                                                WR       178
532    3070 Y=U(2)                                                                 WR       179
534    3080 KK=(KCNF-KY-1)/512                                                     WR       180
541    3090 N=2*KEPS(KQ)/KK                                                        WR       181
546    3100 NN= MIN0  (N,NMAX(KQ))                                                 WR       182
552    3110 GO TO (3150,3200),KQ                                                   WR       183
      C3144                                                                        WR       184
560    3150 KE=M+1-NN                                                              WR       185
563    3160 F(1)=A(KE)*Y                                                           WR       186
566    3162 KE=KE+1                                                                WR       187
570    3170 DO 3180 I=KE,M                                                         WR       188
575    3180 F(1)=(F(1)+A(I))*Y                                                     WR       189
602    3190 GO TO 3250                                                             WR       190
      C3194                                                                        WR       191
603    3200 KE=M+1-NN                                                              WR       192
606    3210 F(4)=AL(KE)*Y                                                          WR       193
611    3220 KE=KE+1                                                                WR       194
613    3230 DO 3240 I=KE,M                                                         WR       195
620    3240 F(4)=(F(4)+AL(I))*Y                                                    WR       196
      C3244                                                                        WR       197
625    3250 J=(KQ-1)*3                                                             WR       198
630    3260 W(J+1)=WC(J+1)*F(J+1)                                                  WR       199
633    3270 W(J+2)=WC(J+2)*F(J+1)                                                  WR       200
636    3280 W(J+3)=WC(J+3)*F(J+1)                                                  WR       201
641    3290 GO TO 3550                                                             WR       202
      C3294                                                                        WR       203
      C3296                                    EXP                                 WR       204
642    3300 J=(KQ-1)*M                                                             WR       205
646    3310 E=A(J+I)*X                                                             WR       206
651    3320 E1= EXP(E)/2.0                                                         WR       207
```

```
 657   3330 E2=0.25/E1                                                  WR       208
 661   3340 FC=(E1+E2)                                                  WR       209
 663   3350 FS=(E1-E2)                                                  WR       210
 665   3360 IF (E-0.1)3370,3370,3450                                    WR       211
 670   3370 E1=E*E                                                      WR       212
 672   3380 E2=E1*E1                                                    WR       213
 674   3390 FSS=1.0+E1/6.0+E2/120.0                                     WR       214
 701   3400 GO TO 3452                                                  WR       215
      C3444                                                             WR       216
 702   3450 FSS=FS/E                                                    WR       217
 704   3452 FS=X*FS                                                     WR       218
      C3454                                                             WR       219
 706   3460 I=(KQ-1)*3                                                  WR       220
 711   3462 F(I+1)=A(J+3)*FSS-A(J+2)*FC-1.0                             WR       221
 720   3470 F(I+2)=A(J+4)*FSS-FS*A(J+5)*FC+A(J+1)                       WR       222
 730   3480 F(I+3)=A(J+6)*FSS+A(J+7)*FS                                 WR       223
          1            +(A(J+8)-A(J+1)*D(2))*FC+A(J+9)                  WR       224
 743   3490 J=I                                                         WR       225
      C3494                                                             WR       226
 745   3500 W(J+1)=WC(J+1)*F(J+1)                                       WR       227
 750   3510 W(J+2)=WC(J+2)*F(J+2)                                       WR       228
 753   3520 W(J+3)=WC(J+3)*F(J+3)                                       WR       229
      C3544                                                             WR       230
 756   3550 GO TO (3600,3650),KQ                                        WR       231
      C3594                                                             WR       232
      C3596                                     ATTRACTIVE PART         WR       233
 764   3600 IF (AM) 3610,3650,3610                                      WR       234
 765   3610 KB=KA                                                       WR       235
 767   3620 KQ=2                                                        WR       236
 770   3630 GO TO 3050                                                  WR       237
      C3644                                                             WR       238
      C3646 FINISH                                                      WR       239
 772   3650 U(3)=W(1)-W(4)                                              WR       240
 774   3660 U(4)=W(2)-W(5)                                              WR       241
 777   3670 U(5)=W(3)-W(6)                                              WR       242
1002   3680 IF(L(6))4200,5000,4200                                      WR       243
      C3992                                                             WR       244
      C3994                          DIAGNOSTIC PRINT                   WR       245
      C3996                                                             WR       246
      C3998                                     PRELIM                  WR       247
1004   4000 CALL PRIN(13HPREL. WR  CC$,6,CC)                            WR       248
1007        CALL PRIN(3HWN$,6,WN)                                       WR       249
1014   4010 IF (L(1)-2)4020,4030,4020                                   WR       250
1016   4020 CALL PRIN(2HA$,30,A)                                        WR       251
1021        CALL PRIN(3HAL$,30,AL)                                      WR       252
1026   4030 GO TO 5000                                                  WR       253
      C4048                                     MAIN INITIAL            WR       254
1027   4100 CALL PRIN(13HMAIN WR  C  $,6,C)                             WR       255
1032        CALL PRIN(3HWC$,6,WC)                                       WR       256
1037   4120 IF (L(1)-1)4130, 4140,4130                                  WR       257
1041   4130 CALL PRIN(2HA$,9,A)                                         WR       258
1044        CALL PRIN(4HAL $,9,AL)                                      WR       259
1051   4140 GO TO 5000                                                  WR       260
      C4194                                     MAIN INTEGRATE          WR       261
1052   4200 CALL PRIN(2HF$,6,F)                                         WR       262
1055        CALL PRIN(13HW (WR ROUT) $,6,W)                             WR       263
1062   4210 GO TO 5000                                                  WR       264
      C4994                                                             WR       265
1063   5000 RETURN                                                      WR       266
      C                                                                 WR       267
```

```
1064          END                                                                             HK

              SUBROUTINE HKW(K)                                                               HK*
         C    KISTIAKOWSKY-WILSON EQUATION OF STATE                                           HK*
         C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - --         HK*
         C    K=1: EOS, CALLED FROM GEM(2)                                                    HK*
         C    K=2: MUS, CALLED FROM XIM(2)                                                    HK*
         C K=1                                                                                HK*
         C   INPUT                                                                            HK*
         C    T,V=TAU,THETA=GM(1),(2). (FOR KW,VSTAR=TSTAR=1)                                 HK*
         C    XI=EMX - (GAS) MOLE FRACTIONS                                                   HK*
         C    KI=XPG - COVOLUMES. NOTE: THIS ARRAY IS COVOLUMES                               HK*
         C    KR=KIM(1) - NO. SPECIES                                                         HK*
         C   OUTPUT                                                                           HK*
         C    XE - X*EXP(BETA*X)=Z-1.LOCAL, USED BY K=2 ENTRY.                                HK*
         C                                                                                    HK*
         C                 FOR KW, RSTARIJ FOR LJO.                                           HK*
         C K=2                                                                                HK*
         C   INPUT (SEE DEFINITIONS ABOVE)                                                    HK*
         C    XE FROM K=1                                                                     HK*
         C    GM FROM K=1                                                                     HK*
         C    KI=XPG                                                                          HK*
         C   NOTES                                                                            HK*
         C    1. UNLIKE LJO, FOR WHICH MIX PART IS DONE IN XIM-XIMS,                          HK*
         C       FOR KW EVEREVERYTHING IS DONE HERE.                                          HK*
         C------------------------------------------------------------------------------------ HK*
   3          COMMON Z(4000)                                                                  HK*
   3          DIMENSION                                                                       HK*
             1 EMX    (            20),GM     (            40),GP     (             20) HK*
             2,KTM    (            10),XMU    (            20),XMT    (             30) HK*
             3,XPG    (      20,     20)                                                      HK*
   3          EQUIVALENCE                                                                     HK*
             1 (Z( 1170),EMX    ) ,(Z( 1490),GM     ) ,(Z( 1470),GP     )                     HK*
             2,(Z( 1681),KIM    ) ,(Z( 2240),XMU    ) ,(Z( 2210),XMT    )                     HK*
             3,(Z( 2660),XPG    )                                                             HK*
         C                                                                                    HK*
         C                            KISTIAKOWSKY-WILSON EQUATION OF STATE                   HK*
         C                                                                                    HK*
         C                                                                                    HK*
   3          EQUIVALENCE (GP(1),ALP),(GP(2),BET),(GP(3),TH)                                  HK*
   3          EQUIVALENCE (GM(1),V),(GM(2),T),(GM(12),X)                                      HK*
   3          EQUIVALENCE (XMT(18),HK)                                                        HK*
   3          EQUIVALENCE (KIM(1),KR)                                                         HK*
         C                                                                                    HK*
         C                                                                                    HK*
         C                                                                                    HK*
   3          GO TO (100,500),K                                                               HK*
         C------------------------------------ K=1, EOS -------------------------------------- HK*
  11       100 HK=0                                                                           HK*
  12       110 DO 120 I=1,KR                                                                  HK*
  21       120 HK=HK+EMX(I+1)*XPG(I)                                                          HK*
         C                                                                                    HK*
  25       150 X=HK/(V*(T+TH)**ALP)                                                           HK*
  34       160 E= EXP(BET*X)                                                                  HK*
  42       170 XE=X*E                                                                         HK*
         C                                                                                    HK*
  44       200 GM(3)=XE+1.0                                                                   HK*
  47       210 GM(4)=ALP*T*XE/(T+TH)                                                          HK*
  53       212 GM(6)=(E-1.0)/BET-ALOG(GM(3))                                                  HK*
```

```
 62      220 GM(9)=GM(3)-(1.0+BET*X)*GM(4)                                    HK*        59
 67      230 GM(10)=-(1.0+BET*X)*XE                                           HK*        60
 73      240 GM(11)=GM(4)*(2.0-(1.0+ALP*(1.0+BET*X))*T/(T+TH) )               HK*        61
105      250 GM(5)=GM(4)+XE                                                   HK*        62
107      260  GM(7)=GM(6)+XE                                                  HK*        63
111      270 GM(8)=GM(5)-GM(7)                                                HK*        64
       C                                                                      HK*        65
113      400 GO TO 2000                                                       HK*        66
       C-------------------------------- K=2, MUS ----------------------------HK*        67
114      500 DO 510 I=1,KR                                                    HK*        68
123      510 AMU(I)=GM(5)+(XPG(I)/HK-1.0)*XE                                  HK*        69
       C                                                                      HK*        70
       C 520              NOTE- GEM MOVES F/RT FROM GM(7) TO GM(5)            HK*        71
       C                                                                      HK*        72
131     2000 RETURN                                                           HK*        73
132          END                                                              HK*        74


             SUBROUTINE SEM (K,L)                                             SEM         2
       C                                                                      SEM         3
       C                        SOLID EQ. OF STATE ADAPTOR                    SEM         4
       C                                                                      SEM         5
       C                                  REVISION I - FOR NEW SEMS CODE      SEM         6
       C                                              W.F. 10/61              SEM         7
       C                                                                      SEM         8
       C                                                                      SEM         9
       C     SEM                                                              SEM        10
                                                                              SEM        11
  6          COMMON Z(4000)                                                   SEM        12
  6          DIMENSION                                                        SEM        13
            1 KEN    (      6,     10),KON    (      6,     10),CAR    (    10,     8) SEM  14
            2,CONT   (             20),EV     (             20),FUB    (     6,    10) SEM  15
            3,KAL    (             20),KEV    (             20),SP     (           20) SEM  16
            4,SPC    (             20),SM     (             20),TMS    (           20) SEM  17
            5,THER   (             50)                                    SEM        18
  6          DIMENSION CE(10)                                                 SEM        19
  6          EQUIVALENCE                                                      SEM        20
            1 (Z( 1620),KEN    ) ,(Z( 1690),KON    ) ,(Z(  920),CAR    )      SEM        21
            2,(Z(  460),CONT   ) ,(Z(  680),EV     ) ,(Z( 1410),FUB    )      SEM        22
            3,(Z( 1600),KAL    ) ,(Z(  900),KEV    ) ,(Z( 1840),SP     )      SEM        23
            4,(Z( 1860),SPC    ) ,(Z( 1820),SM     ) ,(Z( 1990),TMS    )      SEM        24
            5,(Z( 1920),THER   )                                              SEM        25
       C                                                                      SEM        26
       C                                  LOCAL EQ                            SEM        27
       C                                                                      SEM        28
  6          EQUIVALENCE (CAR(51),CE),(CONT(2),R)                             SEM        29
            1            ,(THER(1),P),(THER(3),T),(SM(I),VS)                  SEM        30
  6          GO TO (1000,10),K                                                SEM        31
       C 994                                                                  SEM        32
       C 996                    PRELIMINARY                                   SEM        33
       C 998                                                                  SEM        34
 13     1000 CALL REAP (                                                      SEM        35
            1  54HOX       G, CPR, AL, V0, T0, E0R / C0, C1, C2, C3, C4  $    SEM        36
            2  ,12,SP)                                                        SEM        37
 20     1001 KAL(4)=1                                                         SEM        38
 21     1002 IF(SP(2))1004,1003,1004                                          SEM        39
 22     1003 KAL(4)=0                                                         SEM        40
       C                                                                      SEM        41
 23     1004 CALL SEMS(1)                                                     SEM        42
 27     1006 SM(9 )=0.8                                                       SEM        43
```

```
      C                                                                     SEM     44
 31    1010 CALL DOUT (3HSEM,1)                                             SEM     45
 36    1020 GO TO 300                                                       SEM     46
      C1098                                                                 SEM     47
      C                                                                     SEM     48
      C                                 SES MAIN                            SEM     49
 37      10 KEM(2)=KEM(2)+1                                                 SEM     50
 41      20 IF (KAL(4)) 40,100,40                                           SEM     51
      C                                                                     SEM     52
 42      40 CALL SEMS(2)                                                    SEM     53
      C                                                                     SEM     54
 46      50 GO TO 200                                                       SEM     55
      C                                                                     SEM     56
      C                                 CALC. INCOMPRESSIBLE SOLID OUTPUT   SEM     57
 47     100 SM(9)=1.0                                                       SEM     58
 51     102 SM(10)=1.0                                                      SEM     59
 53     104 SM(1)=SP(4)                                                     SEM     60
 55     106 SM(2)=0.0                                                       SEM     61
 56     108 SM(3)=P*VS/(R*T)                                                SEM     62
 62     110 SM(4)=0.0                                                       SEM     63
 63     112 SM(5)=SM(3)                                                     SEM     64
 65     114 SM(6)=0.0                                                       SEM     65
 66     116 SM(7)=SM(3)                                                     SEM     66
 70     118 SM(8)=P                                                         SEM     67
 72     200 CALL DOUT (3HSEM,2)                                             SEM     68
 77     300 RETURN                                                          SEM     69
                                                                            SEM     70
      C              ARGS  K=1, PREL.                                       SEM     71
      C                    K=2, MAIN                                        SEM     72
      C                    L=1, ISOTHERM                                    SEM     73
      C                    L=2, ISENTROPE                                   SEM     74
      C                                                                     SEM     75
      C       SPECS                                                         SEM     76
      C              INPUT                                                  SEM     77
      C                    SP     SEPS INPUT (SEE SEPS)                     SEM     78
      C                    SPC    SEPS OUTPUT (SEE SEPS)                    SEM     79
      C                    T      TEMP                                      SEM     80
      C                    VS     -SOLID VOL                                SEM     81
      C              OUTPUT                                                 SEM     82
      C                    SM     SES IMPERFECTION THERMO FNS-SEE SEMS      SEM     83
      C                             HERE E,H,A,F,S FOR T,P=1 ATM HAVE BEEN  SEM     84
      C                             SUBTRACTED TO FORM IMPERFECTION FNS.    SEM     85
      C                                                                     SEM     86
100           END                                                           SEM     87

              SUBROUTINE SEMS (K)                                           SEMS     2
      C                                                                     SEMS     3
      C                    NEW SES SUBROUTINE                               SEMS     4
      C                           WITH SINGLE ITERATION FOR V(P,T)          SEMS     5
      C                           INPUT - P,T                               SEMS     6
      C                           OUTPUT - V AND SES IMP. THERMO FNS        SEMS     7
      C                           K=1 FOR PREL                              SEMS     8
      C                           K=2 FOR MAIN                              SEMS     9
      C                                                                     SEMS    10
      C       W. F. -10/61                                                  SEMS    11
      C                                                                     SEMS    12
      C                                                                     SEMS    13
                                                                            SEMS    14
  3           COMMON Z(4000)                                                SEMS    15
```

```
 3          DIMENSION
           1 CAR    (     10,      8),EV     (                 20),FOR    (      6,      10)
           2,KON    (      6,     10),SM     (                 20),SP     (              20)
           3,THER   (             50)
 3          DIMENSION C(5),CN(5),CG(5),CG1(5),CS(10) , KCS(2)
 3          EQUIVALENCE
           1 (Z(  920),CAR    ) ,(Z(  680),EV     ) ,(Z( 1410),FOR    )
           2,(Z( 1690),KON    ) ,(Z( 1820),SM     ) ,(Z( 1840),SP     )
           3,(Z( 1920),THER   )
      C
      C
      C                      ≠ARGUMENTS≠
 3          EQUIVALENCE
           1        (THER(1),P),(THER(3),T)
           2        ,(FOR(11),FORI),(FOR(23),YL),(KON(47 ),KONI)
           3        ,(CAR(41),CS),(CS(8),KCS)
           4        ,(EV(1),E1),(EV(2),E2)
      C
      C
      C
 3          EQUIVALENCE
           1        (SP(1),G),(SP(3),ALPH),(SP(4),V0),(SP(5),T0)
           2        ,(SP(8),C),(SP(13),A),(SP(14),G1)
           3        ,(SP(15),G2),(SP(16),CONST)
           4        ,(SP(18),CN),(SP(24),CG),(SP(30),CG1)
           5        ,(SM(9),Y),(SM(10),YI),(SM(11),TC)
           6        ,(SM(12),T1),(SM(13),PH),(SM(15),WEEG)
           7        ,(SM(16),P2),(SM(17),Y1I),(SM(18),X)
           8        ,(SM(19),YU)
      C
      C
      C
 3        20 GO TO (100,1000),K
      C                                 PRELIM
      C
11        100 R=8.31434E-5
13        112 A=(R*SP(2)/(ALPH*V0))*(G/(G+1.0))
22        110 G1=1.0/(G+1.0)
25        120 G2=0.5+1.0/G
      C
31        150 CN(1)=G1
33        160 DO 180 I=2,4
35        170 FI=I
36        180 CN(I)= CN(I-1)*(G1-(FI-1.0))/FI
      C
45        200 DO 230 I=1,5
47        210 FI=I-1
52        220 CG(I)=C(I)/(G+FI)
56        230 CG1(I)=C(I)/(G+FI+1.0)
      C
64        250 E1=0.0
65        260 E2=0.0
66        270 DO 290 I=1,5
70        280 E1=E1+CG(I)
73        290 E2=E2+CG1(I)
76        300 CONST=0.5*E1-G2*E2
      C
102           GO TO 2000
      C
      C                                 MAIN
```

