LA-6250

C.3

UC-45

Issued: December 1976

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

by

Wildon Fickett

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

UNITED STATES
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161
Price: Printed Copy $6.00 Microfiche $3.00

CONTENTS

CONTENTS (contd)

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

by

Wildon Fickett

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, ..., a_n, d, ΔH_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^0 in place of $\Delta H_f(T_0)$ and setting

$[H^o(T_0) - H^o_0]/RT_0$ for each species to zero. This has the advantage of making the TIP input simpler and independent of T_0. 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 $\underset{\sim}{\rho}_0$

$\underset{\sim}{\rho}_0$ - 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_0) 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 in the gas phase. 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 ideal and imperfection 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 <u>mixture rules</u>, described next.

<u>4. Mixture (XIM)</u>. 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.

<u>5. Chemical Equilibrium (EQM)</u>. 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

$$\mathcal{E}\,(T,\ p) = e_c \quad ,$$

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

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

Here we have defined, in terms of the NBS notation

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

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

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

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

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

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

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

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_o is

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

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 $y = V/V_o$ (with V_o 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_o as a parameter (together with argument T), the quantity supplied by TIM for this calculation is

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

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

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

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

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

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

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

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

- <u>Computation</u>

Given p, T, the function defining y is

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

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

$$y_1 = \left[1 + \left(p - p_2(y)\right)\Big/A\right]^{1/(\Gamma+1)}, \quad A = (Cp/\alpha\ V_0)\ \left[\Gamma/(\Gamma+1)\right]$$

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

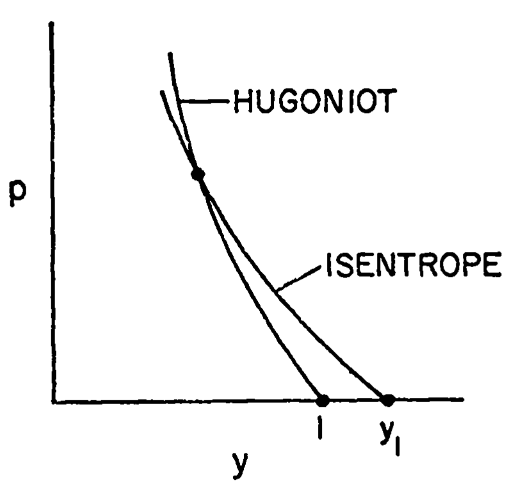


Fig. 1. Solid Hugoniot and isentrope.

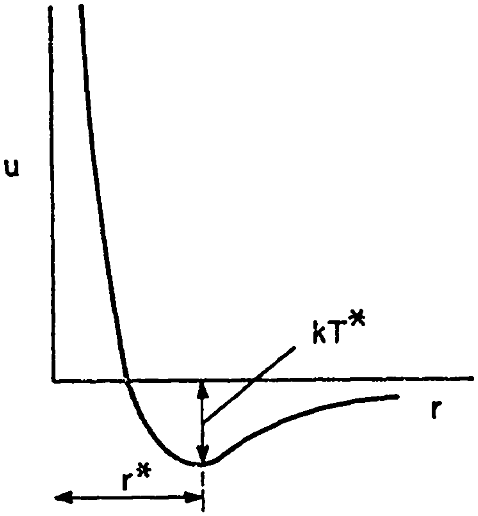


Fig. 2. Intermolecular potential for LJD EOS.

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

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 cell potential 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

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

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

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

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	=	$-1/2\ A_n Zn/(n-m)$	$-1/2\ A_m Zm/(n-m)$
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.

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

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

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

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

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

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

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

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

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

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

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

The series is used for computation.

b. Exponential Form.

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

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

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

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

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

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

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

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 $(0,b^*)$

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

$$\vdots$$

$$y_8 = y_9 \cong 0.1$$

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

$$\vdots$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

<u>4. One-Fluid Mixing</u>. 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

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

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

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

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

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

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

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

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.)

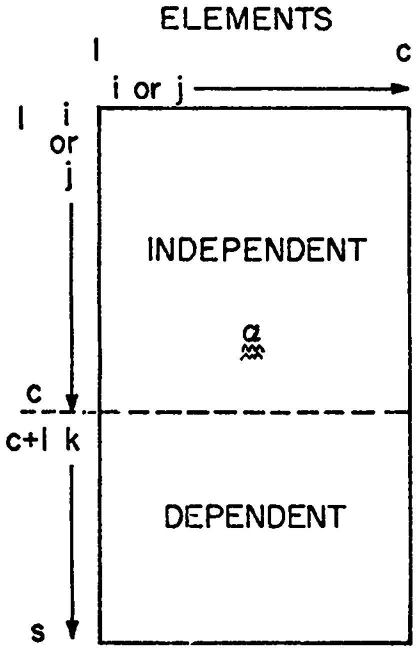


Fig. 3. The α-matrix.

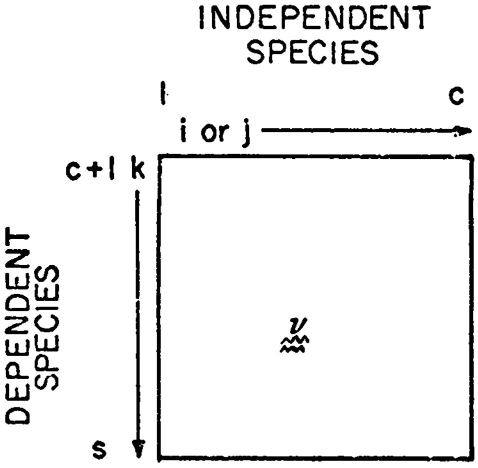


Fig. 4. The ν-matrix.

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

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

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

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

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

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

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

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

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

$$\nu_k = \sum\nolimits_j' \nu_{kj}$$

$$\bar{q}_i = q_i \Big/ \sum\nolimits_j' q_j$$

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

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

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

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

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)

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

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

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

```
     $\tilde{F}_s \leftarrow F^i_s + F'_s$                              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) $\leftarrow$ 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 $\bar{r}^*$, 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	$j(p) - 1$ $j(p) = \left[\frac{v/v_0}{\gamma(\gamma+1 - p_0/p)}\right]^{-\gamma}$
Hugoniot	CH	HUG	T_1 = previous (3000) $x_2 = x_1 - f_1/f_1'$ [c]	$T > T_{min}$ $T < T_{max}$	T/1000	$20\left[\frac{h(T;T_0) - h_0(T_0;T_0)}{(p-p_0)v_0} - \frac{1}{2}\left(1 + \frac{v}{v_0}\right)\right]$ [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) $x_2 = x_1 - f_1/f_1'$	$V_g > V_{g\,min}$ $V_g < V_{g\,max}$	$\ell n\, V_g$	$\ell n \left[\tilde{p}(V_g, T)/p\right]$
Solid EOS	CS	SEMS	x_1 = previous (0.8) $x_2 = r x_1$	$x > x_{min}$ $x < 1+\alpha(T-T_0)$	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 nth (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)

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

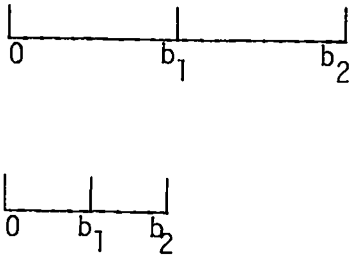
TABLE IV

ALGORITHM FOR THE CELL INTEGRAL

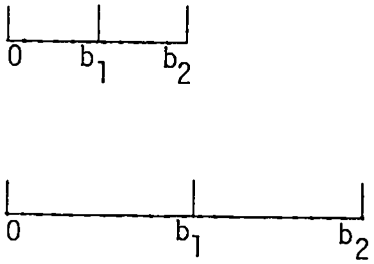
```
$\alpha$ $b_2 \leftarrow b'$, $b_1 \leftarrow b'/2$                              b' is upper limit from
                                                               last entry
  $I \leftarrow \tilde{I}\ (0,b_1)$                                     first segment
  if ($b_1$ just right):  done
  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)
```

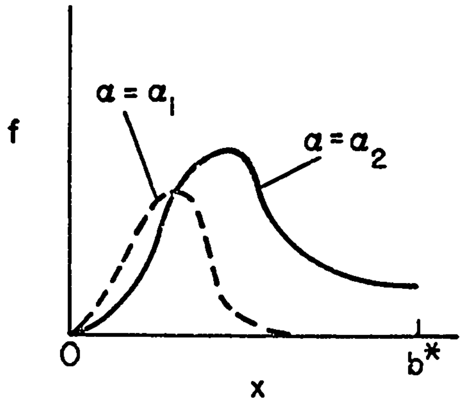


Fig. 5. Integrands for the LJD cell integral.

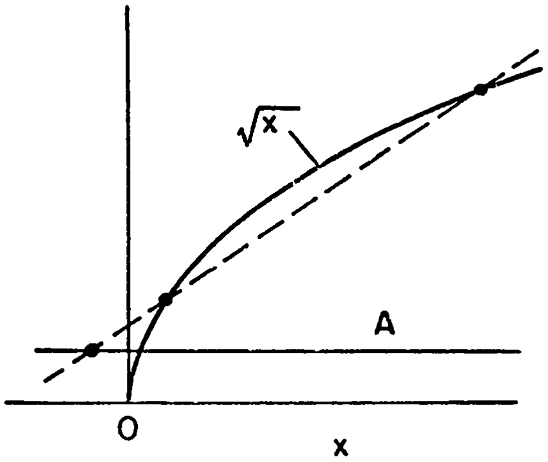


Fig. 6. Iterative solution of $f(x) = x^{1/2} - A = 0$ by FROOT.