```
      C                                                                 SEMS
103    1000 CS(4)=Y                                                     SEMS
105    1020 CS(2)=Y*FOBI                                                SEMS
107    1030 YU=1.0+ALPH*(T-T0)                                          SEMS
113    1040 KCS(1)=0                                                    SEMS
      C                                                                 SEMS
      C                              ITERATE ON Y=V/V0                  SEMS
114    1100 CALL FROOTT (CS,KONI)                                       SEMS
120    1110 KEXIT=KCS(2)                                                SEMS
122    1120 GO TO (1500,1150,1130,1140),KEXIT                           SEMS
132    1130 CALL DBUG (4HSEMS,1)                                        SEMS
136    1132 GO TO 1500                                                  SEMS
137    1140 CALL DBUG (4HSEMS,1)                                        SEMS
143    1142 GO TO 1500                                                  SEMS
      C                              FUNCTION                           SEMS
144    1150 IF (CS(2)-YU) 1180,1180,1160                                SEMS
147    1160 CS(2)=YU                                                    SEMS
151    1170 GO TO 1200                                                  SEMS
152    1180 IF (YL-CS(2)) 1200,1200,1190                                SEMS
155    1190 CS(2)=YL                                                    SEMS
      C                                                                 SEMS
157    1200 Y=CS(2)                                                     SEMS
      C                                 CALC. P2(Y)                     SEMS
161    1210 PH=C(5)                                                     SEMS
163    1220 E1=CG(5)                                                    SEMS
165    1230 E2=CG1(5)                                                   SEMS
167    1250 DO 1290 I=1,4                                               SEMS
171    1260 KE=5-I                                                      SEMS
173    1270 PH=PH*Y+C(KE)                                               SEMS
176    1280 E1=E1*Y+CG(KE)                                              SEMS
201    1290 E2=E2*Y+CG1(KE)                                             SEMS
      C                                                                 SEMS
206    1300 WEEG=(0.5-G2*Y)*PH                                          SEMS
212    1310 YG=Y**G                                                     SEMS
      C                                                                 SEMS
216    1320 P2=-(G/Y)*WEEG+G*(G/Y)*                                     SEMS
          1            (0.5*E1-G2*Y*E2-CONST/YG)                        SEMS
      C                                                                 SEMS
      C                                 CALC Y1, Y11, SEPARATE ON Y     SEMS
231    1350 IF (Y-1.0) 1700,1800,1800                                   SEMS
      C                                                                 SEMS
      C                                                                 SEMS
      C                                                                 SEMS
235    1400 CS(3)=2.0E-6*(TC-T)                                         SEMS
      C                                                                 SEMS
240    1470 CALL DOUT (4HSEMS,1)                                        SEMS
244    1480 GO TO 1100                                                  SEMS
      C                                                                 SEMS
      C                              CALCULATE OUTPUT                   SEMS
245    1500 SM(1)=Y*V0                                                  SEMS
247    1510 SM(7)=P*SM(1)/(R*T)                                         SEMS
253    1520 SM(3)=(1.0+1.0/G)*SM(7)+V0*WEEG/(R*T)-SP(2)*(1.0-T0/T)      SEMS
265    1530 SM(6)=SP(2)*ALOG(T1/T)                                      SEMS
274    1540 SM(5)=SM(3)-SM(6)                                           SEMS
276    1550 SM(2)=SM(3)-SM(7)                                           SEMS
300    1560 SM(4)=SM(5)-SM(7)                                           SEMS
302    1572 GO TO 2000                                                  SEMS
      C                                                                 SEMS
      C                                                                 SEMS
      C                              CALC. FN. FOR Y LESS THAN 1        SEMS
```

```
      C                                                                                   SEMS   136
305    1700 X=(P-P2)*YG*Y/A                                                               SEMS   137
310    1710 YG1=1.0+X                                                                     SEMS   138
313    1720 Y11=CN(4)*X                                                                   SEMS   139
315    1730 DO 1740 I=1,3                                                                 SEMS   140
317    1732 KE=4-I                                                                        SEMS   141
321    1740 Y11=(Y11+CN(KE))*X                                                            SEMS   142
326    1742 Y1=Y11+1.0                                                                    SEMS   143
      C                                                  CALC. T                          SEMS   144
331    1750 T1=Y11/ALPH+T0                                                                SEMS   145
334    1760 TC=T1*(YG1/Y1)/YG                                                             SEMS   146
340    1770 GO TO 1400                                                                    SEMS   147
      C                                             CALC. FN. FOR Y OVER 1                SEMS   148
      C                                                                                   SEMS   149
341    1800 X=P/A                                                                         SEMS   150
343    1810 YG1=1.0+X                                                                     SEMS   151
346    1820 Y11=CN(4)*X                                                                   SEMS   152
350    1830 DO 1850 I=1,3                                                                 SEMS   153
352    1840 KE=4-I                                                                        SEMS   154
354    1850 Y11=(Y11+CN(KE))*X                                                            SEMS   155
361    1860 Y11=Y-1.0+Y*Y11                                                               SEMS   156
365    1862 Y1=Y11+1.0                                                                    SEMS   157
      C                                                  CALC. T                          SEMS   158
370    1870 T1=Y11/ALPH+T0                                                                SEMS   159
373    1880 TC=T1*YG1*Y/(Y11+1.0)                                                         SEMS   160
400    1890 GO TO 1400                                                                    SEMS   161
      C                                                                                   SEMS   162
401    2000 RETURN                                                                        SEMS   163
402         END                                                                           SEMS   164


            SUBROUTINE TIM (K)                                                            TIM      2
      C                                                                                   TIM      3
      C                              ITF ADAPTOR                                          TIM      4
      C                                                                                   TIM      5
      C                 REVISION 1. FIX TIM FOR TIMS REVISION 1                           TIM      6
      C                       W.F. DEC. 61                                                TIM      7
      C                                                                                   TIM      8
      C     TIM                                                                           TIM      9
                                                                                          TIM     10
   3        COMMON Z(4000)                                                                TIM     11
   3        DIMENSION                                                                     TIM     12
           1 CONT   (    20) ,EA     (   200) ,EMX    (    20)                            TIM     13
           2,HE     (    10) ,KEN    (    60) ,KIM    (    10)                            TIM     14
           3,THER   (    50) ,TMS    (    20) ,TMG    (    20)                            TIM     15
           4,TP      (20,10)                                                              TIM     16
   3        DIMENSION KE(2),TH(5)                                                         TIM     17
   3        EQUIVALENCE                                                                   TIM     18
           1 (Z(   460),CONT   ) ,(Z(   480),EA     ) ,(Z( 1170),EMX    )                 TIM     19
           2,(Z( 1590),HE     ) ,(Z( 1620),KEN    ) ,(Z( 1680),KIM    )                   TIM     20
           3,(Z( 1920),THER   ) ,(Z( 1990),TMS    ) ,(Z( 1970),TMG    )                   TIM     21
           4,(Z( 2010),TP     )                                                           TIM     22
      C                              LOCAL EQ,DIM                                         TIM     23
   3        EQUIVALENCE (KIM(2),KS),(KIM(4),KN),(CONT(3),ATM)                             TIM     24
           1            ,(THER(1),P),(THER(3),T)                                          TIM     25
      C                                                                                   TIM     26
      C   98                                                                              TIM     27
   3    100 GO TO (1000,2000),K                                                           TIM     28
      C 996                                                                               TIM     29
      C 998                                        PRELIMINARY                            TIM     30
```

```
 11    1000 CALL READ (                                                    TIM        31
            1  60HOX  KS,KN/ T BOUNDS/ FIT COEFFS.-A1 TO AN,D,DEL,HF,HR...$ TIM        32
            2 ,-2,KE)                                                      TIM        33
 18         CALL READ(0,2,TH(4))                                           TIM        34
 20    1010 KS=KE(1)                                                       TIM        35
 22    1020 KN=KE(2)                                                       TIM        36
 24    1030 KE1=KN+5                                                       TIM        37
 26    1040 DO 1070 I=1,KS                                                 TIM        38
 30    1050 CALL READ (0,KE1,EA)                                           TIM        39
 34    1060 DO 1070 J=1,KE1                                                TIM        40
 44    1070 TP(I,J)=EA(J)                                                  TIM        41
 52         GO TO 3000                                                     TIM        42
      C1996                                                                TIM        43
      C1998                              MAIN                              TIM        44
 52    2000 KEN(3)=KEN(3)+1                                                TIM        45
 54    2010 TH(1)=T                                                        TIM        46
 56    2060 KE(1)=KS                                                       TIM        47
 60    2070 KE(2)=KN                                                       TIM        48
 62    2080 TH(2)=P/ATM                                                    TIM        49
 64    2090 TH(3)=HE(3)                                                    TIM        50
      C2100                                                                TIM        51
 66    2110 CALL TIMS (KE,TH,TP,EMX,TMS,TMG)                               TIM        52
 74    2120 CALL DOUT (3HTIM,1)                                            TIM        53
      C2900                                                                TIM        54
100    3000 RETURN                                                         TIM        55
      C                                                                    TIM        56
      C                                                                    TIM        57
101         END                                                            TIM        58


            SUBROUTINE TIMS (K,TH,A,X,G,F)                                 TIMS        2
      C                                                                    TIMS        3
      C                          IDEAL GAS THERMO FNS SUBROUTINE           TIMS        4
      C             REVISION 1.-CONST. CP EXTENSIONS                       TIMS        5
      C                   W. F. DEC. 61                                    TIMS        6
      C                                                                    TIMS        7
      C                          K(1)=KS, NO. OF SPECIES                   TIMS        8
      C                          K(2)=KN, DEGREE OF FIT                    TIMS        9
      C                          TH(1)=T IN DEGREES K.                     TIMS       10
      C                          TH(2)=PINATM.                             TIMS       11
      C                          TH(3)=T SUB ZERO                          TIMS       12
      C                        TH(4)=TMIN                                  TIMS       13
      C                        TH(5)=TMAX                                  TIMS       14
      C                          A - COEFFICIENT MATRIX (SEE WRITE-UP)     TIMS       15
      C                          X - MOLE FRACTIONS  (X(1) FOR SOLID)      TIMS       16
      C                                                                    TIMS       17
      C     IDEAL GAS THERMODYNAMIC FUNCTIONS                              TIMS       18
      C               INPUT                                                TIMS       19
      C               OUTPUT                                               TIMS       20
      C                          G - TOTAL THERMO FUNCTIONS FOR GAS,SOLID  TIMS       21
      C                          F - FREE ENERGIES AT T,P                  TIMS       22
      C                                    RELATIVE TO ELEMENTS AT 0 KELVIN TIMS      23
      C     TIMS                                                           TIMS       24
 16         COMMON Z(4000)                                                 TIMS       25
 16         DIMENSION K(2),TH(5),A (20,10),X(20),G(20),F(20)               TIMS       26
           1,EA(80),C(20),H(20),S(20),GI(20)                               TIMS       27
 16         EQUIVALENCE                                                    TIMS       28
           1 (Z(  480),EA     )                                            TIMS       29
           1          ,(EA(1),C),(EA(21),H),(EA(41),S)                     TIMS       30
           2,(EA(61),GI)                                                   TIMS       31
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      C                                                                                    TIMS        32
      C                                                                                    TIMS        33
      C    2 E                                                                             TIMS        34
  16       3           R=1.98719E-3                                                        TIMS        35
  20       4            KS=K(1)                                                            TIMS        36
  21       5            N=K(4)                                                             TIMS        37
  23       6            T=TH(1)                                                            TIMS        38
  25       7            PLOG=ALOG(TH(2))                                                   TIMS        39
  34       8            T0=TH(3)                                                           TIMS        40
  34          TMIN=TH(4)                                                                   TIMS        41
  34          TMAX=TH(5)                                                                   TIMS        42
      C    9 I(E)                                                                          TIMS        43
  41      10            DO 20 I=1,80                                                       TIMS        44
  46      20            EA(I)=0.0                                                          TIMS        45
      C                                 BOUND T1 TO FIT RANGE                              TIMS        46
  53      30 IF(T-TMAX) 60,60,40                                                           TIMS        47
  56      40 T1=TMAX                                                                       TIMS        48
  60      50 GO TO 110                                                                     TIMS        49
  61      60 IF(T-TMIN) 70,70,90                                                           TIMS        50
  64      70 T1=TMIN                                                                       TIMS        51
  66      80 GO TO 110                                                                     TIMS        52
  67      90 T1=T                                                                          TIMS        53
      C  100 I                                           ALL SPECIES                       TIMS        54
  71     110 DO 290 I=1,KS                                                                 TIMS        55
      C  112  (I(E))                                             J=N,1 FOR SERIES          TIMS        56
  73     120            J=N                                                                TIMS        57
  75     130            FJ=J                                                               TIMS        58
  77     140            AIJ=A(I,J+1)                                                       TIMS        59
 103     150 H(I)=(H(I)+AIJ)*T1                                                            TIMS        60
 107     160 C(I)=(C(I)+(FJ +1.0)*AIJ)*T1                                                  TIMS        61
 115     170 S(I)=(S(I)+((FJ+1.0)/FJ)*AIJ)*T1                                              TIMS        62
 124     180            J=J-1                                                              TIMS        63
 126     190            IF  (J)130,210,130                                                 TIMS        64
      C  200 E                                           ADD FIRST TERMS                   TIMS        65
 127     210            AIJ=A(I,1)                                                         TIMS        66
 132     220            H(I)=H(I)+AIJ                                                      TIMS        67
 135     230            C(I)=C(I)+AIJ                                                      TIMS        68
 140     240 S(I)=S(I)+AIJ*ALOG(T1)+A(I,N+2)-PLOG                                          TIMS        69
      C                                                                                    TIMS        70
      C                                         ADD CONST CP FUNCTIONS OUTSIDE             TIMS        71
 155     250 IF  (T-T1) 260,290,260                                                        TIMS        72
 157     260 H(I)=( T1*H(I)+C(I)*(T-T1)  )/T                                               TIMS        73
 165     270 S(I)=S(I)+C(I)*ALOG(T/T1)                                                     TIMS        74
      C                                                                                    TIMS        75
 200     290 F(I)=H(I)-S(I)+A(I,N+3)/(R*T)                                                 TIMS        76
      C  300 I(E)                                                  MIXTURE SUMS            TIMS        77
 213     310            DO 360 I=2,KS                                                      TIMS        78
 215     312            XI=X(I)                                                            TIMS        79
 217     320 GI(2)=GI(2)+XI*(H(I)+A(I,N+3)/(R*T))                                          TIMS        80
 230     330            GI(3)=GI(3)+XI*C(I)                                                TIMS        81
 230         FXI=0.0                                                                       TIMS        82
 234         IF(XI.GT.0.0)FXI=XI*ALOG(XI)                                                  TIMS        83
 244     340            GI(4)=GI(4)+XI*S(I)-FXI                                            TIMS        84
 251     350            GI(5)=GI(5)+XI*A(I,N+4)                                            TIMS        85
 257     360 GI(6)=GI(6)+XI*(H(I)-(T0/T)*A(I,N+5)+A(I,N+4)/(R*T))                          TIMS        86
      C  370 E                                                                             TIMS        87
 301     380            GI(1)=GI(2)-1.0                                                    TIMS        88
      C  400 E                                           PURE PHASE                        TIMS        89
 304     410 GI(7)=H(1)+A(1,N+3)/(R*T)                                                     TIMS        90
 312     420            GI(8)=C(1)                                                         TIMS        91
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314      430           GI(9)=S(1)*PLOG                                                   TIMS        92
316      440 GI(10)=F(1)-PLOG                                                            TIMS        93
320      450 GI(11)=A(1,N+4)                                                             TIMS        94
323      460 GI(12)=H(1)-(T0/T)*A(1,N+5)+GI(11)/(R*T)                                     TIMS        95
334      470           F(1)=GI( 0)                                                       TIMS        96
       C 500 I(E)                               STORE GI                                 TIMS        97
336      510           DO 520 I=1,12                                                     TIMS        98
343      520           G(I)=GI(I)                                                        TIMS        99
350      600           RETURN                                                            TIMS       100
351          END                                                                         TIMS       101

             SUBROUTINE XIM (K,L)                                                        XIM          2
       C     GAS (MIXTURE) EQUATION OF STATE AT T, P, XI                                 XIM          3
       C           K=1   READ INPUT DATA (PREL.)                                         XIM          4
       C           K=2   MAIN CALCULATION                                                XIM          5
       C           L SPECIFIES PORTION OF EQ CODE FROM                                   XIM          6
       C                 WHICH XIM IS CALLED (SEE WRITEUP)                               XIM          7
       C    INPUT                                                                        XIM          8
       C      T,P=THER(3),(1)                                                            XIM          9
       C      XI - (GAS) MOLE FRACTIONS                                                  XIM         10
       C    OUTPUT                                                                       XIM         11
       C      XMT - MIXTURE STATE                                                        XIM         12
       C      XMU - MU*S                                                                 XIM         13
       C    ROUTINES                                                                     XIM         14
       C      XIMS - DETAILED CALCULATIONS FOR LH, CS, 1-FLUID.                          XIM         15
       C           CALLS GEP(2) IN MIDDLE FOR REF. STATE FOR MU*S                        XIM         16
       C      GEP(1/2) - PURE STATE POINT (REGULAR/LH EXPANSION)                         XIM         17
       C-----------------------------------------------------------------------------    XIM         18
       C                                    REVISION 1 - ADD KW EQ N. OF STATE           XIM         19
       C                                                 W.F.  9/81                      XIM         20
       C                                                                                 XIM         21
       C                                                                                 XIM         22
       C                                                                                 XIM         23
       C     XIM                                                                         XIM         24
                                                                                         XIM         25
    5        COMMON Z(4000)                                                              XIM         26
    6        DIMENSION                                                                   XIM         27
            1 CONT   (            20),EA     (           200),EMX    (           20) XIM         28
            2,GP     (            20),GM     (            40),GMT    (     3,    20) XIM         29
            3,KAL    (            20),KIM    (            10),THER   (           50) XIM         30
            4,XMT    (            30),XMU    (            20),XPF    (    20,    20) XIM         31
            5,XPG    (     20,    20),XPR    (            20),XPT    (           20) XIM         32
            6 , KEN(6,10)                                                                XIM         33
    6        DIMENSION KE(2),E1(6)                                                       XIM         34
            1,SXG(20),SXF(20)                                                            XIM         35
    6        EQUIVALENCE                                                                 XIM         36
            1 (Z(  460),CONT   ) ,(Z(  480),EA    ) ,(Z( 1170),EMX   )                   XIM         37
            2,(Z( 1470),GP     ) ,(Z( 1490),GM    ) ,(Z( 1530),GMT   )                   XIM         38
            3,(Z( 1600),KAL    ) ,(Z( 1680),KIM   ) ,(Z( 1920),THER  )                   XIM         39
            4,(Z( 2210),XMT    ) ,(Z( 2240),XMU   ) ,(Z( 2260),XPF   )                   XIM         40
            5,(Z( 2660),XPG    ) ,(Z( 3060),XPR   ) ,(Z( 3080),XPT   )                   XIM         41
            6 ,(Z(1620),KEN)                                                             XIM         42
       C                                                                                 XIM         43
       C     LOCAL EQUIVIM                                                               XIM         44
       C                                                                                 XIM         45
    6        EQUIVALENCE                                                                 XIM         46
            1 (CONT(2),R),(GP(5),RSTA),(GP(6),TSTA),(GP(7),VSTA)                         XIM         47
            2,(KIM(1),KR),(THER(1),P),(THER(3),T)                                        XIM         48
            3,(XMT(16),RSTAT),(XMT(17),TSTAT),(XMT(18),VSTAT)                            XIM         49
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              4,(EA(21),SXG),(EA(41),SXF)                                           XIM      50
          C                                                                         XIM      51
  6         80 GO TO (100,800),K                                                    XIM      52
          C - - - - - - - - - - - - - - - - - - - - - - -PRELIM - - - - - - - - - - - XIM      53
 14        100 CALL READ (                                                          XIM      54
              154R*X K9,KAL/ SCP,SCT,R*REF,T*REF,N,M/ (R*)/ (T*)   S                XIM      55
              1 ,-2,KE)                                                             XIM      56
 17             CALL READ(0,6,E1)                                                   XIM      57
 22             CALL READ(0,KE,XPR)                                                 XIM      58
 25             CALL READ(0,KE,XPT)                                                 XIM      59
 32        110 KR=KE(1)                                                             XIM      60
 34        120 KAL(5)=KE(2)                                                         XIM      61
 36        130 DO 150 I=1,KR                                                        XIM      62
 40        140 XPR(I)=XPR(I)*E1(1)                                                  XIM      63
 43        150 XPT(I)=XPT(I)*E1(2)                                                  XIM      64
          C 160                                                                     XIM      65
 46        170 DO 200 I=1,KR                                                        XIM      66
 50        180 DO 200 J=1,KR                                                        XIM      67
 52        190 XPG(I,J)=(XPR(I)+XPR(J))/2.0                                         XIM      68
 60        200 XPF(I,J)= SQRT (XPT(I)*XPT(J))                                       XIM      69
          C 208                                                                     XIM      70
 75        210 XMT(11)=E1(3)                                                        XIM      71
 77        220 XMT(12)=E1(4)                                                        XIM      72
101        230 XMT(13)=E1(5)                                                        XIM      73
103        240 XMT(14)=E1(6)                                                        XIM      74
105        250 IF (KAL(5)-9) 300,260,300                                            XIM      75
107        260 DO 270 I=1,KR                                                        XIM      76
115        270 XPG(I)=E1(3)*CONT(5)*XPR(I)**3                                       XIM      77
121        300 GO TO 6000                                                           XIM      78
          C------------------------------------ MAIN ---------------------------- XIM      79
122        800 KE=KAL(5)+1                                                          XIM      80
124        802 KEN(4)=KEN(4)+1                                                      XIM      81
          C                              CHECK FOR KIASTOWSKY-WILSON                XIM      82
126        804 IF (KAL(5)-9) 810,806,810                                            XIM      83
130        806 CALL GEP(1)                                                          XIM      84
134        808 CALL HKW(2)                                                          XIM      85
          C                                                                         XIM      86
140        809 GO TO 1100                                                           XIM      87
          C                                                                         XIM      88
141        810 GO TO (1000,2000,3000,4000,4000),KE                                  XIM      89
          C--------------------------------------------------------------------- XIM      90
          C 990                           NO MIX (ZERO)                             XIM      91
          C 998                                                                     XIM      92
152        1000 GO TO (1020,6000,1100),L                                            XIM      93
          C1010                                         NO MIX-ONE                  XIM      94
161        1020 CALL GEP(1)                                                         XIM      95
165        1030 DO 1040 I=1,KR                                                      XIM      96
172        1040 XMU(I)=GM(5)                                                        XIM      97
174        1050 GO TO 6000                                                          XIM      98
          C1098                                         NO MIX-THREE                XIM      99
          C                                                   MIXTURE=REF. FLUID    XIM     100
175        1100 XMT(1)=GM(15)                                                       XIM     101
177        1110 XMT(2)=GM(4)                                                        XIM     102
201        1120 XMT(3)=GM(17)                                                       XIM     103
203        1130 XMT(4)=GM(20)                                                       XIM     104
205        1140 XMT(5)=GM(5)                                                        XIM     105
207        1150 XMT(6)=GM(11)                                                       XIM     106
211        1160 XMT(7)=GM(10)                                                       XIM     107
213        1170 XMT(8)=GM(9)                                                        XIM     108
215        1180 GO TO 6000                                                          XIM     109
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      C------------------------------------------------------------------------- XIM      110
      C1090                          IDEAL MIXING (ONE)                          XIM      111
      C1098                                                                      XIM      112
216    2000 GO TO (2030,6000,2200),L                                             XIM      113
      C2010                                                                      XIM      114
      C2020                                    IDEAL -ONE                        XIM      115
225    2030 DO 2110 I=1,KR                                                       XIM      116
227    2040 TSTA=XPT(I)                                                          XIM      117
231    2050 RSTA=XPR(I)                                                          XIM      118
233    2060 VSTA=CONT(5)*RSTA**3                                                 XIM      119
236    2070 CALL GEP(1)                                                          XIM      120
242    2080 GMT(1,I)=GM(15)                                                      XIM      121
245    2090 GMT(2,I)=GM(17)                                                      XIM      122
250    2100 GMT(3,I)=GM(5)                                                       XIM      123
253    2110 XMU(I)=GM(5)                                                         XIM      124
257    2120 GO TO 6000                                                           XIM      125
      C                                        IDEAL -THREE                      XIM      126
260    2200 XMT(1)=0.0                                                           XIM      127
261    2210 XMT(3)=0.0                                                           XIM      128
262    2220 XMT(5)=0.0                                                           XIM      129
263    2230 DO 2250 I=1,KR                                                       XIM      130
265    2240 XMT(1)=EMX(I+1)*GMT(1,I)+XMT(1)                                      XIM      131
271    2250 XMT(3)=EMX(I+1)*GMT(2,I)+XMT(3)                                      XIM      132
275    2260 XMT(5)=EMX(I+1)*GMT(3,I)+XMT(5)                                      XIM      133
      C2270                                                                      XIM      134
303    2280 XMT(7)=P*XMT(1)/(R*T) -1.0                                           XIM      135
310    2290 XMT(2)=XMT(3)-XMT(7)                                                 XIM      136
312    2300 XMT(4)=XMT(5)-XMT(7)                                                 XIM      137
314    2310 XMT(6)=XMT(3)-XMT(5)                                                 XIM      138
316    2320 XMT(8)=XMT(1)-R*T/P                                                  XIM      139
322    2330 GO TO 6000                                                           XIM      140
      C------------------------------------------------------------------------- XIM      141
      C2090                          LH (TWO)                                    XIM      142
      C2098                                                                      XIM      143
323    3000 GO TO (3010,3100,3400),L                                             XIM      144
      C3004                                                                      XIM      145
      C3006                                    LH-ONE                            XIM      146
332    3010 RSTA=XMT(11)                                                         XIM      147
334    3020 TSTA=XMT(12)                                                         XIM      148
336    3030 VSTA=CONT(5)*RSTA**3                                                 XIM      149
341    3040 CALL GEP(1)                                                          XIM      150
      C                                                                          XIM      151
      C                                           LH-TWO                         XIM      152
345    3100 CALL XIMS (1)                                                        XIM      153
351    3120 GO TO 6000                                                           XIM      154
      C3398                                    LH-THREE                          XIM      155
352    3400 CALL GEP(2)                                                          XIM      156
354         GO TO 6000                                                           XIM      157
      C------------------------------------------------------------------------- XIM      158
      C                                        CS (THREE) AND ONE FLUID (FOUR)   XIM      159
356    4000 GO TO (4010,4100,6000),L                                             XIM      160
      C4004                                                                      XIM      161
      C4006                                    CS, 1-FLUID - ONE                 XIM      162
365    4010 CALL XIMS (0)                                                        XIM      163
371    4020 TSTA=TSTAT                                                           XIM      164
373    4030 RSTA=RSTAT                                                           XIM      165
375    4040 VSTA=VSTAT                                                           XIM      166
377    4050 CALL GEP(1)                                                          XIM      167
      C                                        CS, 1-FLUID - TWO                 XIM      168
403    4100 CALL XIMS (1)                                                        XIM      169
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405          GO TO 6000                                                          XIM          170
       C                                                                         XIM          171
407     6000 CALL DOUT(3HXIM,1)                                                  XIM          172
414     6010 RETURN                                                              XIM          173
       C                                                                         XIM          174
415          END                                                                 XIM          175


             SUBROUTINE XIMS (K)                                                 XIMS           2
       C THIS ROUTINE HAD HAD PUNCHES IN COL 73, REMOVED FOR PHOTOSTORE          XIMS           3
       C                                                                         XIMS           4
       C     PERFORM DETAILED CALCULATIONS FOR XIM                               XIMS           5
       C                                                                         XIMS           6
       C                                                                         XIMS           7
       C     XIMS                                                                XIMS           8
                                                                                 XIMS           9
  3          COMMON Z(4000)                                                      XIMS          10
  3          DIMENSION                                                           XIMS          11
           1  XPF    (20,20), XPG    (20,20), CONT    (    20)                   XIMS          12
           2,EA     (  200) ,EMX    (    20) ,GM     (    40)                    XIMS          13
           3,GP     (   20) ,KAL    (    20) ,KIM    (    10)                    XIMS          14
           4,XMO    (   20) ,XMT    (    30) ,EV     (    20)                    XIMS          15
  3          DIMENSION BILK(15)                                                  XIMS          16
  3          DIMENSION SXG(20),SXF(20),SRN(20),STN(20)                           XIMS          17
  3          EQUIVALENCE                                                         XIMS          18
           1 (Z( 2260),XPF    ) ,(Z( 2060),XPG    ) ,(Z(  460),CONT   )          XIMS          19
           2,(Z(  480),EA     ) ,(Z( 1170),EMX    ) ,(Z( 1490),GM     )          XIMS          20
           3,(Z( 1470),GP     ) ,(Z( 1600),KAL    ) ,(Z( 1680),KIM    )          XIMS          21
           4,(Z( 2240),XMO    ) ,(Z( 2210),XMT    ) ,(Z(  680),EV     )          XIMS          22
       C                                                                         XIMS          23
  3          EQUIVALENCE (KIM(1),KR),(KIM(2),KS),(KIM(3),KC),(KIM(4),KN)         XIMS          24
  3          EQUIVALENCE (XMT(16),RSTAT),(XMT(17),TSTAT),(XMT(18),VSTAT)         XIMS          25
           1,            (GP(5),RSTA),(GP(6),TSTA),(GP(7),VSTA)                  XIMS          26
       C                                                                         XIMS          27
       C      704 TO 7090 (N,M FOR ONE FLUID)                                    XIMS          28
  3           EQUIVALENCE (XMT(1),BILK(2))                                       XIMS          29
       C                                                                         XIMS          30
  3           EQUIVALENCE                                                        XIMS          31
           1(EA(21),SXG),(EA(41),SXF),(EA(61),SRN),(EA(81),STN)                  XIMS          32
       C                                                                         XIMS          33
       C   90                        CALCULATE BAR- T*,R* / MOO II,4             XIMS          34
  3     100 DO 130 I=1,KR                                                        XIMS          35
  5     120 SXF(I)=0.0                                                           XIMS          36
  7     130 SXG(I)=0.0                                                           XIMS          37
 12     140 TSTAT=0.0                                                            XIMS          38
 13     150 RSTAT=0.0                                                            XIMS          39
       C 190                                       L-BRANCH- CS OR 1-FLUID       XIMS          40
 14     200 KQ=KAL(5)                                                            XIMS          41
 16     210 GO TO (1500,300,300,400),KQ                                          XIMS          42
       C 290                                                CS(OR LR)            XIMS          43
 26     300 DO 350 I=1,KR                                                        XIMS          44
 30     310 DO 330 J=1,KR                                                        XIMS          45
 32     320 SXF(I)=EMX(J+1)*XPF(I,J)+SXF(I)                                      XIMS          46
 37     330 SXG(I)=EMX(J+1)*XPG(I,J)+SXG(I)                                      XIMS          47
 45     340 TSTAT=EMX(I+1)*SXF(I)+TSTAT                                          XIMS          48
 50     350 RSTAT=EMX(I+1)*SXG(I)+RSTAT                                          XIMS          49
 55     360 GO TO 700                                                            XIMS          50
       C 390                                                ONE-FLUID            XIMS          51
 56     400 EV(11)=0.0                                                           XIMS          52
 57     410 EV(12)=0.0                                                           XIMS          53
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```
 50      500 DO 550 I=1,KR                                                    XIPS     54
 62      510 DO 530 J=1,KR                                                    XIPS     55
 64      520 SXF(I)=FMX(J+1)*XPF(1,J)*XPG(1,J)**BILK(14)    +SXF(I)           XIPS     56
 77      530 SXG(I)=FMX(J+1)*XPF(I,J)*XPG(I,J)**BILK(15)      +SXG(I)         XIPS     57
113      540 EV(11)=FMX(I+1)*SXF(I)+EV(11)                                    XIPS     58
116      550 EV(12)=FMX(I+1)*SXG(I)+EV(12)                                    XIPS     59
123      600 E3=1.0/(BILK(14)-BILK(15))                                       XIPS     60
126      610 E4=BILK(14)*E3                                                   XIPS     61
130      620 E5=BILK(15)*E3                                                   XIPS     62
132      630 TSTAT=EV(12)**E4/EV(11)**E5                                      XIPS     63
142      640 RSTAT=(EV(11)/EV(12))**E3                                        XIPS     64
       C                                  REJOIN-CALC. VSTA                   XIPS     65
147      700 VSTAT=CONT(5)*RSTAT**3                                           XIPS     66
       C 800                                                                  XIPS     67
       C 810                        CALC MUS IF K=1                           XIPS     68
152     1000 IF (K)1010,1500,1010                                             XIPS     69
       C                                                                      XIPS     70
153     1010 CALL GEP(2)                                                      XIPS     71
       C1090                                 I-BRANCH- CS OR 1-FLUID          XIPS     72
       C                                                LH                    XIPS     73
156     1100 GO TO (1500,1150,1200,1300),KW                                   XIPS     74
166     1150 DO 1160 I=1,KR                                                   XIPS     75
175     1160 XMU(I)=GM(5)                                                     XIPS     76
            1        +GM(4)*(2.0*(SXF(I)/XMT(12)-1.0)-(TSTAT/TSTA-1.0))       XIPS     77
            2        +3.0*GM(10)*(2.0*(SXG(I)/XMT(11)-1.0)-(RSTAT/RSTA -1.0)) XIPS     78
216     1170 GO TO 1500                                                       XIPS     79
       C1190                                            CS                    XIPS     80
217     1200  DO 1220 I=1,KR                                                  XIPS     81
221     1210 STN(I)=2.0*(SXF(I)/TSTAT-1.0)                                    XIPS     82
224     1220 SRN(I)=2.0*(SXG(I)/RSTAT-1.0)                                    XIPS     83
234     1230 GO TO 1400                                                       XIPS     84
       C1290                                            ONE-FLUID             XIPS     85
235     1300 DO 1320 I=1,KR                                                   XIPS     86
237     1310 STN(I)= -2.0-2.0*E3*(BILK(15)*SXF(I)/EV(11)                      XIPS     87
            1              -BILK(14)*SXG(I)/EV(12))                           XIPS     88
251     1320 SRN(I)= 2.0*E3*(SXF(I)/EV(11)-SXG(I)/EV(12))                     XIPS     89
       C1390                                 REJOIN FOR MU CALC.              XIPS     90
261     1400 DO 1410 I=1,KR                                                   XIPS     91
270     1410 XMU(I)=XMT(5)+3.0*XMT(7)*SRN(I)+XMT(2)*STN(I)                    XIPS     92
277     1500 RETURN                                                           XIPS     93
300          END                                                              XIPS     94


             SUBROUTINE EQP                                                   EQP       2
       C                         EQ PRELIMINARY                               EQP       3
       C           REVISION  1 ERROR IN STATEMENT 520                         EQP       4
       C               LOOP GOES TO KS, NOT 10                                EQP       5
       C                    W.F.  3/60                                        EQP       6
       C                                                                      EQP       7
       C     EQP                                                              EQP       8
                                                                              EQP       9
  1          COMMON Z(4000)                                                   EQP      10
  1          DIMENSION                                                        EQP      11
            1 EPAL  (      20,      6),EPA    (         20),EPA1  (        20) EQP     12
            2,EPC   (              10),EPW    (         10),FLAB  (    12,  8) EQP     13
            3,KAL   (              20),KIM    (         10),KON   (     6, 10) EQP     14
  1          DIMENSION KEPA(20),KEPA1(20),KEPAL(20,6),KEPC(10)                EQP      15
  1          DIMENSION KE1(12),L(12)                                          EQP      16
  1          EQUIVALENCE                                                      EQP      17
            1 (Z( 1210),EPAL  ) ,(Z( 1190),EPA   ) ,(Z( 1330),EPA1  )         EQP      18
```

```
            2,(Z( 1350),EPC    ) ,(Z( 1360),EPQ    ) ,(Z( 3100),FLAB   )
            3,(Z( 1600),KAL    ) ,(Z( 1680),KIM    ) ,(Z( 1690),KON    )
       C
  1           EQUIVALENCE (KIM(2),KS),(KIM(3),KC)
            2              ,(EPA,KEPA),(EPA1,KEPA1),(EPAL,KEPAL)
            3              ,(EPC,KEPC)
       C
  1           EQUIVALENCE (FLAB(49),L)
       C
       C
  1        80 KAL(6)=1
  2       100 CALL READ (
             1   30H0X    C,S,P,-,PP,PHI / CAP Q   $
            2 ,-6,KEPC)
  5           CALL READ(0,KEPC,EPQ)
 10       110 KC=KEPC(1)
 12       120 KS=KEPC(2)
 14       130 READ(10,140 )              (KE1(I),I=1,12)
          140 FORMAT (12A6)
 22       150 DO 160 I=1,KS
 24       160 READ(10,170 )             L(I),(KEPAL(I,J),J=1,KC)
          170 FORMAT (A6,11I6)
 46       180 READ(10,200 )              (KEPA(I),I=1,KS)
 55       190 READ(10,200 )              (KEPA1(I),I=1,KS)
          200 FORMAT (12I6)
       C
 64       300 WRITE(9,310 )               (KE1(I),I=1,KS)
          310 FORMAT (6H0       ,12A6/)
 73       320 DO 330 I=1,KS
 75       330 WRITE(9,340 )               L(I),(KEPAL(I,J),J=1,KC)
             1                ,KEPA(I),KEPA1(I)
          340 FORMAT (6H       ,A6,11I6)
       C 490
124       500 DO 510 I=1,10
131       510 EPC(I)=KEPC(I)
133       520  DO 530 I=1,KS
135       530 EPA(I)=KEPA(I)
140       540 EPA1(I)=KEPA1(I)
144       550 DO 570 I=1,KS
146       560 DO 570 J=1,KC
156       570 EPAL(I,J)=KEPAL(I,J)
163       580 KAL(6)=1
       C 590
164       600 CALL EQPS(KON(1,8),EPC,EPQ,EPAL,EPAL(1,2),EPA,EPA1)
       C 690
174      1000 RETURN
       C
175           END


              SUBROUTINE EQM
       C              EQUILIBRIUM COMPOSITION AND STATE AT T,P
       C    INPUT
       C      P,T=THER(1),(3). IMPLICIT FOR GEP VIA XIM-XIMS
       C      SM - STATE OF SOLID
       C      IMG - IDEAL STATE
       C    OUTPUT
       C      XI=EMX - (GAS) MOLE FRACTIONS
       C      XMT - GAS (MIXTURE) STATE
       C    VARIABLES
```