```
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 ρ_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	($\ell n\,\hat{s}$ 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; $\ell n\,\hat{s}$ (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    FOB
 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     F-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 1.4940 E-03 -4.2896E-07 6.2644 E-11 -3.4991E-15 -2.81   E+00
 0.0     E+00 0.0     F+00 4.2457 E-01
3.1499  F+00 5.8718 E-04 -1.3665E-07 1.6756 E-11 -8.2278E-16 4.673  E+00
 0.0     E+00 0.0     F+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 1.18370F-03 -2.1492E-07 2.28480E-11 -1.0874E-15 3.19230E+00
 -5.7107E+01 -5.7798E+01 3.99610E+00
 3.377  E+00 5.60470E-04 -1.5606E-07 2.04140E-11 -1.0944E-15 5.93    E+00
 2.1477 F+01 2.16   E+01 3.7032 E+00
 3.2375 E+00 2.3187 E-04 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 F-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     M2 - BEST MCM SET FROM OTHER SOURCES ,GMX-10-54,P43
      7      2
 1.0     E+00 1.0     F+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   SAM   RDX, RHO=1.8, CO2-ARBITRARY COMPOSITION GUESS
     0
 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    DETCNATION HUGONIOT
   0.3            0.2            0.0
CON   CJ     CJ LOCUS
   1.6            1.8
CON   PV     CJ ISENTROPE
     3      1
     0.0            0.0
     0.3            0.2
CON   REND
CON   JEND
```

Calculation

```
MES1 - 744:620                           MES1 - SHORT TEST - CJ. HUG. ISENTHOPE
TICKET13M.      .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 FPS(CC.CH.CM.CG.CS.C)/ RATIOS/ DP.DT.EPSIN.OUT/ FROOT  ROUNDS
       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-MR) .W (NOW 1)  / N.M.AN.AM.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 -7.90150E+00  6.66560E+00
      -2.03920E+00  0.
```

```
CON   TIP
    KS,KN/ T BOUNDS/ FIT COEFFS.-A1 TO AN,D,DEL,HF,HR...
    8     4
      1.60000E+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
      3.28220E+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
      5.93600E+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   EGF
     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       PBAR*           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    3.8000514E+00  1.4179073E+02  2.3377078E+01  3.1776524E+00  4.7999481E+00  1.8252305E+00  5.7533602E-01

CON    DBUG


       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 -1.5737643E+00  1.6336280E+01  2.9987042E+00  1.4021508E-05  1.2958093E-03
            5    9.5110041E+00  4.9433074E+00 -1.5735481E+00  1.6335343E+01  1.4995168E+00  5.4543140E-11  0.
            6    3.8183535E+00  1.1149935E+00 -1.4354516E-01  6.9590543E+00  0.              0.              0.
            7    3.8000467E+00  1.4179416E+02  2.3376993E+01  3.1776524E+00  4.7999481E+00  1.8252305E+00  5.7533602E-01
```

```
CAR - CC/CH/CH/CG/CS/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           7.5917720     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
F06          5.0000E-05    2.0000E-06    1.2000E-05    7.0000E-07    1.0000E-07             0             0     1.0000000     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^^^^^^^    EQP^^^^^^^    ^^^^^^^^^^    SAM^^^^^^^    TED^^^^^^^    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         MESI^-^SHO    RT^TESTA-^    CJ,^HUG,^I    SENTROPE^^    ^^^^^^^^^^    ^^^^^^^^^^    ^^^^^^^^^^             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    BEW^HMIG(P    MIBAR3+()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     5.3330000   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     4.7999481     1.8252305      .5753360      .8664209     3.0700306     5.7377295    3.1992E-05             0             0
THER           .3600000      .6246080    2.0000E+03             0             0      .0629970     1.5056645      .3472286   -6.8373E-03      .0572649
        11    -.1163169     -.0142156    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             .4476100     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       25.2846180  25.2846180  16.9160201  19.3734848  12.0822775  29.8665753  21.6020048           0           0           0
XPF      120.0000000 120.0000000 128.6856635 125.3794241  66.0333250 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    TED    DETONATION HUGONIOT

MES1 - 76AUG20                              MES1 - SHORT TEST - CJ. HUG. ISENTROPE                                          09/02/76
TFICKETIGN.      .255 SEC ON RUN.      .306 SEC ON JOB                                                                TED - HUGONIOT
   P-TABLE
      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     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   4.4058543E-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  1.9896503E+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  4.0869243E+03  1.8578651E-01  6.6908030E-01  1.6000000E+00  1.4015000E+00
               2   4.5145347E-01  2.3055305E-02  7.4780944E-05  8.1163490E+00  8.8812807E-01  9.0044771E+00  1.0942458E-01
               3   1.1136433E+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  2.5193527E+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     2.4894704E-01  7.2997845E-01  3.9844666E+03  1.9324864E-01  7.1567857E-01  1.8000000E+00  1.4418736E+00
           2     4.0554358E-01  2.5069501E-02  7.2603689E-05  7.8696632E+00  1.1353011E+00  9.0049643E+00  1.4426299E-01
           3     1.0003748E+01  1.8666819E+00  2.1540388E+01  7.5174255E+00  1.1353011E+00  2.9950458E+00  5.6811003E-01
           4     1.0858513E+01  2.3172328E+00 -1.0528061E+00  7.1597479E+00  2.8287812E+00  9.9076675E-03  1.7121838E-01
           5     1.0926612E+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     3.8070314E+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     2.4894704E-01  7.2997845E-01  3.9844666E+03  1.9324864E-01  7.1567857E-01  1.8000000E+00  1.4418736E+00
           2     4.0554358E-01  2.5069501E-02  7.2603689E-05  7.8696632E+00  1.1353011E+00  9.0049643E+00  1.4426299E-01
           3     1.0003748E+01  1.8666819E+00  2.1540388E+01  7.5174255E+00  1.1353011E+00  2.9950458E+00  5.6811003E-01
           4     1.0858513E+01  2.3172328E+00 -1.0528061E+00  7.1597479E+00  2.8287812E+00  9.9076675E-03  1.7121838E-01
           5     1.0926612E+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     3.8070314E+00  1.3593882E+02  2.3506133E+01  2.7034071E+00  3.2774684E+00  1.5822509E+00  5.2242984E-01

POINT  8   1     3.0000000E-01  6.8133790E-01  4.1506194E+03 -6.2285136E-01  7.1567857E-01  1.8000000E+00  1.4504140E+00
           2     3.7852106E-01  3.2457083E-02  7.2603704E-05  7.8061860E+00  1.2020925E+00  9.0082785E+00  1.5399230E-01
           3     9.3357347E+00  2.3147033E+00  2.1532467E+01  8.0983612E+00  1.2020925E+00  2.9917379E+00  4.6827416E-01
           4     1.0172292E+01  2.6091067E+00 -1.0716390E+00  7.8259305E+00  2.8558995E+00  1.6623390E-02  1.4410009E-01
           5     1.0232402E+01  2.5989927E+00 -1.0849242E+00  7.8780844E+00  1.3296342E+00  1.6855346E-05  0.
           6     3.8882459E+00  4.7078891E-01 -1.4269568E-01  3.3736489E+00  0.             0.             0.
           7     3.8053098E+00  1.3685726E+02  2.3474259E+01  2.7056370E+00  3.4509657E+00  1.6450713E+00  5.5429430E-01

POINT  9   1     2.0000000E-01  7.9167471E-01  3.7817053E+03 -2.6341168E-01  7.1567857E-01  1.8000000E+00  1.4302499E+00
           2     4.3981928E-01  1.7418127E-02  7.2603722E-05  7.9482801E+00  1.0543765E+00  9.0026566E+00  1.3265467E-01
           3     1.0852025E+01  1.3666470E+00  2.1545919E+01  6.9027591E+00  1.0543765E+00  2.9973496E+00  6.9044635E-01
           4     1.1723572E+01  2.0172005E+00 -1.0273858E+00  6.4571326E+00  2.7938894E+00  5.3018977E-03  2.0611114E-01
           5     1.1802219E+01  1.9967990E+00 -1.0485454E+00  6.5071586E+00  1.2551761E+00  5.6424670E-06  0.
           6     4.2819856E+00  2.4994174E-01 -1.0180381E-01  2.7236865E+00  0.             0.             0.
           7     3.8088931E+00  1.3480486E+02  2.3540636E+01  2.6914850E+00  3.1134498E+00  1.5283198E+00  4.8657312E-01

CON    RENO

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 $\underset{\approx}{Q}$, by giving the two renumberings $\underset{\sim}{a}^1$ and $\underset{\sim}{a}^0$. Recall the definition of a_i^1: 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 $\hat{s}$,

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

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

$\underset{\sim}{a}$, $\underset{\sim}{\alpha}$, 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										

$\underset{\sim}{\nu}$ 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

$$\begin{aligned} W(p) &= - W_p + K + I(p) \\ &= I(p) - \frac{1}{2} u_1^2 \\ &= e_1 - \frac{1}{2} u_1^2 - e_i(p) \quad . \end{aligned}$$

We remark that $W(p_0)$ differs little from the heat of reaction q as conventionally defined -- the energy change in the surroundings for reaction to products at T_0, p_0. 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 $T_0 = 300$ K, $p_0 = 1$ atm. For state 2, the calculated temperature is 518 K and the mean γ is 1.25.