```
      C       F-TILDE=EMG - FREE ENERGIES FOR EQMS
      C       EMN - PHASE MOLE NUMBERS FROM EQMS
      C       RSTAT=XMT(16),(17) - RSTAR-BAR
      C       RSTA,TSTA=GP - RSTAR FOR GEP
      C     ROUTINES
      C       XIM - MIXTURE EOS VIA GEP, INCLUDING MU#S
      C       EQMS - COMPOSITION AT FIXED F-TILDE
   1          COMMON Z(4000)
   1          DIMENSION
             1 EMG   (           20),EMN    (          20),EMX    (          20)
             2,FOH   (      6,   10),GP     (          20),GM     (          40)
             3,KAL   (           20),KEN    (     6,   10),KEV    (          20)
             4,KIM   (           10),KON    (     6,   10),SM     (          20)
             5,TMG   (           20),XMU    (          20),XMT    (          30)
             7,EA(200),FV(20)
   1          EQUIVALENCE
             1 (Z( 1010),EMG   ),(Z( 1030),EMN    ),(Z( 1170),EMX    )
             2,(Z( 1410),FOH   ),(Z( 1470),GP     ),(Z( 1490),GM     )
             3,(Z( 1600),KAL   ),(Z( 1620),KEN    ),(Z(  900),KEV    )
             4,(Z( 1680),KIM   ),(Z( 1690),KON    ),(Z( 1820),SM     )
             5,(Z( 1970),TMG   ),(Z( 2240),XMU    ),(Z( 2210),XMT    )
             7,(Z(480),EA),(Z(680),EV)
      C
   1          EQUIVALENCE (FOH(15),EPS),(KIM(2),KS)
   1          EQUIVALENCE (GP(5),RSTA),(XMT(16),RSTAT)
   1          EQUIVALENCE  (GM (15) , VR)
      C
   1      100 KEN(5)=KEN(5)+1
      C                                          BACK HERE FOR OUTER (LH OR 1-FLUID)
   3      200 CALL XIM(2,1)
   6      210 EMG(1)=TMG(1)+SM(5)
      C
  10      300 CALL DOUT (3HEQM,1)
      C                                          BACK HERE FOR INNER (ALL)
  13      500 DO 520 I=1,KS
  15      510 EMG(I+1)=TMG(I+1)+XMU(I)
  20      520 EA(I)=EMX(I)
      C                                          SKIP FOR FX. COMP.
  24      600 IF (KAL(6)) 800,2000,800
      C
  25      800 KEV(1)=KAL(6)
  27      810 KEV(2)=KON(2,7)
  31      820 KEV(3)=KON(3,7)
  33      830 KEV(4)=0
      C
  34      850 KEN(13)=KEN(13)+1
      C                                          EQUIL. XI AT FIXED F-TILDE (EMG)
  36      900 CALL EQMS (KEV,EMX,EMN,EMG)
      C
  42      910 DO 920 I=1,6
  50      920 KEN(I,7)=KEV(I+6)
      C
  52      950 CALL DOUT (3HEQM,2)
      C                                          DIFF FOR INNER CONV., NEXT#X
  55     1000 EV=0.0
  56     1010 DO 1050 I=1,KS
  60     1020 EV=EV+ ABS(EMX(I)-EA(I))
  64     1030 IF (KEN(13)-1) 1050,1050,1040
  67     1040 EMX(I)=(EMX(I)+EA(I))/2.0
  73     1050 CONTINUE
```

```
      C                                                                                                      EQM      72
 76    1070 CALL COUT (3HEQM,3)                                                                              EQM      73
      C                                                  INNER CONVERGENCE TEST                              EQM      74
101    1100 IF (EV-FMH(16)) 1300,1300,1110                                                                   EQM      75
104    1110 CALL XIM(2,2)                                                                                    EQM      76
107    1120 GO TO 500                                                                                        EQM      77
      C                                                  OUTER CONVERGENCE TEST                              EQM      78
110    1300 IF ((KAL(5)-3)*(KAL(5)-4)) 2000,1310,2000                                                        EQM      79
114    1310 IF ( ABS(RSTA-RSTAI)-EPS) 1320,200,200                                                           EQM      80
121    1320 VR=XMT(1)                                                                                        EQM      81
      C                                                                                                      EQM      82
      C                                                  CALC FINAL THERMO                                   EQM      83
123    2000 CALL XIM(2,3)                                                                                    EQM      84
126    2004 CALL COUT (3HEQM,3)                                                                              EQM      85
      C                                                                                                      EQM      86
131    3000 RETURN                                                                                           EQM      87
      C                                                                                                      EQM      88
      C                                                                                                      EQM      89
132         END                                                                                              EQM      90
      C*********************************************************************                                 MES       2
      C*    4. CALCULATION CONTROLS                                          *                               MES       3
      C*********************************************************************                                 MES       4


            SUBROUTINE MES                                                                                   MES       5
      C                                                                                                      MES       6
      C     MIXTURE EQUATION OF STATE CONTROL                                                                MES       7
      C            CALCULATE EQUATION OF STATE AT                                                            MES       8
      C            GIVEN T AND P                                                                             MES       9
      C                                                                                                      MES      10
      C                               REPLACE (CALL SEM) BY (CALL SEP)                                       MES      11
      C                               IF SES REQUIRES ITER. FOR V(P,T).                                      MES      12
      C   INPUT                                                                                              MES      13
      C     THER(1),(3) - P,T (IMPLICIT)                                                                     MES      14
      C   OUTPUT - SEE COUT                                                                                  MES      15
      C                                                                                                      MES      16
      C     MES                                                                                              MES      17
                                                                                                             MES      18
  1         COMMON Z(4000)                                                                                   MES      19
  1         DIMENSION KEN(60)                                                                                MES      20
                                                                                                             MES      21
  1         EQUIVALENCE                                                                                      MES      22
           1 (Z( 1620),KEN    )                                                                              MES      23
      C                                                                                                      MES      24
  1         KEN(11)=0                                                                                        MES      25
  1         KEN(12)=0                                                                                        MES      26
  1         KEN(13)=0                                                                                        MES      27
  1         KEN(6)=KEN(6)+1                                                                                  MES      28
  1         KEN(14)=KEN(14)+1                                                                                MES      29
  6         CALL COUT (3HMES,1)                                                                              MES      30
      C                                                                                                      MES      31
 10         CALL TIM(2)                                                                                      MES      32
 12         CALL SEM (2,1)                                                                                   MES      33
 14         CALL EQM                                                                                         MES      34
 15         CALL TIM(2)                                                                                      MES      35
 17         CALL COUT                                                                                        MES      36
      C                                                                                                      MES      37
 20         CALL COUT (3HMES,2)                                                                              MES      38
 22         RETURN                                                                                           MES      39
      C                                                                                                      MES      40



 23         END                                                                                              MES      41
```

```
            SUBROUTINE COUT                                                  COUT
    C       CALCULATE MES OUTPUT                                             COUT
    C       CALLED FROM MES                                                  COUT
    C                                                                        COUT
    C     INPUT - EOS ROUTINES OUTPUT                                        COUT
    C       EMN(1), EMN(2) - NS, NG                                          COUT
    C       TMS - IDEAL                                                      COUT
    C       THER(1), (3) - P,T                                               COUT
    C       XMT - GAS                                                        COUT
    C       SM - SOLID                                                       COUT
    C       HE - INITIAL                                                     COUT
    C       EMS - MOLE FRACTIONS                                             COUT
    C       EMG - MU SUB I PRIME (IMPERF. CHEM. POTENTIALS)                  COUT
    C     OUTPUT                                                             COUT
    C       REST OF EMN - PHASE COMPOSITION                                  COUT
    C       THER - THERMO FUNCTIONS                                          COUT
    C       FN - MOLE NUMBERS                                                COUT
    C       FMU - CHEM. POTENTIALS                                           COUT
  1         COMMON Z(4000)                                                   COUT
  1         DIMENSION                                                        COUT
           1 CONT    (    20) ,EMG    (    20) ,EMN    (    20)             COUT
           2,EMX     (    20) ,EV     (    20) ,FN     (    20)             COUT
           3,FMU     (    20) ,HE     (    10) ,KIM    (    10)             COUT
           4,SM      (    20) ,THER   (    50) ,TMS    (    20)             COUT
           5,XMT     (    30)                                                COUT
  1         EQUIVALENCE                                                      COUT
           1 (Z(  480),CONT   ) ,(Z( 1010),EMG    ) ,(Z( 1030),EMN    )     COUT
           2,(Z( 1170),EMX    ) ,(Z(  680),EV     ) ,(Z( 1390),FN     )     COUT
           3,(Z( 1370),FMU    ) ,(Z( 1590),HE     ) ,(Z( 1680),KIM    )     COUT
           4,(Z( 1820),SM     ) .(Z( 1920),THER   ) ,(Z( 1990),TMS    )     COUT
           5,(Z( 2210),XMT    )                                              COUT
    C                                                                        COUT
  1         EQUIVALENCE (CONT(2),R),(CONT(4),CALMB)                          COUT
  1         EQUIVALENCE (THER(1),P),(THER(3),T)                              COUT
  1         EQUIVALENCE (THER(6),Q),(THER(8),V),(THER(9),E)                  COUT
  1         EQUIVALENCE (THER(1 ),H),(THER(11),A),(THER(12),F)               COUT
  1         EQUIVALENCE (THER(13),S),(THER(15),VM)                           COUT
  1         EQUIVALENCE (KIM(7).KS)                                          COUT
  1         EQUIVALENCE (HE(5),V0),(HE(7),H0)                                COUT
  1         EQUIVALENCE (SM(1),VS)                                           COUT
  1         EQUIVALENCE (EMN(4),XG),(EMN(5),XS),(EMN(6),BN)                  COUT
  1         EQUIVALENCE (TMS(2),HGIO),(TMS(4),SGIO),(TMS(6),HMGID)           COUT
           1                ,(TMS(7),HSIO),(TMS(9),SSID),(TMS(12),HHSIO)     COUT
           2               ,(TMS(5).HFG),(TMS(11),HFS)                       COUT
  1       8 EMN(3)=EMN(2)+EMN(1)                                             COUT
  3      10 XG=EMN(1)/EMN(3)                                                 COUT
  5      20 XS=EMN(2)/EMN(3)                                                 COUT
  7      30 VM=XG*XMT(1)+XS*VS                                               COUT
 13      40 THER(21)=P*VM/(R*T)                                              COUT
 17      50 THER(17)=XG*(HGIO+XMT(3))+XS*(HSIO+SM(3))                        COUT
 25      60 THER(20)=XG*(SGIO+XMT(6))+XS*(SSIO+SM(6))                        COUT
 33      70 THER(16)=THER(17)-THER(21)                                       COUT
 35      80 THER(19)=THER(17)-THER(20)                                       COUT
 37      90 THER(18)=THER(19)-THER(21)                                       COUT
 41     100 BN=EMN(3)/HE(4)                                                  COUT
 43     110 EV=BN*R*T                                                        COUT
 46     120 V=BN*VM                                                          COUT
```

```
 50      130 E=FV*THER(16)                                              COUT      59
 52      140 H=FV*THER(17)                                              COUT      60
 54      150 A=FV*THER(18)                                              COUT      61
 56      160 F=FV*THER(19)                                              COUT      62
 60      170 S=RN*R*THER(20)                                            COUT      63
 63      172 THER(14)=FV*(XG*(HMGID+XM(3))+XS*(HMSID+SM(3)))            COUT      64
 72      190 THER(2)=V/V0                                               COUT      65
 74      200 Q=-UN*CALMB*(XG*HFG+XS*HFS)+HU+RN*R*HE(3)                  COUT      66
105      210 THER(7)=1/CALMB                                            COUT      67
107      220 FN(1)=EMN(2)                                               COUT      68
111      230 DO 240 I=2,KS                                              COUT      69
117      240 FN(I)=EMX(I)*EMN(1)                                        COUT      70
121      250 DO 260 I=1,KS                                              COUT      71
123          E1=0                                                       COUT      72
123          IF (EMX(I).NE.0) E1=ALOG(EMX(I))                           COUT      73
130      260 FMO(I)=FMG(I)+E1                                           COUT      74
135      270 FMO(1)=EMG(1)                                              COUT      75
       C                                                                COUT      76
137      300 RETURN                                                     COUT      77
       C     SPECS                                                      COUT      78
       C           INPUT                                                COUT      79
       C                 P,T,ROUTINE OUTPUTS                            COUT      80
       C           OUTPUT                                               COUT      81
       C                 THER-E REF.STATE IS ELEMENTS AT 0 K.           COUT      82
       C                 MOLE NUMBERS                                   COUT      83
140          END                                                        COUT      84


             SUBROUTINE POUT(K)                                         POUT       2
       C                                                                POUT       3
       C                                                                POUT       4
       C                                                                POUT       5
       C           PRINT OUTPUT                                         POUT       6
       C                                                                POUT       7
       C                 K=1   PRINT LABELS                             POUT       8
       C                 K=2   MAIN PRINT                               POUT       9
       C                 K=3   DIFFERENTIATION PRINT                    POUT      10
       C                                                                POUT      11
       C                 PRINT POINT NUMBER AND P,V,T,RHO ON LINE       POUT      12
       C                                                                POUT      13
       C                                                                POUT      14
       C                 REVISION 1. ADD PUNCH OUTPUT (KAL(11) ON)      POUT      15
       C                       W. F. 10/16/61                           POUT      16
       C                                                                POUT      17
       C                                                                POUT      18
       C     POUT                                                       POUT      19
                                                                        POUT      20
  3          COMMON Z(4000)                                             POUT      21
  3          DIMENSION                                                  POUT      22
            1 EMN    (           20),FN     (           20),GM     (      40) POUT  23
            2,HE     (           10),KAL    (           20),KEN    (   6,  10) POUT  24
            3,SM     (           20),THER   (           50),XMT    (      30) POUT  25
            4,FLAB   (    12,     8) ,KIM(10)                               POUT      26
  3          EQUIVALENCE                                                POUT      27
            1 (Z( 1030),EMN   ) ,(Z( 1390),FN    ) ,(Z( 1490),GM    )   POUT      28
            2,(Z( 1590),HE    ) ,(Z( 1600),KAL   ) ,(Z( 1620),KEN   )   POUT      29
            3,(Z( 1820),SM    ) ,(Z( 1920),THER  ) ,(Z( 2210),XMT   )   POUT      30
            4,(Z( 3100),FLAB  )   ,(Z(1680),KIM)                        POUT      31
        C                                                               POUT      32
  3          EQUIVALENCE (KIM(2),KS)                                    POUT      33
```

```
      C
  3     10 GO TO (100,180,300),K
      C  96                         LABELS
      C  98
 12    100 WRITE(9,7100)
 17    120 WRITE(9,7120)
 24    140 WRITE(9,7130)
 30        IF(0.EQ.0) GO TO 400
      C          --- SKIP PUNCH
 32    142 IF (KAL(11)) 400,150,400
      C
 33    150 WRITE(9,7150)                 ((FLAB(J,I),J=1,12),I=1,4)
 50    160 WRITE(9,7160)
 55    162 WRITE(9,7162)                 (FLAB(I,5),I=1,KS)
 65    164 WRITE(9,7164)
 72    170 GO TO 400
      C 176                         REG.PRINT
      C 178
 73    180 KEM(9)=KEM(9)+1
 75    200 WRITE(9,7200)                 KEM(9)
          1           , (THER(I),I=1,5),HE(1),THER(7)
          2           , THER(8),THER(9),THER(13),(EMN(I),I=1,3),EMN(7)
124    230 WRITE(9,7210)                 THER(15),THER(16),
          1THER(20),THER(21),(FN(I),I=1,3),XMT(1),XMT(2),
          2XMT(6),XMT(7),(FN(I),I=4,6),GM(15),GM(4),GM(11),
          3GM(10),(FN(I),I=7,9),SM(1),SM(2),SM(6),SM(7),(FN(I),I=10,12)
          4 , (XMT(I+15 ), I=1,3)
210    240 CALL DOUT (4HPOUT,1)
213        IF(0.EQ.1) GO TO 400
      C          --- SKIP PUNCH
215    242 IF (KAL(11)) 400,250,400
      C
216    250 WRITE(9,7250)
          1,HE(1),THER(1),THER(2),THER(3),THER(4),THER(5)
          2,THER(8),THER(9),XMT(16),XMT(18),XMT(17),THER(7)
          3,EMN(2),EMN(1),EMN(3),SM(1),XMT(1),THER(15)
          4,(FN(I),I=1,12)
271    260 GO TO 400
      C 296                         DIFF. PRINT
      C 298
272    300 WRITE(9,7300)                 (THER(I),I=22,25)
301    310 CALL DOUT (4HPOUT,2)
304        IF(0.EQ.0) GO TO 400
      C          ---SKIP PUNCH
306    312 IF (KAL(11)) 400,320,400
      C
307    320 WRITE(9,7320)
          1THER(22),THER(23),THER(24),THER(25),THER(27)
326    400 RETURN
      7100 FORMAT (1H0,7X,13HOUTPUT LABELS//12X,1H1,6X,
          11HP,14X,4HV/V0,11X,1HT,14X,1HU,14X,1HO,14X,3HRHO,12X,4HGCAL
          2/12X,1H2,6X,1HV,14X,1HE,14X,1HS,14X,2HNG,13X,2HNS,13X,1HN,14X
          36HSUPSAT )
      C
      7120 FORMAT (12X,1H3,6X,1HV,14X,4HE/RT,11X,3HS/R,12X,5HPV/RT,
          110X,2HN1,13X,2HN2, 3X,2HN3 / 12X,1H4,6X,11HDU. FOR GAS,
          249X,6HN4,N5,N6/12X,1H5,6X,12HDU. FOR REF.,48X,8HN7,N8,N9
          3/12X,1H6,6X,13HDU. FOR SOLID,47X,11HN10,N11,N12 )
      C
      7130 FORMAT (12X,1H7,6X,5HRBAR*,10X,5HTBAR*,10X,5HVBAR*,10X
```

```
         1            ,5HGAMMA,10X,5HALPHA,10X,4HBETA,11X,1HC )             POUT          94
      C                                                                     POUT          95
      C                                                                     POUT          96
       7200 FORMAT (1H0,6HPOINT 12,3X                                       POUT          97
         1            ,3H1  1P7E15.7/12X,3H2  7E15.7)                       POUT          98
      C                                                                     POUT          99
       7210 FORMAT (12X,3H3  1P7E15.7/12X,3H4  7E15.7/12X,                  POUT         100
         13H5  7E15.7/12X3H6  7E15.7 /  2X,3H7  3E15.7)                     POUT         101
      C                                                                     POUT         102
       7300 FORMAT (1H+,14X,45X, 1P4E15.7)                                  POUT         103
      C                                                                     POUT         104
      C                         PUNCH FORMATS                               POUT         105
       7150 FORMAT                                                          POUT         106
         1         (2H$1 11A6,A5 / (2H$0 11A6,A5 ))                         POUT         107
327    7160 FORMAT (                                                        POUT         108
         14H$01 3HRHO 9X,1HP 11X,4HV/V0 8X,1HT 11X,1HU 11X,1HD              POUT         109
         2/4H$ 2 1HV 11X,1HE 11X,4HRBAR 8X,4HVBAR 8X,4HTBAR 8X,1HQ          POUT         110
         3/4H$ 3 2HUS 10X,2HNG 10X,1HN 11X,2HVS 10X,2HVG 10X,1HV  )         POUT         111
327    7162 FORMAT (1H$ 6A12)                                               POUT         112
327    7164 FORMAT (                                                        POUT         113
         1/4H$   5HGAMMA 7X,5HALPHA 7X,4HBETA 8X,1HC 11X,6HCJ FN            POUT         114
         7 )                                                                POUT         115
327    7250 FORMAT (2H$0 1PE11.4 ,5E12.4 / (1H$ 6E12.4) )                   POUT         116
327    7320 FORMAT (2H$  1PE11.4 ,5E12.4)                                   POUT         117
327         END                                                             POUT         118


            SUBROUTINE MESC(KG,ASUC)                                        MESC           2
      C                                                                     MESC           3
      C     CALCULATE MIXTURE EQUATION OF STATE                             MESC           4
      C             AT GIVEN T AND                                          MESC           5
      C                     P     FOR KG=1                                  MESC           6
      C                     V      FOR KG=2                                 MESC           7
      C                     S      FOR KG=3                                 MESC           8
      C                     E      FOR KG=4                                 MESC           9
      C                                                                     MESC          10
      C             ITERATE ON T UNDER CONTROL OF FROOT,                    MESC          11
      C             USING MES FOR FUNCTION CALCULATION                      MESC          12
      C                                                                     MESC          13
      C                                                                     MESC          14
      C                                       ALL USE SAME FROOT CALL,      MESC          15
      C                                              BRANCH ON FUNCTION     MESC          16
      C                                                                     MESC          17
      C                     REVISION 1.CALC INTEGRAL PDV ON ISE             MESC          18
      C                         W. F. 1/3/62                                MESC          19
      C      MESC                                                           MESC          20
                                                                            MESC          21
  6         COMMON Z(4000)                                                  MESC          22
  6         DIMENSION                                                       MESC          23
           1 KEN    (    60) ,KON    ( 6,10) ,CAR    (    80)               MESC          24
           2,FOB    (    60) ,THER   (    50)                               MESC          25
           5,CONT(20),HE(10)                                                MESC          26
  6         DIMENSION   ASUC  ( 10)                                         MESC          27
      C     ASUC - INITIAL STATE ON CURVE - SEE SUC                         MESC          28
  6         EQUIVALENCE                                                     MESC          29
           1 (Z( 1620),KEN   ) ,(Z( 1690),KON    ) ,(Z(  920),CAR    )      MESC          30
           2,(Z( 1410),FOB   ) ,(Z( 1920),THER  )                           MESC          31
           5,(Z(460), CONT),(Z(1590),HE)                                    MESC          32
      C                                                                     MESC          33
  6         DIMENSION CM(10),KCM(2)                                         MESC          34
```

```
  6          EQUIVALENCE (CAR(21),CM),(CM(8),KCM)                              MESC      35
  6          EQUIVALENCE (THER(8),V),(THER(13),S),(THER(9),E)                 MESC      36
  6          EQUIVALENCE (THER(3),T)                                          MESC      37
       C                                                                      MESC      38
  6        4 KEN(14)=0                                                        MESC      39
  7        6 KEN(8)=KEN(8)+1                                                  MESC      40
 11        8 KEN(16)=KEN(16)+1                                                MESC      41
 13       10 IF (KG-1) 30,15,30                                               MESC      42
 15       15 T=ASUC(1)                                                        MESC      43
 16       20 CALL MES                                                         MESC      44
 21       25 GO TO 200                                                        MESC      45
 22       30 KCM(1)=0                                                         MESC      46
 23       35 CM(4)=T                                                          MESC      47
 25       40 CM(2)=T*FOB( 9)                                                  MESC      48
 27       45 CALL FRGOTT (CM,KON(3,8))                                        MESC      49
 34       46 KEXIT=KCM(2)                                                     MESC      50
 36       50 GO TO (200,80,70,60), KEXIT                                      MESC      51
 46       60 CALL DBUG (4HMESC,1)                                             MESC      52
 53       62 GO TO 200                                                        MESC      53
 54       70 CALL DBUG (4HMESC,2)                                             MESC      54
 61       72 GO TO 200                                                        MESC      55
 62       80 T=CM(2)                                                          MESC      56
 64          CALL MES                                                         MESC      57
 65          I=KG-1                                                           MESC      58
 70          GO TO (90,100,110),I                                             MESC      59
 76       90 CM(3)=V-ASUC(3)                                                  MESC      60
100       95 GO TO 120                                                        MESC      61
101      100 CM(3)=(( EXP((S/ASUC(4))*ALOG(ASUC(1))))/ASUC(1))-1.             MESC      62
116      105 GO TO 120                                                        MESC      63
117      110 CM(3)=E-ASUC(5)                                                  MESC      64
121      120 CALL DOUT (4HMESC,1)                                             MESC      65
126      125 GO TO 45                                                         MESC      66
       C                                         CALC. ISE INTEGRAL PDV       MESC      67
127      200 IF (KG-3) 220,210,220                                            MESC      68
131      210 THER(4)=(HE(8)-THER(9))/CONT(4)                                  MESC      69
       C                                                                      MESC      70
134      220 CALL DOUT (4HMESC,2)                                             MESC      71
141      300 RETURN                                                           MESC      72
142          END                                                              MESC      73


             SUBROUTINE HUG                                                   HUG        2
       C                              DETONATION HUGONIOT POINT               HUG        3
       C   NOTES                                                              HUG        4
       C     1. SPECIAL SECOND GUESS - FROM FIRST                             HUG        5
       C        ARG AND FUNC AND SLOPE SAVED IN FOB(8)                        HUG        6
       C        FROM PREVIOUS ITER                                            HUG        7
  1          COMMON Z(4000)                                                   HUG        8
  1          DIMENSION                                                        HUG        9
            1  CAR    ( 10,8), KEN    ( 6,10), KON    ( 6,10)                 HUG       10
            2,FOB    (    60) ,HE     (    10) ,THER   (    50)               HUG       11
  1          DIMENSION CM(10),KCM(2)                                          HUG       12
  1          EQUIVALENCE                                                      HUG       13
            1 (Z(  920),CAR    ) ,(Z( 1620),KEN    ) ,(Z( 1690),KON    )      HUG       14
            2,(Z( 1410),FOB    ) ,(Z( 1590),HE     ) ,(Z( 1920),THER   )      HUG       15
       C                                                                      HUG       16
       C                                                                      HUG       17
  1          EQUIVALENCE (THER(1),P),(THER(3),T),(THER(4),U)                  HUG       18
  1          EQUIVALENCE (THER(5),D),(THER(8),V),(THER(14),HH)                HUG       19
  1          EQUIVALENCE (HE(2),P0),(HE(6),V0),(HE(7),H0)                     HUG       20
```

```
  1          EQUIVALENCE (FOB(21),TL),(FOB(22),TU)                          HUG        21
  1          EQUIVALENCE (CAR(11),CH),(CH(8),KCH)                           HUG        22
       C                                                                    HUG        23
       C     CALCULATE HUGONIOT POINT AT GIVEN P,                           HUG        24
       C           ITERATE ON T UNDER CONTROL OF FROOT,                     HUG        25
       C           USING MES IN FUNCTION CALCULATION                        HUG        26
       C                                                                    HUG        27
       C                 TL AND TU ARE BOUNDS ON ITERATION T                HUG        28
       C                                                                    HUG        29
  1        4 KEN(14)=0                                                      HUG        30
  2        6 KEN(15)=KEN(15)+1                                              HUG        31
  4        8 KEN(7)=KEN(7)+1                                                HUG        32
  6       10 IF (T)20,12,20                                                 HUG        33
  7       12 T=3000.0                                                       HUG        34
 11       20 CH(4)=T/1000.                                                  HUG        35
 13       30 KCH(1)=0                                                       HUG        36
 14       40 CALL FROOTT (CH,KON(2,8))                                      HUG        37
 17       42 KEXIT=KCH(2)                                                   HUG        38
 21       50 GO TO (150,72,70,60),KEXIT                                     HUG        39
 31       60 CALL DBUG (3HHUG,1)                                            HUG        40
 34       62 GO TO 150                                                      HUG        41
 35       70 CALL DBUG (3HHUG,2)                                            HUG        42
 40       71 GO TO 150                                                      HUG        43
 41       72  IF (KON (2,8)) 81,75,81                                       HUG        44
 42       75 IF (KCH(1)-2) 81,76,81                                         HUG        45
 44       76 CH(2)=CH(4)-CH(5)/FCB(8)                                       HUG        46
 47       81 T=CH(5)*1000.                                                  HUG        47
 51       82 IF (TU-T) 83,83,85                                             HUG        48
 54       83 T=TU                                                           HUG        49
 56       84 GO TO 90                                                       HUG        50
 57       85 IF (T-TL) 86,90,90                                             HUG        51
 62       86 T=TL                                                           HUG        52
 64       90 CALL MES                                                       HUG        53
 65       92 D=V0* SQRT((P-P0)/(V0-V))                                      HUG        54
 75       94 U= SQRT((P-P0)*(V0-V))                                         HUG        55
104       95 CH(2)=T/1000.                                                  HUG        56
106      100 CH(3)=20.*P*((HH-H0)/((P-P0)*V0)-0.5*(1.0+V/V0))               HUG        57
121      110 CALL DOUT (3HHUG,1)                                            HUG        58
124      120 GO TO 40                                                       HUG        59
125      150 IF (KCH(1)-2) 200,200,151                                      HUG        60
130      151 FOR(8)=(CH(7)-CH(3))/(CH(6)-CH(2))                             HUG        61
134      200 RETURN                                                         HUG        62
       C                                                                    HUG        63
       C                                                                    HUG        64
135          END                                                            HUG        65


             SUBROUTINE GAMM(K1,K2)                                         GAMM        2
       C                                                                    GAMM        3
       C                                                                    GAMM        4
       C     CALCULATE EQUATION OF STATE DERIVATIVES                        GAMM        5
       C           BYNUMERICAL DIFFERENCING OF P AND T                      GAMM        6
       C           USING MES FOR EQ. OF STATE POINTS                        GAMM        7
       C                                                                    GAMM        8
       C     INPUT                                                          GAMM        9
       C           (1) K1=1 - DIFFERENTIATE WITH CURRENT CONDITION          GAMM       10
       C                         (FIXED OR EQUILIBRIUM COMPOSITION)         GAMM       11
       C           (2) K2=1 - DIFFERENTIATE AT FIXED COMPOSITION            GAMM       12
       C                                                                    GAMM       13
       C           (3) THER    (1) P       CENTER POINT QUANTITIES          GAMM       14
```

```
     C                       (3) T
     C                       (8) V
     C                       (21) PV/RT
     C
     C             (4) EMN   (3) N
     C
     C       OUTPUT
     C             SUCG      (1) GAMMA
     C                       (2) ALPHA
     C                       (3) BETA
     C                       (4) C (SOUND SPEED)
     C                       (5) CJ FUNCTION
     C                           =((V/V0)/(GAM/(GAM+1-P/P0)) )**(-GAM)-1
     C                       (6) CAP GAMMA (ISOTHERMAL)
     C                       (7) CP/R
     C                       (9) (D LN V/D T) (CONSTANT P)
     C
     C             ABOVE OUTPUT IS FORMED FOR EITHER
     C                   OR BOTH CONDITIONS AND PLACED IN
     C                   APPROPRIATE THER LOCATIONS
     C
     C       DATA]
     C             FOB              (13) R - P+ =PC*R
     C             FOB              (14) DEL - T+ =TC*(1.0+DEL)
     C             DER              (1) PC
     C                                (2)VC
     C                                (3)TC
     C                                (4)PC*VC/R*TC
     C                                (5)V+
     C                                (6)V-
     C                                (7)H+
     C                                (8)H-
     C             E2                 SAVE NC
     C
     C       GAMM

 5           COMMON Z(4000)
 6           DIMENSION
            1 DER    (    10) ,EMN    (    20) ,FOB    (    60)
            2,HF     (    10) ,KAL    (    20) ,THER   (    50)
            3,SUCG   (    20)
 6           EQUIVALENCE
            1 (Z( 1000),DER    ) ,(Z( 1030),EMN    ) ,(Z( 1410),FOB    )
            2,(Z( 1590),HF     ) ,(Z( 1600),KAL    ) ,(Z( 1920),THER   )
            3,(Z( 1900),SUCG   )
     C
 6           EQUIVALENCE (THER(1),P),(THER(3),T),(THER(8),V)
     C   18                                 SAVE CENTER VALUES
 8       20 DER(1)=P
10       30 DER(2)=V
12       40 DER(3)=T
14       50 DER(4)=THER(21)
16       60 E2=EMN(3)
     C   98                         MAIN CODE /TEST ARGS.
     C
20      100 IF (K2) 110,400,110
21      110 IF (KAL(6)) 200,400,200
     C  198                                 DIFF. AT FIX. COMP.
22      200 LM=KAL(6)
24      210 KAL(6)=0
```

```
 25      220 K=1                                                              GAMM      75
 26      230 GO TO 1000                                                       GAMM      76
       C 298                                     SET OUTPUT                   GAMM      77
 27      300 THER(26)=SUCG(1)                                                 GAMM      78
 31      310 THER(30)=SUCG(2)                                                 GAMM      79
 33      320 THER(29)=SUCG(4)                                                 GAMM      80
 35      330 THER(28)=SUCG(5)                                                 GAMM      81
 37      340 KAL(6)=LM                                                        GAMM      82
 41      350 CALL DOUT (4HGAMM,1)                                             GAMM      83
       C 398                               DIFF. AT EQ.COMP.                  GAMM      84
 46      400 IF (K1)410,600,410                                               GAMM      85
 47      410 K=2                                                              GAMM      86
 50      420 GO TO 1000                                                       GAMM      87
       C 498                                     SET OUTPUT                   GAMM      88
 51      500 THER(22)=SUCG(1)                                                 GAMM      89
 53      510 THER(23)=SUCG(2)                                                 GAMM      90
 55      520 THER(24)=SUCG(3)                                                 GAMM      91
 57      530 THER(25)=SUCG(4)                                                 GAMM      92
 61      540 THER(27)=SUCG(5)                                                 GAMM      93
 63      550 CALL DOUT (4HGAMM,1)                                             GAMM      94
       C 598                                                                  GAMM      95
 70      600 RETURN                                                           GAMM      96
       C 994                                                                  GAMM      97
       C 996                         DIFFERENCE SUBROUTINE                    GAMM      98
       C 998                               DELTA P                            GAMM      99
 71     1000 P=FOB(13)*DER(1)                                                 GAMM     100
 73     1004 T=DER(3)                                                         GAMM     101
 75     1010 CALL MES                                                         GAMM     102
100     1020 DER(5)=V                                                         GAMM     103
102     1030 P=DER(1)/FOB(13)                                                 GAMM     104
104     1040 CALL MES                                                         GAMM     105
107     1050 DER(6)=V                                                         GAMM     106
111     1060 SUCG(6)=-2.0*ALOG(FOB(13))/ALOG(DER(5)/DER(6))                   GAMM     107
       C1096                                                                  GAMM     108
       C1098                               DELTA T                            GAMM     109
124     1100 P=DER(1)                                                         GAMM     110
125     1104 T=DER(3)*(1.0+FOB(14))                                           GAMM     111
131     1110 CALL MES                                                         GAMM     112
134     1120 DER(5)=V                                                         GAMM     113
136     1130 DER(7)=THER(17)*T*EMN(3)                                         GAMM     114
141     1140 T=DER(3)*(1.0-FOB(14))                                           GAMM     115
144     1150 CALL MES                                                         GAMM     116
147     1160 DER(6)=V                                                         GAMM     117
151     1170 DER(8)=THER(17)*T*EMN(3)                                         GAMM     118
154     1180 SUCG(7)=(DER(7)-DER(8))/(2.0*DER(3)*FOB(14)*E2)                  GAMM     119
162     1190 SUCG(8)=ALOG(DER(5)/DER(6))/(2.0*DER(3)*FOB(14))                 GAMM     120
       C1296                                                                  GAMM     121
       C1298                               CALC. OUTPUT                       GAMM     122
174     1300 T=DER(3)                                                         GAMM     123
176     1302 V=DER(2)                                                         GAMM     124
200     1304 E1=DER(4)*T*SUCG(8)/SUCG(7)                                      GAMM     125
204     1310 SUCG(1)=SUCG(6)/(1.0-SUCG(6)*E1*T*SUCG(8))                       GAMM     126
211     1320 SUCG(3)=1.0/(SUCG(1)*E1)                                         GAMM     127
214     1330 SUCG(2)=SUCG(1)*SUCG(3)-1.0                                      GAMM     128
217     1340 SUCG(4)= SQRT(SUCG(1)*DER(1)*DER(2))                             GAMM     129
226     1350 SUCG(5)=(V/HE(6))/(SUCG(1)/(SUCG(1)+1.0-HE(2)/DER(1)))           GAMM     130
234     1360 SUCG(5)=SUCG(5)**(-SUCG(1))-1.0                                  GAMM     131
       C                                                                      GAMM     132
242     1400 GO TO (300,500),K                                                GAMM     133
       C                                                                      GAMM     134
```

```
      C
250         END

            SUBROUTINE PV(IDMY)
      C
      C     CALCULATE ISOTHERM,ISOCHORE,ISENTROPE,
      C            OR CONSTANT-ENERGY POINTS
      C            AT VALUES OF P IN PT ARRAY
      C            (FOR KAL(8)=1,2,3,4)
      C   INPUT
      C     SUC(1), (2) - TC,PC (INITIAL POINT)
      C     KAL(1), KAL(2) - DIFF SWITCHES
      C     KAL(8) - 1,2,3,4 FOR CONSTANT T,V,S,E
      C     PT - PRESSURE TABLE
      C   OUTPUT
      C     PRINTED POINT OUTPUT
      C----------
      C     REVISION 1.LEAVE P CORRECT ON EXIT
      C                   FOR RESTART OPTION
      C                          W. F. 3/1/62
      C
      C     PV

  3         COMMON Z(4000)
  3         DIMENSION
           1 KAL    (    20) ,KEN    (    60) ,PT     (    50)
           2,SUC    (    20) ,THER   (    50)
  3         EQUIVALENCE
           1 (Z( 1600),KAL    ) ,(Z( 1620),KEN    ) ,(Z( 1750),PT     )
           2,(Z( 1880),SUC    ) ,(Z( 1920),THER   )
      C
  3         EQUIVALENCE (THER(1),P),(THER(3),T)
  3         EQUIVALENCE (THER(8),V),(THER(9),E),(THER(13),S)
      C
  3       8 KEN(16)=0
      C
  4      12 CALL POUT (1)
  7      14 T=SUC(1)
 11      16 P=SUC(2)
 13      40 CALL MES
 15      50 CALL POUT(2)
 20      55 SUC(3)=V
 22      56 SUC(4)=S
 24      57 SUC(5)=E
 26      60 IF (KAL(1)+KAL(2)) 70,112,70
 30      70 CALL GAMM (KAL(1),KAL(2))
 34      90 CALL POUT(3)
 37     112 I=1
 40     114 IF (PT(I)) 200,200,116
 42     116 P=PT(I)
 44     120 CALL MESC (KAL(8),SUC)
 50     122 CALL POUT(2)
 53     124 IF (KAL(1)+KAL(2)) 130,140,130
 55     130 CALL GAMM (KAL(1),KAL(2))
 61     134 CALL POUT(3)
 64     140 I=I+1
 66     142 GO TO 114
 67     200 RETURN
 70         END
```

```
            SUBROUTINE TED
      C
      C     DETONATION HUGONIOT CONTROL
      C           CALCULATE DET. HUG. POINTS AT P VALUES
      C           FOUND IN PT ARRAY
      C
      C   INPUT
      C     KAL(1), KAL(2) - DIFF SWITCHES
      C     PT - PRESSURE TABLES
      C   OUTPUT
      C     PRINTED POINT OUTPUT
      C----------
      C
      C     REVISION 1.LEAVE P CORRECT ON EXIT
      C                 FOR RESTART OPTION
      C                       W. F. 3/1/62
      C
      C     TED

 1          COMMON Z(4000)
 1          DIMENSION
           1 KAL    (    20) ,PT     (    50)
           2, THER (50)
 1          EQUIVALENCE
           1 (Z( 1600),KAL    ) ,(Z( 1750),PT     )
           2 , (Z(1920),THER)
      C
 1          EQUIVALENCE (THER(1),P)
      C
      C                                            SET TGUESS ON FIRST ENTRY
 1       12 CALL POUT(1)
 3       20 I=1
 4       30 IF(PT(I)) 200,200,40
 6       40 P=PT(I)
10       50 I=I+1
12       60 CALL HUG
13       70 CALL POUT(2)
15       80 IF (KAL(1)+KAL(2)) 100,30,100
17      100 CALL GAMM (KAL(1),KAL(2))
22      150 CALL POUT(3)
24      180 GO TO 30
25      200 RETURN
      C
26          END

            SUBROUTINE CJ
      C
      C     CALCULATE CJ LOCUS AT VALUES OF RHO ZERO
      C           IN ROT TABLE
      C
      C           ITERATE ON P ALONG HUGONIOT UNTIL
      C           CJ CONDITION IS SATISFIED
      C   INPUT
      C     KAL(1), KAL(2) - DIFF SWITCHES
      C     ROT - INITIAL-DENSITY TABLE
      C   OUTPUT
      C     PRINTED POINT OUTPUT
      C----------
```