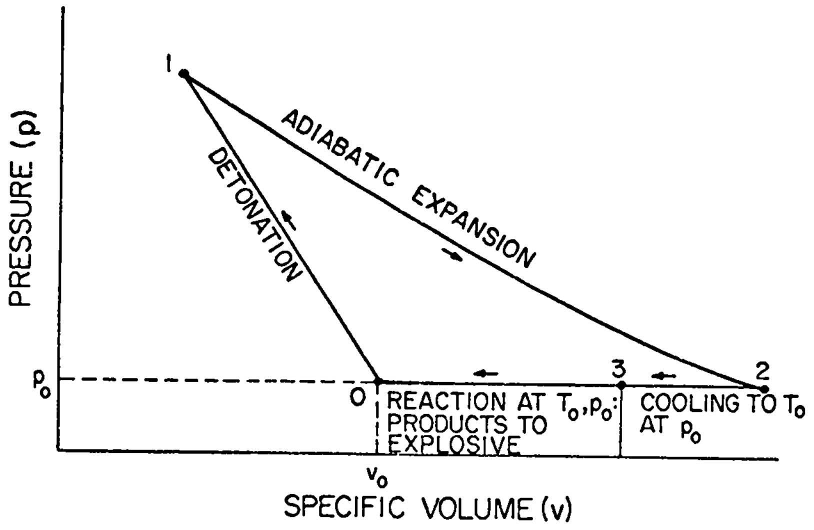


Fig. B-1. Closed cycle of energy changes in the p-v plane.

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-5H-1, DET. PROD. LJD EOS   / W. FICKETT, 74                   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           EQPS PACKAGE (SEC. 3)                                              MESO
     C           REAP (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, 4HSALT, 3HFUB, 1H                                         MESO
           2, 3HUIP, 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 , 4HFCRM, 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 SEHR                                                               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       59
      C*********************************************************************** MESO       60
      C*    2. UTILITY                                                       * MESO       61
      C*********************************************************************** MESO       62


            SUBROUTINE DBUG(A,B)                                               DBUG        2
      C       OLD ERR ROUTINE                                                  DBUG        3
      C         CHANGE DBUG CALLS TO ERR CALLS AS NEEDED                       DBUG        4
 6            CALL ERR(A,B,4LDBUG)                                             DBUG        5
 7          RETURN                                                             DBUG        6
10          END                                                                DBUG        7


            SUBROUTINE ERR(ISUB,IMES,ERRD)                                     ERR         2
      C*********************************************************************** ERR         3
      C     ERROR CONTROL                                                      ERR         4
      C     ARGS - ROUTINE, MESSAGE, DATA (10 WORDS)                           ERR         5
      C++++++++++++++++++++++++++++++++++ COMMONS +++++++++++++++++++++++++++ ERR         6
10          COMMON Z(4000)                                                     ERR         7
10          DIMENSION KON(60), CONT(20)                                        ERR         8
10          EQUIVALENCE (Z(460),CONT), (Z(1690),KON)                           ERR         9
10          EQUIVALENCE (CONT(9),OUT),(KON(6),QERRGAT)                         ERR        10
10          COMMON /SERRC/ SERRCA(16)                                          ERR        11
      C++++++++++++++++++++++++++++++++++ LOCALS ++++++++++++++++++++++++++++ ERR        12
10          DIMENSION ILAB(5)                                                  ERR        13
            DATA ILAB/30H/////// ERROR (ERR CALL) IN - ,1H ,1L                 ERR        14
      C++++++++++++++++++++++++++++++++++ EXECUTE +++++++++++++++++++++++++++ ERR        15
10          ILAB(4)=ISUB                                                       ERR        16
      C---------------------------------- 1. CHECK GATE - WARN IF CLOSED      ERR        17
10          IF(QERRGAT.EQ.0.) GOTO 150                                         ERR        18
12          PRINT 130, ILAB                                                    ERR        19
        130 FORMAT(/// 30X,4(*//////*),* ERR RE-ENTERED FROM  *,5A10///)       ERR        20
21      150 QERRGAT = QERRGAT + 1.0                                            ERR        21
23          IF(QERRGAT .GT. 1.) CALL EXIT                                      ERR        22
      C---------------------------------- 2. PRINT HEAD ARGS, ERP ---------- ERR        23
26          CALL HEAD (ILAB)                                                   ERR        24
32          CALL PRIN (IMES, 10, ERRD)                                         ERR        25
36          IF (ISUB.EQ.4LSERR) CALL UMPPK(OUT,SERRCA)                         ERR        26
44          CALL TRACE                                                         ERR        27
47          CALL ERP(3LERR)                                                    ERR        28
      C---------------------------------- 3. TERMINAL LINE ----------------- ERR        29
51          PRINT 860                                                          ERR        30
        860 FORMAT(///21(5H*****),* END OF RUN AFTER ERR* ///)                 ERR        31
61          CALL CON(1.)                                                       ERR        32
63          END                                                                ERR        33


            SUBROUTINE ERP(L)                                                  ERP         2
      C     DIAGNOSTIC COMMON PRINT                                            ERP         3
 3          COMMON Z(4000)                                                     ERP         4
 3          EQUIVALENCE                                                        ERP         5
           1 (Z( 920),CAR ),(Z( 460),CONT),(Z(1000),DER ),(Z(1010),EMG )       ERP         6
           2,(Z(1030),EPN ),(Z(1170),EMX ),(Z(1370),FMU ),(Z(1390),FN  )       ERP         7
           3,(Z(1410),FOB ),(Z(1490),GM  ),(Z(1470),GP  ),(Z(1590),HE  )       ERP         8
           4,(Z(1600),KAL ),(Z(1620),KEN ),(Z(1680),KIM ),(Z(1690),KON )       ERP         9
           5,(Z(1750),PT  ),(Z(1800),ROT ),(Z(1820),SM  ),(Z(1840),SP  )       ERP        10
           6,(Z(1880),SUC ),(Z(1900),SUCG),(Z(1920),THER),(Z(1970),TMG )       ERP        11
           7,(Z(1990),TMS ),(Z(2010),TP  ),(Z(2210),XMT ),(Z(2240),XMU )       ERP        12
           8,(Z(2260),XPF ),(Z(2660),XPG ),(Z(3060),XPR ),(Z(3080),XPT )       ERP        13
```