```
      C                       CONST. V DET. P CALCD FROMQ,GAMMA           CJ
      C                       W. F. 11/21/61                              CJ
      C                                                                   CJ
      C                 REVISION 2. SAVE INITIAL E FOR INTEGRAL PDV       CJ
      C                       W. F. 1/3/62                                CJ
      C                                                                   CJ
      C                                                                   CJ
      C      CJ                                                           CJ
                                                                          CJ
   1         COMMON Z(4000)                                               CJ
   1         DIMENSION                                                    CJ
            1 CAR    (     10,     8),HE     (          10),KAL    (   20) CJ
            2,KON    (      6,    10),ROT    (          20),THER   (   50) CJ
            3,KEN(60)                                                     CJ
   1         DIMENSION CC(10),KCC(2)                                      CJ
   1         EQUIVALENCE                                                  CJ
            1 (Z( [illegible]),CAR   ) ,(Z( 1590),HE    ) ,(Z( 1600),KAL   )   CJ
            2,(Z( 1690),KON   ) ,(Z( 1800),ROT   ) ,(Z( 1920),THER  )   CJ
            3,(Z(1620),KEN)                                               CJ
      C                                                                   CJ
      C                                                                   CJ
   1         EQUIVALENCE (CAR(1),CC),(CC(8),KCC)                          CJ
   1         EQUIVALENCE (HE(6),V0),(HE(2),P0),(HE(1),RHO)                CJ
   1         EQUIVALENCE (THER(1),P),(THER(22),GAM),(THER(26),GAM0)       CJ
   1         EQUIVALENCE (THER(8),V)                                      CJ
   1         EQUIVALENCE (THER(6),Q)                                      CJ
   1       6 KEN(15)=0                                                    CJ
   2       8 KEN(16)=0                                                    CJ
      C   10 Q+Q+E                               INPUT, OUTPUT LABEL      CJ
   3      30         CALL POUT(1)                                         CJ
   5      40         I=1                                                  CJ
      C   50 H1+E                                SET UP FROOTT            CJ
   6      60         RHO=ROT(I)                                           CJ
  10      65         HE(1)=RHO                                            CJ
  12      70         V0=1./RHO                                            CJ
  14      72 IF(P) 80,74,80                                               CJ
  15      74 P=0.3                                                        CJ
  17      80 CC(4)=P                                                      CJ
  21     100         KCC(1)=0                                             CJ
      C  110 W(G2,G3,G4,G5)                      FROOTT                   CJ
  22     120         CALL FROOTT(CC,KON (1,8))                            CJ
  25     130         KEXIT=KCC(2)                                         CJ
  27     140         GO TO (365,200,180,160), KEXIT                       CJ
      C  150 H5+Q                                FROOT ERROR EXIT 1       CJ
  37     160 CALL DBUG (2HCJ,1)                                           CJ
  42     170 GO TO 365                                                    CJ
  43     180 CALL DBUG (2HCJ,1)                                           CJ
  46     190 GO TO 365                                                    CJ
  47     200 IF (KON(1,8)) 260,204,260                                    CJ
  50     204 IF (KCC(1)-2) 260,210,260                                    CJ
  52     210 E1=GAM                                                       CJ
  54     220 IF(GAM)240,230,240                                           CJ
  55     230 E1=GAM0                                                      CJ
  57     240 E2=V0*E1/(E1+1.0-P0/P)                                       CJ
  64     250 CC(2)=P*(V/E2)**E1                                           CJ
      C                                                                   CJ
  72     260 IF (KCC(1)-2)280,280,262                                     CJ
  75     262 E1=GAM                                                       CJ
  77     264 IF(GAM)268,266,266                                           CJ
 100     266 E1=GAM0                                                      CJ
```

```
102     268 IF(CC(2)-0.5*RHO*Q*(E1-1.0)) 270,280,280                                  CJ        75
111     270 CC(2)=0.5*RHO*Q*(E -1.0)                                                  CJ        76
      C                                                                               CJ        77
116     280 P=CC(2)                                                                   CJ        78
120     282 KEN(15)=0                                                                 CJ        79
121     284 CALL HUG                                                                  CJ        80
      C                                                                               CJ        81
122     286 IF (KAL(7)) 320,290,320                                                   CJ        82
123     290 CALL GAMM(1,0)                                                            CJ        83
126     300       CC(3)=THER(27)                                                      CJ        84
130     310 GO TO 340                                                                 CJ        85
131     320 CALL GAMM(0,1)                                                            CJ        86
134     330       CC(3)=THER(28)                                                      CJ        87
136     340       CALL DOUT (2HCJ,1)                                                  CJ        88
141     350       GO TO 120                                                           CJ        89
      C 360 H2+Q+G+G                              OUTPUT POINT                        CJ        90
142     365       P=CC(2)                                                             CJ        91
144     370       CALL HUG                                                            CJ        92
      C                                   SAVE INITIAL E FOR ISE INTEGRAL             CJ        93
145     380 HE(8)=THER(9)-THER(4)**2/2.0                                              CJ        94
152     390       CALL POUT(2)                                                        CJ        95
153     420 CALL GAMM(KAL(1),KAL(2))                                                  CJ        96
155     430.      CALL POUT(3)                                                        CJ        97
      C 440 E+C(G1)                               NEXT RHO VALUE                      CJ        98
160     450       I=I+1                                                               CJ        99
162     460       IF (ROT(I))  60,470,60                                              CJ       100
164     470       RETURN                                                              CJ       101
      C                                                                               CJ       102
      C                                                                               CJ       103
      C                                                                               CJ       104
      C                                                                               CJ       105
165             END                                                                   CJ       106
      C********************************************************************** CON        2
      C*      5. READ CONTROL                                                 CON        3
      C********************************************************************** CON        4


                SUBROUTINE CON (ACON)                                         CON        5
      C********************************************************************** CON        6
      C       INPUT AND CONTROL                                               CON        7
      C       BRANCH ON EACH CON WORD TO READ INPUT PACK                      CON        8
      C       EXECUTE ON TED,PV,CJ                                            CON        9
      C----------                                                             CON       10
      C       MAIN CONTROL -                                       CON(ACON)  CON       11
      C       READ INPUT AND EXECUTE AS DIRECTED                              CON       12
      C       CALLED FROM                                                     CON       13
      C         1. MAIN PROGRAM MESU - ACON=0                                 CON       14
      C         2. ERR - ACON=1 - SKIP THRU NEXT RENO ON INP,                 CON       15
      C             THEN REGULAR (NEXT RUN)                                   CON       16
      C                 REVISION 1. - ADD PUNCH OUTPUT                        CON       17
      C                       W. F. 10/16/61                                  CON       18
      C       REVISION 2 - ADD TC,PC OPTION TO PV                             CON       19
      C                       W. FICKETT 11/20/61                             CON       20
      C                                                                       CON       21
      C       REVISION 3. - ADD RENO AND TIME PRINTS                          CON       22
      C             W.F. 3/8/62                                               CON       23
      C                                                                       CON       24
      C********************************** COMMONS ************************** CON       25
                                                                              CON       26
  3             COMMON Z(4000)                                                CON       27
```

```
 3       DIMENSION                                                      CON
        1 BS     (              40),CAR    (     10,      8),CONT   (          20) CON
        2,EMN    (              20),EMX    (             20),FN     (          20) CON
        3,FLAB   (     12,       6),FUB    (      6,     10),HE     (          10) CON
        4,KAL    (              20),KIM    (             10),KON    (      6,  10) CON
        5,PT     (              50),ROT    (             20),SUC    (          20) CON
        6, THER(40)                                                      CON
 3       EQUIVALENCE                                                    CON
        1 (Z(  400),BS    ) ,(Z(  920),CAR    ) ,(Z(  460),CONT  )      CON
        2,(Z( 1030),EMN   ) ,(Z( 1170),EMX    ) ,(Z( 1390),FN    )      CON
        3,(Z( 3100),FLAB  ) ,(Z( 1410),FUB    ) ,(Z( 1590),HE    )      CON
        4,(Z( 1500),KAL   ) ,(Z( 1680),KIM    ) ,(Z( 1690),KON   )      CON
        5,(Z( 1700),PT    ) ,(Z( 1800),ROT    ) ,(Z( 1880),SUC   )      CON
        6, (Z(1920), THER)                                              CON
    C+++++++++++++++++++++++++++++++++++ LOCALS ++++++++++++++++++++++++ CON
 3       LOGICAL E,NE                                                   CON
 3       DIMENSION E(20),NE(12)                                         CON
 3       EQUIVALENCE (KIM(2),KS)                                        CON
 3       EQUIVALENCE (BS(37),BLANK),(BS(38),FORM),(BS(39),BCON)         CON
 3       EQUIVALENCE (BS(21),BPAS),(BS(36),END)                         CON
 3       EQUIVALENCE (BS(26),BCORE),(BS(27),BDBUG)                      CON
 3       EQUIVALENCE (BS(33),DOLLAR)                                    CON
 3       EQUIVALENCE (BS(35),BREND)                                     CON
 3       EQUIVALENCE ( E(1) , CW1 ) ,     ( E(2), CW )                  CON
    C                                                                   CON
 3       EQUIVALENCE (FLAB(1),RUNLAB),(FLAB(13),HELAB)                  CON
 3       EQUIVALENCE (FLAB(25),CORLAB),(FLAB(37),SPELAB)                CON
    C                                                                   CON
 3       EQUIVALENCE (THER(1),P),(THER(3),T)                            CON
 3       EQUIVALENCE(KON(6), GERRGAT)                                   CON
    C                                                                   CON
 3       DIMENSION RUNLAB(12),HELAB(12),CORLAB(12),SPELAB(12)           CON
    C+++++++++++++++++++++++++++++++++++ EXECUTE +++++++++++++++++++++++ CON
 3       IF(ACON.EQ.0) GOTO 70                                          CON
    C----------------------------------- 1. SCAN TO REND --------------- CON
 4     20 CALL FIO (3HRIT,6H(12A6),12,E,0)                              CON
 10      IF (NE(CW.BREND)) GO TO 20                                     CON
    C----------------------------------- 2. BEGIN RUN ------------------ CON
 15    70 CONTINUE                                                      CON
 15       GERRGAT=1.                                                    CON
 16    80 CALL FIO (3HRIT,13H(2A6,6A10,A8) ,  9, E, 0)                  CON
 21    90 CALL FIO (3HWOT,14H(/1X2A6, 6A10, A8) ,  9, E, 0)             CON
 27       IF(NE(CW1.BCON))                                              CON
        1 CALL ERR(3LCON, 14LBAD INPUT PACK,E)                          CON
    C                                                                   CON
    C                                     SEARCH FOR CON BRANCH         CON
 40   8300 DO 8320 I=1,36                                               CON
 42   8310 IF (CW-BS(I)) 8320,8350,8320                                 CON
    C                                                                   CON
    C                                                                   CON
 45   8320 CONTINUE                                                     CON
 47       CALL ERR(3HCON, 13HBAD CON CARD  , E)                         CON
    C8346                                                               CON
 51   8350 GO TO (100,200,300,400,500,600                               CON
        1           ,700,800,900,1000,1100,1200                         CON
        2           ,1300,1400,1500,1600,1700,1800                      CON
        3           ,1900,2000,2100,2200,2300,2400                      CON
        4           ,2500,2600,2700,2800,2900,3000                      CON
        5           ,3100,3200,3300,3400,3500,3600),I                   CON
    C                                                                   CON
```

```
      C
123      100 GO TO 81
 ..   C 198                                         PAS
      C                                             ZERO COMMON
124      200 CONTINUE
      C          ZERO COMMON
124          DO 210 I=1,2900
131      210  CONT(I)=0.0
133          CALL READIT(E(3))
135          CALL READ(19LBEGIN RUN)
      C
141      250 DO 252 I=1,56
145      252 FLAG(I)=BLANK
147      254 DO 260 I=1,10
154      260 RUNLAB(I)=E(I+2)
156          GOTO 80
      C                                                    SATI
156      300 CONTINUE
155          CALL READ(
            150IDIFF, FX DIFF, GAS, SOLID, MIX, EQ, CJ, PV
            2, -12, KE)
162      302 DO 308 I=1,12
164      304 IF (ISIGN(1,KE(I))) 308,306,306
170      306 NAL(I)=FE(I)
172      308 CONTINUE
174      310 GO TO 80
      C 398                                         FOR
175      400 CALL READ(
            1OL*. FORMAT EPS(CC,CH,CM,CG,CS,C)/ RATIOS/ UP,UT,EPSIN,CO)/ FROOT
            2 BOUNDS*
            2  ,3*,FO))
201      410 DO 429 I=1,5
211      420 CAN(1,I)=FOR(I)
214      430 GO TO 80
215      500 GO TO 80
      C 598                                         DIP
216      600 NOT(7)=)
217      610 CALL DIP1
221      620 GO TO 80
      C 698                                         DIS
222      700 CALL READ (0,-7,KE)
225      710 DO 720 I=1,7
235      720 KON(I,KE)=KE(I+1)
237      730 GO TO 80
      C 798                                         DIG
240      800 CALL READ (8,-1,KE)
244      820 KON(KE,8)=1
246      830 CALL READ (0,3,CAN(5,KE)) .
254      840 GO TO 80
      C 898                                         EMPTY
255      900 GO TO 81
      C 998                                         GEM
256     1000 CALL GEM(1)
261     1010 GO TO 80
      C1098                                         SEM
262     1100 CALL SEM(1,1)
266     1110 GO TO 80
      C1198                                         TIM
267     1200 CALL TIM(1)
272     1210 GO TO 81
```

```
      C1298                                                  XIP                  CON      148
273    1300  CALL XIP (1,0)                                                       CON      149
277    1310 GO TO 80                                                              CON      150
      C1398                                                  EQ                   CON      151
300    1400 CALL EQP                                                              CON      152
302    1410 GO TO 80                                                              CON      153
      C1498                                                  EMPTY                CON      154
303    1500 GO TO 800                                                             CON      155
      C1598                                                  SAM                  CON      156
304    1600 CALL HEAD(18LSAM - INPUT PART 2)                                      CON      157
306         CALL READ (33H  KS/ RHO, P0, T0, M0, HFE/ NI $  ,-1, KS)              CON      158
311         CALL READ(0,5,HE)                                                     CON      159
314         CALL READ(0,KS,FN)                                                    CON      160
320    1610 HE(6)=1.0/HE(1)                                                       CON      161
322    1620 HE(7)=HE(5)*CONT(4)/HE(4)                                             CON      162
325    1630 EMN(2)=FN(1)                                                          CON      163
327    1632 EMN(3)=0.0                                                            CON      164
330    1634 DO 1636 I=1,KS                                                        CON      165
334    1636 EMN(3)=EMN(3)+FN(I)                                                   CON      166
337    1640 EMN(1)=EMN(3)-EMN(2)                                                  CON      167
341    1642 EMN(4)=EMN(1)/EMN(3)                                                  CON      168
343    1644 EMN(5)=EMN(2)/EMN(3)                                                  CON      169
345    1650 DO 1652 I=1,KS                                                        CON      170
353    1652 EMX(1)=FN(I)/EMN(1)                                                   CON      171
      C                                                                           CON      172
356    1660 DO 1662 I=1,10                                                        CON      173
363    1662 HELAB(I)=E(I+2)                                                       CON      174
365    1670 GO TO 80                                                              CON      175
      C1698                                                  TEO                  CON      176
366    1700 CALL HEAD(14LTEO - HUGONIOT)                                          CON      177
370         CALL READ (11H  P-TABLE $, 0, PT)                                     CON      178
      C                                                                           CON      179
374    1710 CALL TEO                                                              CON      180
376    1720 GO TO 80                                                              CON      181
      C1798                                                  PV                   CON      182
377    1800 CALL HEAD (5LLOCUS)                                                   CON      183
401         CALL READ(                                                            CON      184
          150H  BRANCH (1-T,2-V,3-S,4-E) / TC,PC/ P-TABLE $                       CON      185
          2 ,-2,KAL(3))                                                           CON      186
404         CALL READ(0,2,SUC)                                                    CON      187
407         CALL READ(0,0,PT)                                                     CON      188
      C                                                                           CON      189
      C                                                                           CON      190
413    1850 IF(KAL(9)) 1852,1860,1852                                             CON      191
414    1852 SUC(1)=T                                                              CON      192
416    1854 SUC(2)=P                                                              CON      193
      C                                                                           CON      194
420    1860 CONTINUE                                                              CON      195
421         CALL PV                                                               CON      196
422    1870 GO TO 80                                                              CON      197
      C1898                                                  CJ                   CON      198
423    1900 CALL HEAD(2LCJ)                                                       CON      199
425         CALL READ (16H  CJ RHO-TABLE $, 0, ROT )                              CON      200
      C                                                                           CON      201
431    1910 CALL CJ                                                               CON      202
433    1920 GO TO 80                                                              CON      203
      C1998                                                  TEST                 CON      204
434    2000 CALL TEST                                                             CON      205
436    2010 GO TO 80                                                              CON      206
      C2098                                                  CHEC                 CON      207
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437      2100 CALL CHEC                                                         CON     208
441      2110 GO TO 80                                                          CON     209
        C2198                                        EMPTY                      CON     210
442      2200 GO TO 80                                                          CON     211
        C2298                                        SPEC                       CON     212
443      2300 CALL SPEC                                                         CON     213
445      2310 GO TO 80                                                          CON     214
        C2398                                        SPEC1                      CON     215
446      2400 CALL SPEC1                                                        CON     216
450      2410 GO TO 80                                                          CON     217
        C2498                                        EMPTIES                    CON     218
451      2500 GO TO 80                                                          CON     219
        C                                            CORE                       CON     220
452      2600 E(2)=E(4)                                                         CON     221
454      2610 E(1)=E(5)                                                         CON     222
456      2620 CALL CORE (E(3))                                                  CON     223
461      2630 GO TO 80                                                          CON     224
        C2698                                        DBUG                       CON     225
462      2700  CALL ERP(4HCON$)                                                 CON     226
465      2710 GO TO 80                                                          CON     227
        C2798                                        LOAD                       CON     228
466      2800 GO TO 80                                                          CON     229
        C2898                                        EMPTIES                    CON     230
467      2900 GO TO 80                                                          CON     231
470      3000 GO TO 80                                                          CON     232
471      3100 GO TO 80                                                          CON     233
472      3200 GO TO 80                                                          CON     234
473      3300 GO TO 80                                                          CON     235
        C                                            FORM                       CON     236
474      3400 CALL FIO (3HWOT,4H(A6),1,E(3),0)                                  CON     237
502      3410 POL=E(4)-BLANK                                                    CON     238
504      3420 IF (POL) 3430,3440,3430                                           CON     239
505      3430 CALL FIO (5HPRINT,4H(A6),1,E(5),0)                                CON     240
        C                                                                       CON     241
513      3440 IF(E(6)-DOLLAR) 3470,3450,3470                                    CON     242
515      3450 DO 3460 I=1,6                                                     CON     243
522      3460 SPELAB(I)=E(I+6)                                                  CON     244
524      3470 GO TO 80                                                          CON     245
        C                                                                       CON     246
        C                                                                       CON     247
        C                                            REND - END OF RUN          CON     248
525      3500 GO TO 80                                                          CON     249
        C                                                      JEND - END OF JOBCON     250
526      3600 CONTINUE                                                          CON     251
526           CALL HEADE (7HJOBENDS   )                                         CON     252
530           CALL EXIT                                                         CON     253
532      4000 RETURN                                                            CON     254
        C                                                                       CON     255
        C                                   LOAD BUTTON                         CON     256
        C                                                                       CON     257
        C                                                                       CON     258
        C                                                                       CON     259
533           END                                                               CON     260
        C***********************************************************************EQPS      2
        C*    6. OUT OF PLACE                                                  *EQPS      3
        C***********************************************************************EQPS      4
        C***********************************************************************EQPS      5
        C     BRINKLEY-METHOD EQUILIBRIUM-COMPOSITION PKG.                      EQPS      6
        C       TRANSCRIBED TO FORTRAN BY PAUL BIRD, GMX-7,                     EQPS      7
        C         FROM FICKETT≠S ORIGINAL LONGHAND VERSION.                     EQPS      8
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      C       NOTES -                                                          EQPS
      C       1. CHANGES WHEN INCORPORATED INTO REVIVED MES                    EQPS
      C          (MARKED KERSHNER 3/1//76)                                     EQPS
      C         A. MAKE AVECT LOCAL, FILLED FROM ARGS EPA, EPA1,               EQPS
      C             IN EQPS                                                    EQPS
      C         B. EMOL(2) REPLACED BY EMOL(7), IN EQMS                        EQPS
      C*************************************************************************  EQPS