```
          X,(Z( 400),BS  ),(Z( 460),EA  ),(Z( 680),EV  ),(Z(3100),FLAB)          ERR     14
          Y,(Z(1530),GMT ),(Z( 900),KEV),(Z(1860),SPC)                            ERR     15
   3       CALL PRIN(1L , 0, 0 )                                                  ERR     16
   6       CALL PRIN ( L, 0, 0)                                                   ERR     17
  11       CALL POUT(1)                                                           ERR     18
  13       CALL POUT(2)                                                           ERR     19
  15       CALL POUT(3)                                                           ERR     20
  17       CALL PRIN (24LCAR = CC/CH/CM/CG/CS/CE  , 60, CAR)                      ERR     21
  22       CALL PRIN(3LDER,10,DER)                                                ERR     22
  25       CALL PRIN(4LCONT,10,CONT)                                              ERR     23
  30       CALL PRIN(3LEMG,10,EMG)                                                ERR     24
  33       CALL PRIN(3LEMN,10,EMN)                                                ERR     25
  36       CALL PRIN(3LEMX,10,EMX)                                                ERR     26
  41       CALL PRIN(3LFMU,10,FMU)                                                ERR     27
  44       CALL PRIN(2LFN,10,FN)                                                  ERR     28
  47       CALL PRIN(3LFOB,40,FOB)                                                ERR     29
  52       CALL PRIN(2LGM,30,GM)                                                  ERR     30
  55       CALL PRIN(2LGP,10,GP)                                                  ERR     31
  60       CALL PRIN(2LHE,10,HE)                                                  ERR     32
  63       CALL PRIN(2LBS,50,BS)                                                  ERR     33
  66       CALL PRIN(2LEA,80,EA)                                                  ERR     34
  71       CALL PRIN(2LEV,10,EV)                                                  ERR     35
  74       CALL PRIN(4LFLAB,10,FLAB)                                              ERR     36
  77       CALL PRIN(3LGMT,10,GMT)                                                ERR     37
 102       CALL PRIN(3LKEV,10,KEV)                                                ERR     38
 105       CALL PRIN(3LSPC,10,SPC)                                                ERR     39
 110       CALL PRIN(3LKAL,12,KAL)                                                ERR     40
 113       CALL PRIN(3LKON,60,KON)                                                ERR     41
 116       CALL PRIN(3LKEN,20,KEN)                                                ERR     42
 121       CALL PRIN(3LKIM,10,KIM)                                                ERR     43
 124       CALL PRIN(2LPT,10,PT)                                                  ERR     44
 127       CALL PRIN(4LRHOT,10,RHOT)                                              ERR     45
 132       CALL PRIN(2LSM,20,SM)                                                  ERR     46
 135       CALL PRIN(2LSP,20,SP)                                                  ERR     47
 140       CALL PRIN(3LSUC,10,SUC)                                                ERR     48
 143       CALL PRIN(4LSUCG,10,SUCG)                                              ERR     49
 146       CALL PRIN(4LTHER,30,THER)                                              ERR     50
 151       CALL PRIN(3LTMG,10,TMG)                                                ERR     51
 154       CALL PRIN(3LTMS,20,TMS)                                                ERR     52
 157       CALL PRIN(2LTP, 80, TP)                                                ERR     53
 162       CALL PRIN(3LXMT,20,XMT)                                                ERR     54
 165       CALL PRIN(3LXMU,10,XMU)                                                ERR     55
 170       CALL PRIN(3LXPF,10,XPF)                                                ERR     56
 173       CALL PRIN(3LXPG,10,XPG)                                                ERR     57
 176       CALL PRIN(3LXPR,10,XPR)                                                ERR     58
 201       CALL PRIN(3LXPT,10,XPT)                                                ERR     59
 204       RETURN                                                                 ERR     60
 205       END                                                                    ERR     61


           SUBROUTINE FIO (B,FMT,N,A,KL)                                          FIO      2
      C                                                                           FIO      3
      C    B=READ  ,RIT    ,PRINT ,WOI                                            FIO      4
      C    FMT=FORMAT                                                             FIO      5
      C    N=NUMBER OF WORDS OF ARRAY A FOR I.O.                                  FIO      6
      C    FOR N=0,FMT IS HOLLERITH ARGUMENT LABEL                                FIO      7
      C          ,KL IS THE WORD LENGTH OF THE LABEL.                             FIO      8
  14       DIMENSION BS(4),FMT(60), A(10)                                         FIO      9
  14       INTEGER B,FMT,BS                                                       FIO     10
      C                                                                           FIO     11
```

```
      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)
     C      GM - STATE POINT FROM PREVIOUS K=1 CALCULATION
     C           (GEM(2) OUTPUT)
     C      EMX(2...) - (GAS) MOLE FRACTIONS
     C    OUTPUT
     C      XMT - MIXTURE STATE POINT
     C            (NOTE - CHEMICAL POTENTIALS IN XMU ARE
     C             CALCULATED BY CALLER)
     C    VARIABLES
     C      EV - 1,2 - TSTAR AND RSTAR DISPLACEMENTS
     C           3,5 - EXPANSION COEFFICIENTS
     C
 3          COMMON Z(4000)
 3          DIMENSION
           1 CAR    (    80) ,CONT  (    20) ,EV    (    20)
           2,FOB    (    60) ,GM    (    40) ,KEN   (    60)
           3,KON    ( 6,10) ,THER  (    50) ,XMT   (    30)
           4,GP(20)
 3          EQUIVALENCE
           1 (Z(  920),CAR    ) ,(Z(  460),CONT   ) ,(Z(  680),EV     )
           2,(Z( 1410),FOB    ) ,(Z( 1490),GM     ) ,(Z( 1620),KEN    )
           3,(Z( 1690),KON    ) ,(Z( 1920),THER   ) ,(Z( 2210),XMT    )
           4,(Z(1470),GP)
 3          DIMENSION CG(10),KCG(2)
     C
 3          EQUIVALENCE
           1 (CAR(31),CG),(CG(8),KCG)
           2,(CONT(2),R)
           3,(FOB(20),VRU),(FOB(19),VRL)
           4,(GM(15),VR),(GM(10),PG)
           5,(THER(1),P),(THER(3),T)
           6,(GP(5),RSTA),(GP(6),TSTA)
           7,(XMT(16),RSTAT),(XMT(17),TSTAT)
     C
     C
 3        4  GO TO ( 10,300) , K
     C---------------------------------- K=1 - REGULAR ----------------
 11      10 IF (VR) 20,12,50
 12      12 VR=10.0
 14      20 CG(4)=ALOG(VR)
 20      22 CALL DOUT (3HGEP,1)
 24      40 KCG(1)=0
     C
 25      50 CALL FROOTT (CG,KON(4,8))
 31      52 KEXIT=KCG(2)
 33      60 GO TO (150,88,80,70),KEXIT
 43      70 CALL DBUG (3HGEP,1)
 47      72 GO TO 150
 50      80 CALL DBUG (3HGEP,2)
 54      82 GO TO 150
 55      88 IF (KON(4,8)) 92,90,92
 55      90 IF (KCG(1)-2)92,91,92
 60      91 CG(2)=CG(4)-CG(3)*PG/(VR*GM(12))
 65      92 VR= EXP(CG(2))
 71      93 IF (VRU-VR)94,94,96
 74      94 VR=VRU
 76      95 GO TO 98
 77      96 IF (VR-VRL) 97,97,98
102      97 VR=VRL
104      98 KEN(11)=KEN(11)+1
```

```
106      100 CALL GEM(2)
111      105 IF (PG)106,110,110
113      106 IF (VRL-VR/3.)107,97,97
117      107 VR=VR/3.
121      108 GO TO 110
122      110 CG(3)=ALOG(PG/P)
130      112 CG(2)=ALOG(VR)
134      120 CALL COUT (3HGEP,2)
140      130 GO TO 50
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)=-(1*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)
230      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                                                              GEM

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

```
      C 998                                                                                      GEM      59
 11    1000 CALL REAP (                                                                          GEM      60
           1  60H0        POT (1-LJ,2-MCM,3-MR) ,W (NOW 1)  / N,M,AN,AM,R*,T*$                   GEM      61
           1 ,-2,KE)                                                                             GEM      62
 14         CALL REAP(0,6,GP)                                                                    GEM      63
 20    1010 KE(3)=0                                                                              GEM      64
 21    1012 KE(4)=0                                                                              GEM      65
 22    1020 KE (5)=KON(1,4)                                                                      GEM      66
 24    1022 KE (6)=KON(2,4)                                                                      GEM      67
 26    1024 IF (KE(1)-9) 1030,1025,1030                                                          GEM      68
 30    1025 KAL(3)=9                                                                             GEM      69
 31    1026 VSTA=1.0                                                                             GEM      70
 33    1027 TSTA=1.0                                                                             GEM      71
 35    1028 GO TO 3000                                                                           GEM      72
 36    1030 CALL GES(1,KE,GP,GM)                                                                 GEM      73
 43    1040 CALL PRTN(4HV*$ ,1,VSTA)                                                             GEM      74
 47    1050 KAL(3)=1                                                                             GEM      75
 50    1060 GO TO 3000                                                                           GEM      76
      C1994                                                                                      GEM      77
      C1996                        MAIN                                                          GEM      78
      C1998                                                                                      GEM      79
 51    2000 KEN(1)=KEN(1)+1                                                                      GEM      80
 53    2002  E1 = VP                                                                             GEM      81
      C2004                                                                                      GEM      82
      C2006                                       IDEAL                                          GEM      83
 55    2010 IF (KAL(3)) 2200,2050,2200                                                           GEM      84
 56    2050 DO 2060 I=3,15                                                                       GEM      85
 63    2060 GM(I)=0.0                                                                            GEM      86
 65    2070 GM(3)=1.0                                                                            GEM      87
 67    2080 GM(9)=1.0                                                                            GEM      88
 71    2090 GM(14)=1.0                                                                           GEM      89
 73    2100 GO TO 2300                                                                           GEM      90
      C2194                                                                                      GEM      91
      C2196                                       LJD                                            GEM      92
 74    2200 TAU=VR/VSTA                                                                          GEM      93
 76    2210 THETA=T/TSTA                                                                         GEM      94
100    2220 KE(5)=KON(1,4)                                                                       GEM      95
102    2230 KE(6)=KON(2,4)                                                                       GEM      96
      C                                                   KW                                     GEM      97
104    2234 IF (KAL(3)-9) 2240,2236,2240                                                         GEM      98
106    2236 CALL RKW(1)                                                                          GEM      99
111    2238 GO TO 2300                                                                           GEM     100
      C                                                                                          GEM     101
112    2240 CALL GES (2,KE,GP,GM)                                                                GEM     102
      C                                           REARRANGE AND FINISH GM                        GEM     103
117    2300 GM(22)=GM(15)                                                                        GEM     104
121    2310 GM(21)=GM(14)                                                                        GEM     105
123    2320 GM(20)=GM(6)                                                                         GEM     106
125    2330 GM(19)=GM(13)                                                                        GEM     107
127    2340 GM(18)=GM(12)                                                                        GEM     108
131    2350 GM(17)=GM(5)                                                                         GEM     109
133    2352  VP = E1                                                                             GEM     110
135    2360 PG=GM(3)*R*T/VR                                                                      GEM     111
141    2370 GM(15)=VR                                                                            GEM     112
143    2380 GM(12)=(R*T/VR**2)*(GM(10)-GM(3))                                                    GEM     113
150    2390 GM(13)=(R/VR)*GM(9)                                                                  GEM     114
153    2400 GM(14)=-GM(13)/GM(12)                                                                GEM     115
155    2410 E1=GM(11)                                                                            GEM     116
157    2412 E2=GM(7)                                                                             GEM     117
161    2420 GM(11)=GM(8)                                                                         GEM     118
```

```
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. CORREST 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)=0.75541441                                                           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                                                    GES      38
 66      246 BDOWN=0.93778543                                                 GES      39
 70      248 EPS=18.0                                                         GES      40
 72      260 GP(7)=0.426012*GP(5)**3                                          GES      41
 75      300 CALL WR(1,L,GP)                                                  GES      42
102      310 GO TO 5000                                                       GES      43
       C 990                                                                  GES      44
       C 992                          MAIN ENTRY                              GES      45
       C 994                              INITIAL                             GES      46
103     1000 TAU=GM(1)                                                        GES      47
104     1010 THETA=GM(2)                                                      GES      48
106     1012 L(3)=L(3)+1                                                      GES      49
110     1020 IF(TAU)1040,1040,1030                                            GES      50
112     1030 IF(THETA)1040,1040,1050                                          GES      51
114     1040 CALL DBUG(3HGES,1)                                               GES      52
122     1050 CH(1)=TAU                                                        GES      53
124     1060 CALL WR (2,L,CH)                                                 GES      54
132     1070 KE1=0                                                            GES      55
133     1080 IF (L(5)) 4000,1200,4000                                         GES      56
       C1190                              FIND LIMIT                          GES      57
134     1200 W1=B*(1.0+Y(1))                                                  GES      58
137     1210 CALL WR (3,L,W1)                                                 GES      59
145     1220 IF ((W1(3)- ABS(CH(2)))/THETA-EPS) 1400,1400,1250                GES      60
       C1238                                                                  GES      61
       C1240                                  CHECK AND LOWER                 GES      62
153     1250 W2=B*(1.0+Y(3))                                                  GES      63
156     1260 CALL WR (3,L,W2)                                                 GES      64
164     1270 IF ((W2(3)- ABS(CH(2)))/THETA-EPS) 1600,1600,1300                GES      65
172     1300 KE1=KE1+1                                                        GES      66
174     1310 DO 1320 I=1,5                                                    GES      67
201     1320 W1(I)=W2(I)                                                      GES      68
205     1330 B=B*BDOWN                                                        GES      69
207     1340 IF (L(5)) 4100,1250,4100                                         GES      70
       C1394                                                                  GES      71
       C1396                                  RAISE                           GES      72
211     1400 IF (B-BMAX)1450,1410,1410                                        GES      73
214     1410 W2=B*(1.0+Y(3))                                                  GES      74
217     1420 CALL WR (3,L,W2)                                                 GES      75
225     1430 GO TO 1600                                                       GES      76
226     1450 DO 1460 I=1,5                                                    GES      77
233     1460 W2(I)=W1(I)                                                      GES      78
237     1470 B=B*BUP                                                          GES      79
241     1472 IF(L(5))4150,1474,4150                                           GES      80
242     1474 KE1=KE1+1                                                        GES      81
244     1480 IF (B-BMAX) 1520,1520,1490                                       GES      82
247     1490  B=BMAX                                                          GES      83
251     1500 W2=B*(1.0+Y(3))                                                  GES      84
254     1510 CALL WR (3,L,W2)                                                 GES      85
262     1520 W1=B*(1.0+Y(1))                                                  GES      86
265     1530 CALL WR(3,L,W1)                                                  GES      87
273     1540 IF ((W1(3)- ABS(CH(2)))/THETA-EPS) 1550,1600,1600                GES      88
301     1550 IF (B-BMAX) 1450,1600,1600                                       GES      89
       C1596                                  FINISH                          GES      90
304     1600 KE2=KE1+KE2                                                      GES      91
306     1610 L(4)=KE2/L(3)                                                    GES      92
       C1696                                                                  GES      93
       C1698                              INTEGRATE                           GES      94
312     2000 DO 2010 I=1,7                                                    GES      95
317     2010 S(I)=0.0                                                         GES      96