              SUBROUTINE EQPS(KBP,CSP,QATOM,ALPHA,ALPHA12,EPA,EPA1)            EQPS
      C                                                                        EQPS
      C                                                                        EQPS
 17           DIMENSION CSP(6),QATOM(6),ALPHA(20,6),AVECT(20,2),RALPHA(101,6),  EQPS
             1ALPT(6,101),KBP(2)                                               EQPS
 17           DIMENSION QBAR(6),NAVEC(100),XNUMAT(100,6),XNU(100),             EQPS
             1QBARS(6),NAVECS(100),XNUMATS(100,6),XNUS(100)                    EQPS
 17           DIMENSION EPA(1),EPA1(1)                                         EQPS
      C                                                                        EQPS
 17           COMMON /EQUIB/QBAR,NAVEC,XNUMAT,XNU,SUMQ,NS,NC,ND,NP,NPHI,ND1,   EQPS
             1QBARS,NAVECS,XNUMATS,XNUS,SUMQS                                  EQPS
      C                                                                        EQPS
      C                                                                        EQPS
      C*****************************************************************     EQPS
      C     MAKE AVECT LOCAL.  KERSHNER 3/17/76                                EQPS
      C*****************************************************************     EQPS
 17           DO 12 I=1,20                                                     EQPS
 24           AVECT(I,1)=EPA(I)                                                EQPS
 24           AVECT(I,2)=EPA1(I)                                               EQPS
 24        12 CONTINUE                                                         EQPS
      C DEFINE CONTROL CONSTANTS AND REORDER ALPHA ACCORDING TO A-VECTOR       EQPS
 33           NC=CSP(1)                                                        EQPS
 33           NS=CSP(2)                                                        EQPS
 33           NPHI=CSP(6)                                                      EQPS
 33           ND=NS-NC                                                         EQPS
 33           ND1=ND+1                                                         EQPS
 33           NPHI1=NPHI+1                                                     EQPS
 45           IF(NPHI.EQ.1.AND.KBP.EQ.0)GO TO 30                               EQPS
 52           NP=CSP(3)                                                        EQPS
 54        13 KV=1                                                             EQPS
 55        14 NCMP=NC-NP                                                       EQPS
 57           IF(NCMP.LE.0)CALL DBUG(2)                                        EQPS
 62           DO 1 I=1,NS                                                      EQPS
 73           NAVEC(I)=AVECT(I,KV)                                             EQPS
 73           NAV=NAVEC(I)                                                     EQPS
 74           DO 1 J=1,NC                                                      EQPS
111         1 RALPHA(NAV,J)=ALPHA(I,J)                                         EQPS
122           DO 2 J=1,NC                                                      EQPS
131         2 RALPHA(NS+1,J)=QATOM(J)                                          EQPS
133           CALL MATTRA(NS+1,NC,RALPHA,101,ALPT,6)                           EQPS
      C TRANSPOSE ALPHA MATRIX                                                 EQPS
      C SOLVE FOR NU-MATRIX                                                    EQPS
141           CALL LSS(NC,ND1,6,ALPT,ALPT(1,NC+1),DET)                         EQPS
      C TEST FOR ZERO DETERMINANT, EXIT FOR NEW A-VECTOR                       EQPS
151           IF(DET.EQ.0.0)CALL DBUG(2)                                       EQPS
      C TRANSPOSE FOR NU-MATRIX AND SMALL Q                                    EQPS
157           CALL MATTRA(NC,ND+1,ALPT(1,NC+1),6,XNUMAT,100)                   EQPS
175           SUMQ=0.0                                                         EQPS
176           DO 3 J=1,NCMP                                                    EQPS
211         3 SUMQ=SUMQ+XNUMAT(ND+1,J)                                         EQPS
214           DO 4 J=1,NC                                                      EQPS
```

```
232       4 QBAR(J)=XNUMAT(ND+1,J)/SUMQ                                        EQMS     67
234         DO 5 I=1,ND                                                        EQMS     68
241         XNU(I)=0.0                                                         EQMS     69
243         DO 5 J=1,NCMP                                                      EQMS     70
252       5 XNU(I)=XNU(I)+XNUMAT(I,J)                                          EQMS     71
      C PRINT NU-MATRIX AND QBAR                                               EQMS     72
263         WRITE(9,6)(QBAR(J),J=1,NCMP)                                       EQMS     73
271         WRITE(9,7)(XNUMAT(1,J),J=1,NC)                                     EQMS     74
          6 FORMAT(1H0,5X,4HQBAR,5X,  6E15.7)                                  EQMS     75
          7 FORMAT(1H0,5X,6HNU MAT,3X,  6E15.7)                                EQMS     76
          8 FORMAT(10X,I3,2X,  6E15.7)                                         EQMS     77
317         IF(ND.LE.1)GO TO 90                                                EQMS     78
321         DO 9 I=2,ND                                                        EQMS     79
323       9 WRITE(9,8)I,(XNUMAT(I,J),J=1,NC)                                   EQMS     80
352         GO TO (10,15),NPHI                                                 EQMS     81
360      90 IF(NPHI.EQ.1.AND.NP.EQ.1)GO TO 11                                  EQMS     82
367      10 RETURN                                                             EQMS     83
370      11 NP=0                                                               EQMS     84
370         KV=2                                                               EQMS     85
372         GO TO 14                                                           EQMS     86
373      15 GO TO (16,10),KFLAG                                                EQMS     87
401      16 DO 17 I=1,ND                                                       EQMS     88
403         XNUS(I)=XNU(I)                                                     EQMS     89
405         DO 17 J=1,NC                                                       EQMS     90
415      17 XNUMATS(I,J)=XNUMAT(I,J)                                           EQMS     91
425         XNUS(ND1)=NP                                                       EQMS     92
430         DO 18 I=1,NS                                                       EQMS     93
435      18 NAVECS(I)=NAVEC(I)                                                 EQMS     94
437         SUMQS=SUMQ                                                         EQMS     95
440         DO 19 J=1,NC                                                       EQMS     96
451      19 QBARS(J)=QBAR(J)                                                   EQMS     97
453         KFLAG=2                                                            EQMS     98
454         GO TO (20,21),NPS                                                  EQMS     99
465      20 NP=0                                                               EQMS    100
465         KV=2                                                               EQMS    101
467         GO TO 22                                                           EQMS    102
470      21 NP=1                                                               EQMS    103
470         KV=1                                                               EQMS    104
472      22 XNU(ND1)=NP                                                        EQMS    105
475         GO TO 14                                                           EQMS    106
475      30 NP=CSP(5)                                                          EQMS    107
475         NPS=NP+1                                                           EQMS    108
501         GO TO (31,33),NPS                                                  EQMS    109
506      31 NP=1                                                               EQMS    110
506         KV=1                                                               EQMS    111
510      32 KFLAG=1                                                            EQMS    112
511         GO TO 14                                                           EQMS    113
512      33 NP=0                                                               EQMS    114
512         KV=2                                                               EQMS    115
514         GO TO 32                                                           EQMS    116
515         END                                                                EQMS    117


            SUBROUTINE EQMS(KBERR,XCOMP,EMOL,FDAG)                             EQMS      2
      C                                                                        EQMS      3
      C                                                                        EQMS      4
            DATA ITERCYC,EXPLIM,EPSILON/99,600.,1.0E-10/                       EQMS      5
      C                                                                        EQMS      6
 12         DIMENSION XCOMP(100),EMOL(7),FDAG(100)                             EQMS      7
      C**************************************************                      EQMS      8
```

```
      C  EMOL(2) REPLACED BY EMOL(7). 2/10/76
      C*********************************************
 12          DIMENSION XLNKI(100),RXCOMP(100),RFDAG(100),XLNXJ(6),A(6,6),F(6),
            1H(6)
 12          DIMENSION QBAR(6),NAVEC(100),XNUMAT(100,6),XNU(100),
            1QBARS(6),NAVECS(100),XNUMATS(100,6),XNUS(100)
      C
 12          EQUIVALENCE (F,H)
      C
 12          COMMON /EQUIB/QBAR,NAVEC,XNUMAT,XNU,SUMQ,NS,NC,ND,NP,NPHI,ND1,
            1QBARS,NAVECS,XNUMATS,XNUS,SUMQS
      C
      C
      C SET CONSTANTS
 12     1000 NPHFLAG=1
 13     1001 ITERCO=0
 13          NCMP=NC-NP
      C REORDER MOLE FRACTIONS AND FREE ENERGIES
 16          DO 1 I=1,NS
 23          NAV=NAVEC(I)
 23          RXCOMP(NAV)=XCOMP(I)
 23        1 RFDAG(NAV)=FDAG(I)
 30          IF(NPHI.EQ.1.AND.NP.EQ.0)RFDAG(NS)=EXPLIM
      C CALCULATE LNKI
 43          DO 2 I=1,ND
 45          XLNKI(I)=-RFDAG(I+NC)
 50          DO 2 J=1,NC
 57        2 XLNKI(I)=XLNKI(I)+XNUMAT(I,J)*RFDAG(J)
      C
      C CALCULATE LN XJ
 67        3 DO 4 J=1,NCMP
 71        4 XLNXJ(J)=ALOG(RXCOMP(J))
      C CALCULATE MOLE FRACTIONS OF DEPENDENT SPECIES
102          DO 6 I=1,ND
103          XLNXI=XLNKI(I)
105          DO 5 J=1,NCMP
114        5 XLNXI=XLNXI+XNUMAT(I,J)*XLNXJ(J)
120          IF(XLNXI.GT.0.0)XLNXI=0.0
125          IF(XLNXI.LT.-EXPLIM)XLNXI=-EXPLIM
131        6 RXCOMP(I+NC)=EXP(XLNXI)
      C SET UP ITERATION LOOP
143          IF(ITERCO.EQ.0)GO TO 11
144          IF(ITERCO.GT.ITERCYC)GO TO 20
      C TEST FOR CONVERGENCE
147          DO 7 J=1,NCMP
150          IF(ABS(H(J)).GT.EPSILON)GO TO 11
155        7 CONTINUE
      C PASSED CONVERGENCE TEST
      C
      C CALCULATE NUMBER OF MOLES
157          RNOR=1.0
160          DO 8 I=1,ND
170        8 RNOR=RNOR+RXCOMP(I+NC)*(XNU(I)-1.0)
176          EMOL(1)=SUMQ/RNOR
      C CALCULATE XC AND MOLES OF SOLID FOR NP=1
176          EMOL(2)=0.0
201          IF(NP.NE.1)GO TO 81
203          XC=QBAR(NC)
205          DO 80 I=1,NC
220       80 XC=XC-(XNUMAT(I,NC)-QBAR(NC)*(XNU(I)-1.0))*RXCOMP(I+NC)
```

```
231           RXCOMP(NC)=XC                                                EQMS      69
231           EMOL(2)=XC*EMOL(1)                                           EQMS      70
        C RESTORE MOLE FRACTION ORDER                                      EQMS      71
234        81 DO 9 I=1,NS                                                  EQMS      72
243           NAV=NAVEC(I)                                                 EQMS      73
243         9 XCOMP(I)=RXCOMP(NAV)                                         EQMS      74
247           IF(NPHI.EQ.1)GO TO 22                                        EQMS      75
        C EXIT WITH COMPUTED EQUILIBRIUM COMPOSITION                       EQMS      76
253        10 RETURN                                                       EQMS      77
        C                                                                  EQMS      78
        C ENTRY TO CALCULATE CORRECTIONS TO MOLE FRACTIONS                 EQMS      79
254        11 DO 13 J=1,NCMP                                               EQMS      80
256           SUMF=0.0                                                     EQMS      81
257           DO 12 I=1,NR                                                 EQMS      82
272        12 SUMF=SUMF+(XNUMAT(I,J)-GBAR(J)*(XNU(I)-1.0))*RXCOMP(I+NC)    EQMS      83
303        13 F(J)=GBAR(J)-RXCOMP(J)-SUMF                                  EQMS      84
311           DO 14 J=1,NCMP                                               EQMS      85
313           DO 14 JP=1,NCMP                                              EQMS      86
314           A(J,JP)=0.0                                                  EQMS      87
317           IF(J.EQ.JP)A(J,JP)=RXCOMP(J)                                 EQMS      88
322           DO 14 I=1,NR                                                 EQMS      89
340        14 A(J,JP)=A(J,JP)+(XNUMAT(I,J)-GBAR(J)*(XNU(I)-1.0))*RXCOMP(I+NC)*  EQMS      90
             1XNUMAT(I,JP)                                                 EQMS      91
357           CALL LSS(NCMP,1,6,A,F,DET)                                   EQMS      92
363           IF (DET.EQ.0.0)GO TO 20                                      EQMS      93
367           DO 17 J=1,NCMP                                               EQMS      94
370           RXCOMP(J)=RXCOMP(J)*(1.0+F(J))                               EQMS      95
373           IF(RXCOMP(J).LT.EPSILON)RXCOMP(J)=EPSILON                    EQMS      96
377        17 CONTINUE                                                     EQMS      97
402           ITERCO=ITERCO+1                                              EQMS      98
403           GO TO 3                                                      EQMS      99
404        20 CALL DBUG(1)                                                 EQMS     100
406           GO TO 1000                                                   EQMS     101
        C TEST FOR PREVIOUS SOLUTION FOR PHI = 1                           EQMS     102
411        22 IF(NPHFLAG.EQ.2)GO TO 10                                     EQMS     103
414           IF(NP.EQ.1)GO TO 40                                          EQMS     104
        C SATURATION TEST FOR 1-PHASE SOLUTION                             EQMS     105
        C SELECT NON-ZERO ELEMENT OF 2-PHASE NU                            EQMS     106
416           DO 50 I=1,NR                                                 EQMS     107
417           IF(XNUMATS(I,NC).NE.0.0)GO TO 51                             EQMS     108
422        50 CONTINUE                                                     EQMS     109
424           CALL DBUG(2)                                                 EQMS     110
        C LOCATED SPECIES FORMED FROM SOLID                                EQMS     111
430        51 ISP=I                                                        EQMS     112
432           DO 52 I=1,NS                                                 EQMS     113
437           NAV=NAVECS(I)                                                EQMS     114
437           RXCOMP(NAV)=XCOMP(I)                                         EQMS     115
437        52 RFDAG(NAV)=FDAG(I)                                           EQMS     116
444           ZLNKI=-RFDAG(ISP+NC)                                         EQMS     117
447           DO 53 J=1,NC                                                 EQMS     118
462        53 ZLNKI=ZLNKI+XNUMATS(ISP,J)*RFDAG(J)                          EQMS     119
465           XLNS=ALOG(RXCOMP(ISP+NC))-ZLNKI                              EQMS     120
472           NCM1=NC-1                                                    EQMS     121
474           DO 54 J=1,NCM1                                               EQMS     122
500        54 XLNS=XLNS-XNUMATS(ISP,J)*ALOG(RXCOMP(J))                     EQMS     123
514           EMOL(7)=XLNS                                                 EQMS     124
        C**********************************************************        EQMS     125
        C   EMOL(7) SET 2/10/76                                            EQMS     126
        C**********************************************************        EQMS     127
        C TEST FOR SUPERSATURATION                                          EQMS     128
```

```
515          IF(XLNS.LT.0.0)GO TO 10                                   EQMS     129
       C EXCHANGE FOR 2-PHASE SOLUTION                                 EQMS     130
       C                                                               EQMS     131
       C EXCHANGE A-VECTORS, ETC., FOR CHANGE IN NUMBER OF PHASES      EQMS     132
516       30 NPHFLAG=2                                                 EQMS     133
517          DO 31 I=1,ND                                              EQMS     134
521          DO 31 J=1,NC                                              EQMS     135
530          XNUMSV=XNUMATS(I,J)                                       EQMS     136
530          XNUMATS(I,J)=XNUMAT(I,J)                                  EQMS     137
530       31 XNUMAT(I,J)=XNUMSV                                        EQMS     138
541          DO 32 J=1,NC                                              EQMS     139
545          GBARSV=GBARS(J)                                           EQMS     140
546          GBARS(J)=GBAR(J)                                          EQMS     141
546       32 GBAR(J)=GBARSV                                            EQMS     142
551          DO 33 I=1,NS                                              EQMS     143
561          NAV=NAVECS(I)                                             EQMS     144
561          NAVECS(I)=NAVEC(I)                                        EQMS     145
561       33 NAVEC(I)=NAV                                              EQMS     146
564          DO 34 I=1,NDI                                             EQMS     147
574          XNUSAV=XNUS(I)                                            EQMS     148
574          XNUS(I)=XNU(I)                                            EQMS     149
574       34 XNU(I)=XNUSAV                                             EQMS     150
577          SUMGSAV=SUMGS                                             EQMS     151
577          SUMGS=SUMG                                                EQMS     152
577          SUMG=SUMGSAV                                              EQMS     153
577          NP=XNU(N 1)                                               EQMS     154
605          GO TO 1001                                                EQMS     155
       C TEST FOR SATISFACTORY 2-PHASE SOLUTION                        EQMS     156
       C   40 IF(XC.GT.0.0)GO TO 10                                    EQMS     157
       C   STMT. 40 REPLACED BY THE FOLLOWING TWO STATEMENTS.          EQMS     158
       C    KERSHNER 2/10/76                                           EQMS     159
610       40 EMOL(7)=XC                                                EQMS     160
612          IF(XC.GT.0.0)GO TO 10                                     EQMS     161
       C NO SOLID PHASE. GO TO 1-PHASE SOLUTION                        EQMS     162
614          GO TO 30                                                  EQMS     163
614          END                                                       EQMS     164


             SUBROUTINE MATTRA(N,M,A,IA,B,IB)                          MATTRA     2
 16          DIMENSION A(IA,M),B(IB,N)                                 MATTRA     3
 16          DO 1 J=1,M                                                MATTRA     4
 17          DO 1 I=1,N                                                MATTRA     5
 26        1 B(J,I)=A(I,J)                                             MATTRA     6
 37          RETURN                                                    MATTRA     7
 40          END                                                       MATTRA     8


             SUBROUTINE LSS (N,M,I,A,B,DET)                            LSS        2
       C MODIFIED FOR FORTRAN IV HUG                                   LSS        3
 16          DIMENSION A(I,N), B(I,M)                                  LSS        4
 16          DOUBLE PRECISION S1,S2,DOTPRO                             LSS        5
 16          NN=N                                                      LSS        6
 16          MM=M                                                      LSS        7
 16          SN=1.                                                     LSS        8
 21          DO 9 J=1,NN                                               LSS        9
 23          L=J-1                                                     LSS       10
 24          IF (J.EQ.NN) GO TO 7                                      LSS       11
 31          T=ABS(A(J,J))                                             LSS       12
 31          M1=J                                                      LSS       13
 31          M2=J+1                                                    LSS       14
```