       C2048                                                                  GES      97
```

```
323    2050 DO 2550 IG=1,16                                                                GES      98
325    2060 IF(IG-14) 2100,2070,2100                                                       GES      99
327    2070 DO 2080 I=1,5                                                                  GES     100
334    2080 W(I)=W2(I)                                                                     GES     101
340    2082 KE=17-IG                                                                       GES     102
342    2090 GO TO 2400                                                                     GES     103
343    2100 IF(IG-16)2150,2110,2150                                                        GES     104
345    2110 DO 2120 I=1,5                                                                  GES     105
352    2120 W(I)=W1(I)                                                                     GES     106
356    2122 KE=17-IG                                                                       GES     107
360    2130 GO TO 2400                                                                     GES     108
      C                                                                                    GES     109
361    2150 IF(IG-8) 2160,2160,2200                                                        GES     110
364    2160 X=B*(1.0-Y(IG))                                                                GES     111
370    2170 KE=IG                                                                          GES     112
372    2180 GO TO 2300                                                                     GES     113
      C2198                                                                                GES     114
373    2200 KE=17-IG                                                                       GES     115
375    2210 X=B*(1.0+Y(KE))                                                                GES     116
      C2298                                                                                GES     117
401    2300 CALL WR(3,L,W)                                                                 GES     118
      C2398                                          CALC. INTEGRANDS                      GES     119
407    2400 E(1)=A(KE)*W(2)* EXP(-W(3)/THETA)                                              GES     120
421    2410 E(2)=W(4)*E(1)                                                                 GES     121
423    2420 E(3)=W(3)*E(1)                                                                 GES     122
425    2430 E(4)=W(4)*E(2)                                                                 GES     123
427    2440 E(5)=W(3)*E(3)                                                                 GES     124
431    2450 E(6)=W(3)*E(2)                                                                 GES     125
433    2460 E(7)=W(5)*E(1)                                                                 GES     126
      C2498                                                                                GES     127
435    2500 DO 2510 I=1,7                                                                  GES     128
442    2510 S(I)=E(I)+S(I)                                                                 GES     129
      C          ---NOTE - SUM S(I) IS 1/2 INTEGRAL                                        GES     130
      C2538                                                                                GES     131
447    2540 IF (L(5)) 4200,2550,4200                                                       GES     132
450    2550 CONTINUE                                                                       GES     133
      C2994                                                                                GES     134
      C2996                              CALC OUTPUT                                       GES     135
      C2998                                    INTEGRALS                                   GES     136
452    3000 DO 3010 I=2,7                                                                  GES     137
457    3010 S(I)=S(I)/S(1)                                                                 GES     138
464    3020 TM=1./THETA                                                                    GES     139
466    3030 S(1)= 2.0*B*S(1)                                                               GES     140
471    3032 G(12)=TM*CH(3)                                                                 GES     141
473    3040 G(3)=1.0+G(12)-TM*S(2)                                                         GES     142
477    3042 G(13)=-TM*CH(2)                                                                GES     143
501    3050 G(4)=G(13)+TM*S(3)                                                             GES     144
504    3052 G(14)=8.8857662*S(1)                                                           GES     145
506    3060 G(6)=1.0+G(13)-ALOG(G(14))                                                     GES     146
516    3070 IF(G(3))3080,3080,3100                                                         GES     147
520    3080 CALL PRIN(14HGES NEG. KAP $,1,G(3))                                            GES     148
525         CALL PRIN(4HTAU$,1,TAU)                                                        GES     149
533    3090 GO TO 3110                                                                     GES     150
534    3100 G(6)=G(6)-ALOG(G(3))                                                           GES     151
542    3110 E2=TM*TM                                                                       GES     152
544    3120 G(9)=1.0-E2*(S(6)-S(3)*S(2))                                                   GES     153
551    3130 G(10)=TM*CH(4)+E2*(S(4)-S(2)**2-THETA*S(7))                                    GES     154
560    3140 G(11)=E2*(S(5)-S(3)**2)                                                        GES     155
      C                                                                                    GES     156
563    3150 G(5)=G(4)+G(3)-1.0                                                             GES     157
```

```
567     3160 G(7)=G(6)+G(3)-1.0
573     3170 G(8)=G(4)-G(6)
       C
575     3200 DO 3210 I=3,15
602     3210 GM(I)=G(I)
606     3220  IF( L(5)) 4300,5000,4300
       C3094
       C3096                          DIAGNOSTIC PRINT
       C3098
610     4000 CALL PRIN (28H GES DIAG. -TAU,THETA,B     $,0,B)
616     4010 E(1)=TAU
620     4020 E(2)=THETA
622     4030 E(3)=B
624     4040 CALL PRIN (2H $,3,E)
632     4050 GO TO 1200
633     4100 CALL PRIN (2HB$,1,B)
641     4110 GO TO 1250
642     4150 CALL PRIN (2HB$,1,B)
650     4160 GO TO 1474
651     4200 DO 4210 I=1,7
661     4210 E(I)=E(I)/A(KE)
665     4220 E(8)=IG
667     4230 E(9)=X
671     4240 E(10)=W(3)
673     4250 CALL PRIN(7HI,X,W $,3,E(8))
700          CALL PRIN(7HINTS  $,7,E)
706     4260 GO TO 2550
707     4300 CALL PRIN(7HG(OUT)$,15,G)
712          CALL PRIN(7HS(INT)$,S)
       C4090
717     5000 RETURN
720          END


             SUBROUTINE WR(K,L,D)
       C                              GES CELL POTENTIAL
 10       20 DIMENSION CC(6),C(6),WN(6),WC(6),W(6)
            1             ,KFPS(2),NMAX(2),F(6),A(60),AL(30),D(7),L(6)
 10       30 EQUIVALENCE (WN,CC(7)),(KONE,ONE),(KY,Y)
            1             ,(A(31),AL)
 10      200 GO TO (1000,2000,3000),K
       C 090
       C 094                          PRELIM. ENTRY
       C 096
       C 098                                         SET POT. AND EQUIV. ARGS
 17     1000 DO 1004 I=1,6
 21     1002 W(I)=0.0
 23     1004 C(I)=0.0
 25     1006 M=30
 26     1010 GO TO (1020,1040,1060),L
 35     1020 KA=1
 36     1022 KR=1
 37     1030 GO TO 1100
 40     1040 KA=2
 41     1042 KR=2
 42     1050 GO TO 1100
 43     1060 KA=1
 44     1062 KR=2
       C1070
       C
```

```
 45    1100 FN=D(1)                                                        WR        28
 46    1110 FM=D(2)                                                        WR        29
 50    1120 AN=D(3)                                                        WR        30
 52    1130 AM=D(4)                                                        WR        31
      C1190                                                                WR        32
      C1194                                REPULSIVE PART                  WR        33
 54    1200 IF (AN) 1800,1800,1210                                         WR        34
      C                                                                    WR        35
 56    1210 G=FN                                                           WR        36
 60    1212 GB=FM                                                          WR        37
 62    1220 AG=AN                                                          WR        38
 64    1230 KB=KR                                                          WR        39
 66    1240 KQ=1                                                           WR        40
      C1290                                                                WR        41
      C1294                                   CALC.                        WR        42
 67    1300 BB= 12.0*GB/(FN-FM)                                            WR        43
 73    1310 AA=-AG*BB/2.0                                                  WR        44
      C1320                                                                WR        45
 76    1330 GO TO (1350,1650),KB                                           WR        46
      C1344                                                                WR        47
      C1348                                      LJ                        WR        48
104    1350 J=(KQ-1)*M                                                     WR        49
110    1352 KE1=J+M                                                        WR        50
112    1360 A(KE1)=G *(G -1.0)/6.0                                         WR        51
117    1370 E=A(KE1)/4.0                                                   WR        52
122    1380 E1=1.0E-7*E                                                    WR        53
      C1394                                                                WR        54
124    1400 DO 1480 I=2,M                                                  WR        55
126    1410 KE=KE1+1-I                                                     WR        56
131    1420 E2=2*(I-1)                                                     WR        57
134    1440 E3=(G +E2)*((G +E2)-1.0)/((E2+3.0)*(E2+2.0))                   WR        58
144    1450 A(KE)=E3*A(KE+1)                                               WR        59
147    1460 E=E3*E/4.0                                                     WR        60
152    1470 IF(E1-E)1480,1480,1510                                         WR        61
155    1480 CONTINUE                                                       WR        62
      C1498                                                                WR        63
160    1500 CALL FIO (3HWOT,                                               WR        64
           1  53H (1H0,12X,32H A-DIM. TOO SMALL, A30*1/4**30= 1PE15.7),    WR        65
           21,A(J+1),0)                                                    WR        66
      C1508                                                                WR        67
171    1510 NMAX(KQ)=I                                                     WR        68
173    1520 KEPS(KQ)=-ALOG(1.0E-7*A(KE1)/A(KE))/0.6931                     WR        69
      C1544                                                                WR        70
206    1550 J=(KQ-1)*3                                                     WR        71
211    1560 CC(J+1)=AA                                                     WR        72
213    1570 CC(J+2)=-AA*G/3.0                                              WR        73
217    1580 CC(J+3)=-CC(J+2)*G/3.0                                         WR        74
223    1590 WN(J+1)=BB                                                     WR        75
225    1600 WN(J+2)=-BB*G/3.0                                              WR        76
231    1610 WN(J+3)=-WN(J+2)*G/3.0                                         WR        77
235    1620 GO TO 1750                                                     WR        78
      C1644                                                                WR        79
      C1646                                      EXP                       WR        80
236    1650 J=(KQ-1)*3                                                     WR        81
241    1660 CC(J+1)=AA                                                     WR        82
243    1670 CC(J+2)=-AA/3.0                                                WR        83
246    1680 CC(J+3)=AA/9.0                                                 WR        84
251    1690 WN(J+1)=BB                                                     WR        85
253    1700 WN(J+2)=BB  /3.0                                               WR        86
256    1710 WN(J+3)=BB  /9.0                                               WR        87
```

```
      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
```

```
461    2450 GO TO (2500,2600),KQ
      C2494
      C2494.
      C2496                                            ATTRACTIVE PART
467    2500 IF (AM) 2600,2600,2510
471    2510 G=FM
473    2520 KB=KA
475    2530 KQ=2
476    2540 GO TO 2050
      C2594
      C2596                                            WHOLE
477    2600 D(2)=C(1)-C(4)
502    2610 D(3)=C(2)-C(5)
505    2620 D(4)=C(3)-C(6)
510    2630 IF(L(6))4100,5000,4100
      C2990
      C2992
      C2994                                  MAIN ENTRY FOR CELL POTENTIAL
      C2996
      C2998                                            REPULSIVE PART
512    3000 X=D(1)
513    3002 D(2)=X**2
515    3004 IF (AN) 3600,3600,3010
517    3010 KB=KR
521    3020 KQ=1
      C3030
      C3040                                                 CALC.
522    3050 GO TO (3060,3300),KB
      C3054
      C3056                                                     LJ
530    3060 UNF=1.0
532    3070 Y=D(2)
534    3080 KK=(KONF-KY-1)/512
541    3090 N=2*KEPS(KQ)/KK
546    3100 NN= MIN0  (N,NMAX(KQ))
552    3110 GO TO (3150,3200),KQ
      C3144
560    3150 KE=M+1-NN
563    3160 F(1)=A(KE)*Y
566    3162 KE=KE+1
570    3170 DO 3180 I=KE,M
575    3180 F(1)=(F(1)+A(I))*Y
602    3190 GO TO 3250
      C3194
603    3200 KE=M+1-NN
606    3210 F(4)=AL(KE)*Y
611    3220 KE=KE+1
613    3230 DO 3240 I=KE,M
620    3240 F(4)=(F(4)+AL(I))*Y
      C3244
625    3250 J=(KQ-1)*3
630    3260 W(J+1)=WC(J+1)*F(J+1)
633    3270 W(J+2)=WC(J+2)*F(J+1)
636    3280 W(J+3)=WC(J+3)*F(J+1)
641    3290 GO TO 3550
      C3294
      C3296                                                     EXP
642    3300 J=(KQ-1)*M
646    3310 E=A(J+1)*X
651    3320 E1= EXP(E)/2.0
```

```
 657    3330 E2=0.25/E1
 661    3340 FC=(E1+E2)
 663    3350 FS=(E1-E2)
 665    3360 IF (E-0.1)3370,3370,3450
 670    3370 E1=E*E
 672    3380 E2=E1*E1
 674    3390 FSS=1.0+E1/6.0+E2/120.0
 701    3400 GO TO 3452
       C3444
 702    3450 FSS=FS/E
 704    3452 FS=X*FS
       C3454
 706    3460 I=(KQ-1)*3
 711    3462 F(I+1)=A(J+3)*FSS-A(J+2)*FC-1.0
 720    3470 F(I+2)=A(J+4)*FSS-FS*A(J+5)*FC+A(J+1)
 730    3480 F(I+3)=A(J+6)*FSS+A(J+7)*FS
             1            +(A(J+8)-A(J+1)*D(2))*FC+A(J+9)
 743    3490 J=I
       C3494
 745    3500 W(J+1)=WC(J+1)*F(J+1)
 750    3510 W(J+2)=WC(J+2)*F(J+2)
 753    3520 W(J+3)=WC(J+3)*F(J+3)
       C3544
 756    3550 GO TO (3600,3650),KQ
       C3594
       C3596                                    ATTRACTIVE PART
 764    3600 IF (AM) 3610,3650,3610
 765    3610 KB=KA
 767    3620 KQ=2
 770    3630 GO TO 3050
       C3644
       C3646 FINISH
 771    3650 U(3)=W(1)-W(4)
 774    3660 U(4)=W(2)-W(5)
 777    3670 U(5)=W(3)-W(6)
1002    3680 IF(L(6))4200,5000,4200
       C3992
       C3994                            DIAGNOSTIC PRINT
       C3996
       C3998                                    PRELIM
1004    4000 CALL PRIN(13HPREL. WR  CC$,6,CC)
1007         CALL PRIN(3HWN$,6,WN)
1014    4010 IF (L(1)-2)4020,4030,4020
1016    4020 CALL PRIN(2HA$,30,A)
1021         CALL PRIN(3HAL$,30,AL)
1026    4030 GO TO 5000
       C4098                                    MAIN INITIAL
1027    4100 CALL PRIN(13HMAIN WR  C  $,6,C)
1032         CALL PRIN(3HWC$,6,WC)
1037    4120 IF (L(1)-1)4130, 4140,4130
1041    4130 CALL PRIN(2HA$,9,A)
1044         CALL PRIN(4HAL $,9,AL)
1051    4140 GO TO 5000
       C4194                                    MAIN INTEGRATE
1052    4200 CALL PRIN(2HF$,6,F)
1055         CALL PRIN(13HW (WR ROUT) $,6,W)
1062    4210 GO TO 5000
       C4994
1063    5000 RETURN
       C
```

```
1064        END                                                                 WR
                                                                       
            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 LJD.                              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 LJD, 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,KIM   (          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*
 67      230 GM(10)=-(1.0+BET*X)*XE                                                 HK*
 73      240 GM(11)=GM(4)*(2.0-(1.0+ALP*(1.0+BET*X))*T/(T+TH) )                     HK*
105      250 GM(5)=GM(4)*XE                                                         HK*
107      260  GM(7)=GM(6)*XE                                                        HK*
111      270 GM(8)=GM(5)-GM(7)                                                      HK*
       C                                                                            HK*
113      400 GO TO 2000                                                             HK*
       C------------------------------- K=2, MUS ---------------------------------- HK*
114      500 DO 510 I=1,KR                                                          HK*
123      510 AMU(I)=GM(5)+(XPG(I)/HK-1.0)*XE                                        HK*
       C                                                                            HK*
       C 520             NOTE- GEM MOVES F/RI FROM GM(7) TO GM(5)                   HK*
       C                                                                            HK*
131     2000 RETURN                                                                 HK*
132          END                                                                    HK*


             SUBROUTINE SEM (K,L)                                                   SEM
       C                                                                            SEM
       C                           SOLID EQ. OF STATE ADAPTOR                       SEM
       C                                                                            SEM
       C                                        REVISION 1 - FOR NEW SEMS CODE      SEM
       C                                                  W.F. 10/61                SEM
       C                                                                            SEM
       C                                                                            SEM
       C     SEM                                                                    SEM
                                                                                    SEM
  6          COMMON Z(4000)                                                         SEM
  6          DIMENSION                                                              SEM
            1 KEN    (      6,     10),KUN    (      6,     10),CAR    (     10,     8) SEM
            2,CONT   (             20),EV     (             20),FUB    (      6,    10) SEM
            3,KAL    (             20),KEV    (             20),SP     (            20) SEM
            4,SPC    (             20),SM     (             20),TMS    (            20) SEM
            5,THER   (             50)                                                SEM
  6          DIMENSION CE(10)                                                       SEM
  6          EQUIVALENCE                                                            SEM
            1 (Z( 1620),KEN    ) ,(Z( 1690),KUN    ) ,(Z(  920),CAR    )            SEM
            2,(Z(  460),CONT   ) ,(Z(  680),EV     ) ,(Z( 1410),FUB    )            SEM
            3,(Z( 1600),KAL    ) ,(Z(  900),KEV    ) ,(Z( 1840),SP     )            SEM
            4,(Z( 1860),SPC    ) ,(Z( 1820),SM     ) ,(Z( 1990),TMS    )            SEM
            5,(Z( 1920),THER   )                                                    SEM
       C                                                                            SEM
       C                                        LOCAL EQ                            SEM
       C                                                                            SEM
  6          EQUIVALENCE (CAR(51),CE),(CONT(2),R)                                   SEM
            1            ,(THER(1),P),(THER(3),T),(SM(1),VS)                        SEM
  6          GO TO (1000,10),K                                                      SEM
       C 994                                                                        SEM
       C 996                        PRELIMINARY                                     SEM
       C 998                                                                        SEM
 13     1000 CALL REAP (                                                            SEM
            1  54H0X      G, CPR, AL, V0, T0, EOR / C0, C1, C2, C3, C4  S           SEM
            2  ,12,SP)                                                              SEM
 20     1001 KAL(4)=1                                                               SEM
 21     1002 IF(SP(2))1004,1003,1004                                                SEM
 22     1003 KAL(4)=0                                                               SEM
       C                                                                            SEM
 23     1004 CALL SEMS(1)                                                           SEM
 27     1006 SM(9 )=0.8                                                             SEM
```

```
      C
 31    1010 CALL DOUT (3HSEM,1)
 36    1020 GO TO 300
      C1098
      C
      C                          SES MAIN
 37         10 KEN(2)=KEN(2)+1
 41         20 IF (KAL(4)) 40,100,40
      C
 42         40 CALL SEMS(2)
      C
 46         50 GO TO 200
      C
      C                          CALC. INCOMPRESSIBLE SOLID OUTPUT
 47        100 SM(9)=1.0
 51        102 SM(10)=1.0
 53        104 SM(1)=SP(4)
 55        106 SM(2)=0.0
 56        108 SM(3)=P*VS/(R*T)
 62        110 SM(4)=0.0
 63        112 SM(5)=SM(3)
 65        114 SM(6)=0.0
 66        116 SM(7)=SM(3)
 70        118 SM(8)=P
 72        200 CALL DOUT (3HSEM,2)
 77        300 RETURN
      C            ARGS   K=1, PREL.
      C                   K=2, MAIN
      C                   L=1, ISOTHERM
      C                   L=2, ISENTROPE
      C
      C       SPECS
      C            INPUT
      C                   SP     SEPS INPUT (SEE SEPS)
      C                   SPC    SEPS OUTPUT (SEE SEPS)
      C                   T      TEMP
      C                   VS     -SOLID VOL
      C            OUTPUT
      C                   SM     SES IMPERFECTION THERMO FNS-SEE SEMS
      C                            HERE E,H,A,F,S FOR T,P=1 ATM HAVE BEEN
      C                            SUBTRACTED TO FORM IMPERFECTION FNS.
      C
100           END

              SUBROUTINE SEMS (K)
      C
      C                   NEW SES SUBROUTINE
      C                          WITH SINGLE ITERATION FOR V(P,T)
      C                          INPUT - P,T
      C                          OUTPUT - V AND SES IMP. THERMO FNS
      C                          K=1 FOR PREL
      C                          K=2 FOR MAIN
      C
      C       W. F. -10/61
      C
      C

  3           COMMON Z(4000)
```

```
  3        DIMENSION                                                      SEMS      16
          1 CAR    (     10,     8),EV    (            20),FOB   (     6,   10) SEMS      17