```
 34          DO 1 K=M2,NN                                      LSS     15
 35          X=ABS(A(K,J))                                     LSS     16
 41          IF (X.LE.T) GO TO 1                               LSS     17
 44          T=X                                               LSS     18
 45          M1=K                                              LSS     19
 46    1     CONTINUE                                          LSS     20
 51          IF (M1.EQ.J) GO TO 4                              LSS     21
 53          DO 2 K=1,NN                                       LSS     22
 63          T=A(J,K)                                          LSS     23
 63          A(J,K)=A(M1,K)                                    LSS     24
 63    2     A(M1,K)=T                                         LSS     25
 67          SN=-SN                                            LSS     26
 70          IF (MM.LE.0) GO TO 4                              LSS     27
 76          DO 3 K=1,MM                                       LSS     28
106          T=B(J,K)                                          LSS     29
106          B(J,K)=B(M1,K)                                    LSS     30
106    3     B(M1,K)=T                                         LSS     31
116    4     IF (A(J,J).EQ.0.) GO TO 13                        LSS     32
122          DO 6 K=M2,NN                                      LSS     33
124          S1=0.                                             LSS     34
124          S2=0.                                             LSS     35
127          IF (L.EQ.0) GO TO 5                               LSS     36
130          S1=DOTPRO(L,A(J,1),I,A(1,K),1)                    LSS     37
150    5     A(J,K)=(A(J,K)-S1)/A(J,J)                         LSS     38
177          S2=DOTPRO(J,A(K,1),I,A(1,M2),1)                   LSS     39
217    6     A(K,M2)=A(K,M2)-S2                                LSS     40
232    7     IF (MM.LE.0) GO TO 9                              LSS     41
234          IF (A(J,J).EQ.0.) GO TO 13                        LSS     42
240          DO 8 K=1,MM                                       LSS     43
241          S1=0.                                             LSS     44
242          IF (L.EQ.0) GO TO 8                               LSS     45
243          S1=DOTPRO(L,A(J,1),I,B(1,K),1)                    LSS     46
263    8     B(J,K)=(B(J,K)-S1)/A(J,J)                         LSS     47
315    9     CONTINUE                                          LSS     48
320          DET=A(1,1)*SN                                     LSS     49
321          IF (DET.EQ.0.) GO TO 13                           LSS     50
322          IF (N.EQ.1) GO TO 15                              LSS     51
324          DO 10 J=2,NN                                      LSS     52
332    10    DET=DET*A(J,J)                                    LSS     53
335          IF (DET.EQ.0.) GO TO 13                           LSS     54
341          IF (MM.EQ.0) GO TO 15                             LSS     55
342          M3=NN-1                                           LSS     56
344          DO 12 J=1,MM                                      LSS     57
346          DO 11 L=1,M3                                      LSS     58
347          M1=NN-L                                           LSS     59
347          S1=0.                                             LSS     60
347          M2=M1+1                                           LSS     61
347          K=NN-M2+1                                         LSS     62
355          S1=DOTPRO(K,A(M1,M2),I,B(M2,J),1)                 LSS     63
374    11    B(M1,J)=B(M1,J)-S1                                LSS     64
407    12    CONTINUE                                          LSS     65
411          GO TO 15                                          LSS     66
412        13 DET=0.0                                          LSS     67
413    15    RETURN                                            LSS     68
414          END                                               LSS     69

             DOUBLE FUNCTION DOTPRO(N,X,IX,Y,IY)               DOTPRO   2
 14          DIMENSION X(IX,N),Y(IY,N)                         DOTPRO   3
 14          DOUBLE DX,DY,SUM                                  DOTPRO   4
```

```
14           SUM=0.0                                                          DOTPRO      5
15           DO 1 I=1,N                                                       DOTPRO      6
24           DX=X(1,I)                                                        DOTPRO      7
26           DY=Y(1,I)                                                        DOTPRO      8
24         1 SUM=SUM+DX*DY                                                    DOTPRO      9
46           DOTPRO=SUM                                                       DOTPRO     10
50           RETURN                                                           DOTPRO     11
52           END                                                              DOTPRO     12


             SUBROUTINE REAP(LABEL,N,A)                                       REAP        2
      C*******************************************************               REAP        3
      C     THIS ROUTINE IS DESIGNED TO READ AND PRINT SPECIFIED              REAP        4
      C   ARRAYS.                                                             REAP        5
      C                                               KERSHNER 2/13/76        REAP        6
      C*******************************************************               REAP        7
10           DIMENSION LABEL(10),A(N)                                         REAP        8
      C*******************************************************               REAP        9
      C     FORMAT STATEMENTS.                                                REAP       10
      C*******************************************************               REAP       11
          10 FORMAT(12I6)                                                     REAP       12
          20 FORMAT(6E12.7)                                                   REAP       13
          30 FORMAT(5X,12I8)                                                  REAP       14
          40 FORMAT(5X,1P5E13.5)                                              REAP       15
          50 FORMAT(2X,10A10)                                                 REAP       16
10           CALL PRIN (LABEL,0,0)                                            REAP       17
      C*******************************************************               REAP       18
      C     THEN BRANCH ON N TO READ AND PRINT ARRAY A.                       REAP       19
      C*******************************************************               REAP       20
12           IF(N)100,110,150                                                 REAP       21
      C*******************************************************               REAP       22
      C     NEGATIVE N, USE 12I6 FORMAT.                                      REAP       23
      C*******************************************************               REAP       24
15       100 CONTINUE                                                         REAP       25
15           NP=-N                                                            REAP       26
16           READ (10,10)(A(I),I=1,NP)                                        REAP       27
26           PRINT 10,(A(I),I=1,NP)                                           REAP       28
40           RETURN                                                           REAP       29
      C*******************************************************               REAP       30
      C     ZERO N, STOP AFTER READING BLANK FIELD.                           REAP       31
      C*******************************************************               REAP       32
41       110 CONTINUE                                                         REAP       33
41           J=1                                                              REAP       34
41           K=6                                                              REAP       35
43       120 READ(10,20)(A(I),I=J,K)                                          REAP       36
55           DO 130 L=J,K                                                     REAP       37
61           IF(A(L).EQ.0.0)GO TO 140                                         REAP       38
62       130 CONTINUE                                                         REAP       39
64           PRINT 40,(A(I),I=J,K)                                            REAP       40
76           J=K+1                                                            REAP       41
76           K=J+5                                                            REAP       42
101          GO TO 120                                                        REAP       43
104      140 A(L)=0.0                                                         REAP       44
106          PRINT 40,(A(I),I=J,L)                                            REAP       45
120          RETURN                                                           REAP       46
      C*******************************************************               REAP       47
      C     POSITIVE N, USE E12.7 FORMAT.                                     REAP       48
      C*******************************************************               REAP       49
121      150 CONTINUE                                                         REAP       50
121          READ(10,20)(A(I),I=1,N)                                          REAP       51
```

```
14          SUM=0.0                                                      DOTPRO      5
15          DO 1 I=1,N                                                   DOTPRO      6
24          DX=X(1,I)                                                    DOTPRO      7
24          DY=Y(1,I)                                                    DOTPRO      8
24        1 SUM=SUM+DX*DY                                                DOTPRO      9
45          DOTPRO=SUM                                                   DOTPRO     10
50          RETURN                                                       DOTPRO     11
52          END                                                          DOTPRO     12


            SUBROUTINE REAP(LABEL,N,A)                                   REAP        2
      C**********************************************************        REAP        3
      C     THIS ROUTINE IS DESIGNED TO READ AND PRINT SPECIFIED         REAP        4
      C   ARRAYS.                                                        REAP        5
      C                                          KERSHNER 2/13/76        REAP        6
      C**********************************************************        REAP        7
10          DIMENSION LABEL(10),A(N)                                     REAP        8
      C**********************************************************        REAP        9
      C     FORMAT STATEMENTS.                                           REAP       10
      C**********************************************************        REAP       11
         10 FORMAT(12I6)                                                 REAP       12
         20 FORMAT(6E12.7)                                               REAP       13
         30 FORMAT(5X,12I8)                                              REAP       14
         40 FORMAT(5X,1P5E13.5)                                          REAP       15
         50 FORMAT(2X,10A10)                                             REAP       16
10          CALL PRIN (LABEL,0,0)                                        REAP       17
      C**********************************************************        REAP       18
      C     THEN BRANCH ON N TO READ AND PRINT ARRAY A.                  REAP       19
      C**********************************************************        REAP       20
12          IF(N)100,110,150                                             REAP       21
      C**********************************************************        REAP       22
      C     NEGATIVE N, USE 1216 FORMAT.                                 REAP       23
      C**********************************************************        REAP       24
15      100 CONTINUE                                                     REAP       25
15          NP=-N                                                        REAP       26
16          READ (10,10)(A(I),I=1,NP)                                    REAP       27
26          PRINT 10,(A(I),I=1,NP)                                       REAP       28
40          RETURN                                                       REAP       29
      C**********************************************************        REAP       30
      C     ZERO N, STOP AFTER READING BLANK FIELD.                      REAP       31
      C**********************************************************        REAP       32
41      110 CONTINUE                                                     REAP       33
41          J=1                                                          REAP       34
41          K=6                                                          REAP       35
43      120 READ(10,20)(A(I),I=J,K)                                      REAP       36
55          DO 130 L=J,K                                                 REAP       37
61          IF(A(L).EQ.0.0)GO TO 140                                     REAP       38
62      130 CONTINUE                                                     REAP       39
64          PRINT 40,(A(I),I=J,K)                                        REAP       40
76          J=K+1                                                        REAP       41
76          K=J+5                                                        REAP       42
101         GO TO 120                                                    REAP       43
104     140 A(L)=0.0                                                     REAP       44
106         PRINT 40,(A(I),I=J,L)                                        REAP       45
120         RETURN                                                       REAP       46
      C**********************************************************        REAP       47
      C     POSITIVE N, USE E12.7 FORMAT.                                REAP       48
      C**********************************************************        REAP       49
121     150 CONTINUE                                                     REAP       50
121         READ(10,20)(A(I),I=1,N)                                      REAP       51
```

```
131          PRINT 40,(A(I),I=1,N)                                                      REAP        52
143          RETURN                                                                     REAP        53
144          END                                                                        REAP        54
      C************************************************************************************ DUMMY        2
      C*     7. DUMMIES                                                                * DUMMY        3
      C************************************************************************************ DUMMY        4


             SUBROUTINE DOUT                                                            DUMMY        5
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY        6
  1          RETURN                                                                     DUMMY        7
  2          END                                                                        DUMMY        8


             SUBROUTINE DIP1                                                            DUMMY        9
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       10
  1          RETURN                                                                     DUMMY       11
  2          END                                                                        DUMMY       12


             SUBROUTINE TEST                                                            DUMMY       13
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       14
  1          RETURN                                                                     DUMMY       15
  2          END                                                                        DUMMY       16


             SUBROUTINE CHEC                                                            DUMMY       17
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       18
  1          RETURN                                                                     DUMMY       19
  2          END                                                                        DUMMY       20


             SUBROUTINE SPEC                                                            DUMMY       21
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       22
  1          RETURN                                                                     DUMMY       23
  2          END                                                                        DUMMY       24


             SUBROUTINE SPEC1                                                           DUMMY       25
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       26
  1          RETURN                                                                     DUMMY       27
  2          END                                                                        DUMMY       28


             SUBROUTINE CORE                                                            DUMMY       29
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       30
  1          RETURN                                                                     DUMMY       31
  2          END                                                                        DUMMY       32


             SUBROUTINE DOM                                                             DUMMY       33
      C      THIS IS A DUMMY ROUTINE.                                                   DUMMY       34
  1          RETURN                                                                     DUMMY       35
  2          END                                                                        DUMMY       36
      C      CZZ                                                                        CZZ          2
```

APPENDIX D

COMMON STORE

The contents of the common arrays are listed in Table D-I.

•<u>General Notes</u>

(1) If there is a principal routine dealing with an array, its name is given in parentheses at the end of the description line.

(2) A few important equivalent names are given; these are denoted by a preceding equals sign.

(3) A single subscript indicates a one-dimensional array (for example x_i); a double subscript indicates a two-dimensional array.

(4) One-dimensional arrays containing species properties or compositions for the entire system list the solid as the first species. The mole fraction of the solid is $x_s = n_s/n$.

(5) Unless otherwise stated, the units are cm-g-μs or cm-mol-μs.

(6) Unless otherwise stated, all derivatives for the system are at chemical equilibrium.

•<u>Particular Notes</u>

(1) GM - the prime here denotes imperfection quantities with respect to ideal gas at the same temperature and <u>volume</u>. See Sec. IV.C.

(2) THER - the subscript o on quantities near the end of the array denotes a frozen-composition derivative.

TABLE D-I

COMMON STORE

CAR - matrix of FROOT arrays (columns)

1. CC - CJ
2. CH - Hugoniot
3. CM - constant-v, s, e contours
4. CG - gas EOS
5. CS - solid EOS

CONT - constants

1. 1.98719 R(cal)
2. 831439 x 10^{-5} R(Mbar-cm^3/g)
3. 1.01325 x 10^{-6} atm to Mbar
4. 0.04184 kcal to Mbar-cm^3
5. 0.426012 $(N/\sqrt{2})$ x 10^{-24}

DER - differentiation (GAMM)

1. p
2. v
3. T
4. v_+
5. v_-
6. H_+
7. H_-

EMG - $\tilde{F}_i$, "free energies" for equilibrium constants (EQMS)

EMN - phase mole numbers

1. n_g
2. n_s
3. $n = n_g + n_s$
4. $x_g = n_g/n$
5. $x_s = n_s/n$
6. n/M_0 (moles/gram)
7. $\ell n\ s$ (saturation index) or $-n_s$ (all solid evaporated)

EMX - x_i, mole fractions

FMU - μ_i', imperfection chemical potentials

FN - n_i, mole numbers

FOB - knobs

1-6. FROOT ε's
7-12. FROOT r's
13. $\Delta_1 = \Delta\ \ell n\ p$ (GAMM)
14. $\Delta_2 = \Delta T$ (GAMM)
15. ε, equilibrium outer (EQP)
16. ε, equilibrium inner (EQP)
17,18. ---
19-36. FROOT x_{min}, x_{max} in pairs

GM - pure-fluid gas state (sub g) (GEM)

1. $\tau = v/v^*$
2. $\theta = T/T^*$
3. $z = pV/RT$
4. E'/RT
5. F'/RT
6. $(z\theta)_\theta$
7. τz_τ
8. C_v'/R
9. z - RT/p
10. $z-1$
11. S'/R
12. $(\partial p/\partial V)_T$
13. $(\partial p/\partial T)_V$
14. $(\partial V/\partial T)_p$
15. V
16. p
17. H'/RT
18. $(z-1)_\ell = \tau\chi_\tau/\theta$
19. $(E'/RT)_\ell = -\chi/\theta$
20. A'/RT
21. $V_f/V = 2\pi\sqrt{2}\ g(1)$ (V_f = free volume)
22. $b/2$ (integration limit)
23. ---
24. ---
25. γ
26. $p^{-1}\ (\partial E/\partial V)_p$
27. $1/\Gamma$
28. $-(\partial\ \ell n\ p/\partial\ \ell n\ V)_T$
29. C_p'/R
30. $(\partial\ \ell n\ V/\partial T)_p$

GP - gas EOS (GEM)

1. n
2. m
3. A_n
4. A_m
5. $r^* =$ RSTA
6. $T^* =$ TSTA
7. $V^* =$ VSTA

HE - initial (unreacted) state (CON)

1. ρ_0 (g/cm3)
2. p_0 (Mbar)
3. T_0 (K)
4. M_0 (g/mole)
5. ΔH_{f0} (kcal/mole relative to elements at T_0)
6. $v_0 = 1/\rho_0$
7. $h_0\ (T_0;T_0) = (n/M_0)\ \Delta H_{f0}$
8. $e_j - \frac{1}{2} u_j^2$

KAL - option switches, see <u>CON</u>, <u>SWIT</u>

1. equilibrium differentiation
2. fixed composition differentiation
3. gas (0/9/other: ideal/KW/LJD)
4. solid (0 for incompressible)
5. mix 0 no-mix 3 - CS
   1 ideal 4 One-Fluid
   2 LH
6. composition (0/1 for fixed, equilibrium)
7. CJ (0/1 for equilibrium/frozen)
8. contour (1, 2, 3, 4 for constant-T, v, s, e)
9. T_c, p_c choice (0/1 for input/previous)
10. z - 1
11. punch output if ≠ 0

KEN - entry and iteration counts

KIM - sizes

1. r = KR number of gas species
2. s = KS total number of species
3. c = KC number of elements
4. n = KN degree of ideal-function fit

KON - triggers and diagnostic switches

PT - input pressure table (PV, TED)

ROT - input ρ_0 table (CJ)

SM - solid state (sub s) (SEMS)

1. V
2. E'/RT
3. H'/RT
4. A'/RT
5. F'/RT
6. S'/R
7. $z = pV/RT$
8. p
9. $V/V_0 = Y$
10. T
11. T_1

SP - solid EOS (SEMS)

1. Γ
2. C_p/R
3. α
4. V_0
5. T_0
6. E_0/RT_0
7. ---

8-12. c_0-c_4 - Hugoniot fit

13-20. working store

SUC - contour initial state (PV)

1. T_c
2. p_c
3. V_c
4. S_c
5. E_c

SUCG - derivatives working store (GAMM)

1. γ
2. $p^{-1} (\partial e/\partial v)_p$
3. $1/\Gamma$
4. c
5. CJ function j(p) [see THER (28)]
6. $-(\partial \ln p/\partial \ln v)_T$
7. C_p/R
8. $(\partial \ln v/\partial \ln T)_p$

THER - system state (COUT)

1. p
2. v/v_0
3. T
4. u
5. D
6. q (Mbar - cm^3/g)
7. q (kcal/g)
8. v
9. e
10. h
11. a
12. f
13. s
14. $H(T;T_0)/RT$ - relative to elements at T_0
15. V
16. E/RT
17. H/RT
18. A/RT
19. F/RT
20. S/R
21. $z = pV/RT$
22. γ
23. $p^{-1}(\partial e/\partial v)_p$
24. $1/\Gamma$
25. c
26. γ_0 (frozen)
27. $j(p)$ equilibrium
28. $j(p)$ frozen

    where $j(p)$ is the CJ function:

$$j(p) = \left\{v/v_0 \left[\left(\gamma+1 - p_0/p\right)/\gamma\right]\right\}^{-\gamma}$$

29. c_0 (frozen)
30. $p^{-1} (\partial e/\partial v)_p$ frozen

TMG - F_i^i - ideal free energies

TMS - ideal functions (super i) (TIMS)

1. E_g/RT
2. H_g/RT
3. C_g/R
4. S_g/R
5. $\Delta g(T_0)$ } relative to
6. $H_g(T;T_0)/RT$ } elements at T_0
7. H_s/RT
8. C_s/R
9. S_s/R
10. F_s/RT
11. $\Delta s(T_0)$ } relative to
12. $H_s(T;T_0)/RT$ } elements at T_0

TP - <u>CON</u>, <u>TIP</u> strings 3 ..., one row per species

XMT - gas mixture state (sub g) (XIM)

1. V
2. E'/RT
3. H'/RT
4. A'/RT
5. F'/RT
6. S'/R
7. $z-1$
8. $V-RT/p$
9. $\Sigma\, x_i\, x_j\, T^*_{ij}/T^*_r$ (for LH mix)
10. $\Sigma\, x_i\, x_j\, r^*_{ij}/r^*_r$ (for LH mix)
11. r^*_r (for LH mix)
12. T^*_r (for LH mix)
13. n (for One-Fluid mix)
14. m (for One-Fluid mix)
15. V^*_r (for One-Fluid mix)
16. $\bar{r}^* =$ RSTAT (from XIMS)
17. $\bar{T}^* =$ TSTAT (from XIMS)
18. $\bar{V}^* =$ VSTAT (from XIMS)

XMU μ'_i/RT, gas species only (XIM)

XPF - T^*_{ij} (XIM)

XPG - r^*_{ij} (XIM)

XPR - r^*_i (XIM)

XPT - T^*_i (XIM)

REFERENCES

1. W. Fickett, "Calculation of the Detonation Properties of Condensed Explosives," Phys. Fluids <u>6</u>, 997-1006 (1963).

2. W. Fickett, "Detonation Properties of Condensed Explosives Calculated with an Equation of State Based on Intermolecular Potentials," Los Alamos Scientific Laboratory report LA-2712 (December 1962).

3. S. J. Jacobs, "Energy of Detonation," Naval Ordnance Laboratory report NAVORD 4366 (September 1956).

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