          2,KON    (      6,    10),SM    (            20),SP    (          20) SEMS      18
          3,THER   (            50)                                          SEMS      19
  3        DIMENSION C(5),CN(5),CG(5),CG1(5),CS(10) , KCS(2)               SEMS      20
  3        EQUIVALENCE                                                     SEMS      21
          1 (Z(  920),CAR   ) ,(Z(  680),EV    ) ,(Z( 1410),FOB   )        SEMS      22
          2,(Z( 1690),KON   ) ,(Z( 1820),SM    ) ,(Z( 1840),SP    )        SEMS      23
          3,(Z( 1920),THER  )                                              SEMS      24
      C                                                                   SEMS      25
      C                                                                   SEMS      26
      C                    #ARGUMENTS#                                    SEMS      27
  3        EQUIVALENCE                                                     SEMS      28
          1        (THER(1),P),(THER(3),T)                                 SEMS      29
          2        ,(FOB(11),FOBI),(FOB(23),YL),(KON(47 ),KONI)            SEMS      30
          3        ,(CAR(41),CS),(CS(8),KCS)                               SEMS      31
          4        ,(EV(1),E1),(EV(2),E2)                                  SEMS      32
      C                                                                   SEMS      33
      C                                                                   SEMS      34
      C                                                                   SEMS      35
  3        EQUIVALENCE                                                     SEMS      36
          1        (SP(1),G),(SP(3),ALPH),(SP(4),V0),(SP(5),T0)            SEMS      37
          2        ,(SP(8),C),(SP(13),A),(SP(14),G1)                       SEMS      38
          3        ,(SP(15),G2),(SP(16),CONST)                             SEMS      39
          4        ,(SP(18),CN),(SP(24),CG),(SP(30),CG1)                   SEMS      40
          5        ,(SM(9),Y),(SM(10),Y1),(SM(11),TC)                      SEMS      41
          6        ,(SM(12),T1),(SM(13),PH),(SM(15),WEEG)                  SEMS      42
          7        ,(SM(16),P2),(SM(17),Y11),(SM(18),X)                    SEMS      43
          8        ,(SM(19),YU)                                            SEMS      44
      C                                                                   SEMS      45
      C                                                                   SEMS      46
      C                                                                   SEMS      47
  3     20 GO TO (100,1000),K                                              SEMS      48
      C                        PRELIM                                     SEMS      49
      C                                                                   SEMS      50
 11    100 R=8.31439E-5                                                    SEMS      51
 13    102 A=(R*SP(2)/(ALPH*V0))*(G/(G+1.0))                               SEMS      52
 22    110 G1=1.0/(G+1.0)                                                  SEMS      53
 25    120 G2=0.5+1.0/G                                                    SEMS      54
      C                                                                   SEMS      55
 31    150 CN(1)=G1                                                        SEMS      56
 33    160 DO 180 I=2,4                                                    SEMS      57
 35    170 FI=I                                                            SEMS      58
 36    180 CN(I)= CN(I-1)*(G1-(FI-1.0))/FI                                 SEMS      59
      C                                                                   SEMS      60
 45    200 DO 230 I=1,5                                                    SEMS      61
 47    210 FI=I-1                                                          SEMS      62
 52    220 CG(I)=C(I)/(G+FI)                                               SEMS      63
 56    230 CG1(I)=C(I)/(G+FI+1.0)                                          SEMS      64
      C                                                                   SEMS      65
 64    250 E1=0.0                                                          SEMS      66
 65    260 E2=0.0                                                          SEMS      67
 66    270 DO 290 I=1,5                                                    SEMS      68
 70    280 E1=E1+CG(I)                                                     SEMS      69
 73    290 E2=E2+CG1(I)                                                    SEMS      70
 76    300 CONST=0.5*E1-G2*E2                                              SEMS      71
      C                                                                   SEMS      72
102        GO TO 2000                                                      SEMS      73
      C                                                                   SEMS      74
      C                        MAIN                                       SEMS      75
```

```
      C                                                                      SEMS    76
103    1000 CS(4)=Y                                                          SEMS    77
105    1020 CS(2)=Y*FOBI                                                     SEMS    78
107    1030 YU=1.0+ALPH*(T-T0)                                               SEMS    79
113    1040 KCS(1)=0                                                         SEMS    80
      C                                                                      SEMS    81
      C                                        ITERATE ON Y=V/V0             SEMS    82
114    1100 CALL FROOTT (CS,KONI)                                            SEMS    83
120    1110 KEXIT=KCS(2)                                                     SEMS    84
122    1120 GO TO (1500,1150,1130,1140),KEXIT                                SEMS    85
132    1130 CALL DBUG (4HSEMS,1)                                             SEMS    86
136    1132 GO TO 1500                                                       SEMS    87
137    1140 CALL DBUG (4HSEMS,1)                                             SEMS    88
143    1142 GO TO 1500                                                       SEMS    89
      C                                        FUNCTION                      SEMS    90
144    1150 IF (CS(2)-YU) 1180,1180,1160                                     SEMS    91
147    1160 CS(2)=YU                                                         SEMS    92
151    1170 GO TO 1200                                                       SEMS    93
152    1180 IF (YL-CS(2)) 1200,1200,1190                                     SEMS    94
155    1190 CS(2)=YL                                                         SEMS    95
      C                                                                      SEMS    96
157    1200 Y=CS(2)                                                          SEMS    97
      C                                            CALC. P2(Y)               SEMS    98
161    1210 PH=C(5)                                                          SEMS    99
163    1220 E1=CG(5)                                                         SEMS   100
165    1230 E2=CG1(5)                                                        SEMS   101
167    1250 DO 1290 I=1,4                                                    SEMS   102
171    1260 KE=5-I                                                           SEMS   103
173    1270 PH=PH*Y+C(KE)                                                    SEMS   104
176    1280 E1=E1*Y+CG(KE)                                                   SEMS   105
201    1290 E2=E2*Y+CG1(KE)                                                  SEMS   106
      C                                                                      SEMS   107
206    1300 WEEG=(0.5-G2*Y)*PH                                               SEMS   108
212    1310 YG=Y**G                                                          SEMS   109
      C                                                                      SEMS   110
216    1320 P2=-(G/Y)*WEEG+G*(G/Y)*                                          SEMS   111
          1           (0.5*E1-G2*Y*E2-CONST/YG)                              SEMS   112
      C                                                                      SEMS   113
      C                                            CALC Y1, Y11, SEPARATE ON Y SEMS 114
231    1350 IF (Y-1.0) 1700,1800,1800                                        SEMS   115
      C                                                                      SEMS   116
      C                                                                      SEMS   117
      C                                                                      SEMS   118
235    1400 CS(3)=2.0E-6*(TC-T)                                              SEMS   119
      C                                                                      SEMS   120
240    1470 CALL DOUT (4HSEMS,1)                                             SEMS   121
244    1480 GO TO 1100                                                       SEMS   122
      C                                                                      SEMS   123
      C                                        CALCULATE OUTPUT              SEMS   124
245    1500 SM(1)=Y*V0                                                       SEMS   125
247    1510 SM(7)=P*SM(1)/(R*T)                                              SEMS   126
253    1520 SM(3)=(1.0+1.0/G)*SM(7)+V0*WEEG/(R*T)-SP(2)*(1.0-T0/T)           SEMS   127
265    1530 SM(6)=SP(2)*ALOG(T1/T)                                           SEMS   128
274    1540 SM(5)=SM(3)-SM(6)                                                SEMS   129
276    1550 SM(2)=SM(3)-SM(7)                                                SEMS   130
300    1560 SM(4)=SM(5)-SM(7)                                                SEMS   131
302    1572 GO TO 2000                                                       SEMS   132
      C                                                                      SEMS   133
      C                                                                      SEMS   134
      C                                        CALC. FN. FOR Y LESS THAN 1   SEMS   135
```

```
      C                                                                                  SEMS     136
303    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( 1590),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  60H0X  KS,KN/ T BOUNDS/ FIT COEFFS.-A1 TO AN,D,DEL,HF,HR...S    TIM       32
          2 ,-2,KE)                                                          TIM       33
 14              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
      C1096                                                                  TIM       43
      C1098                                   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,IMS,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
```

```
       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             DC 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
```

```
314    430           GI(9)=S(1)+PLOG                                          TIPS      92
316    440 GI(10)=F(1)-PLOG                                                   TIPS      93
320    450 GI(11)=A(1,N+4)                                                    TIPS      94
323    460 GI(12)=H(1)-(T0/T)*A(1,N+5)+GI(11)/(R*T)                           TIPS      95
334    470           F(1)=GI( 0)                                              TIPS      96
     C 500 I(E)                                  STORE GI                     TIPS      97
336    510           DO 520 I=1,12                                            TIPS      98
343    520           G(I)=GI(I)                                               TIPS      99
350    600           RETURN                                                   TIPS     100
351          END                                                              TIPS     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 EQ,DIM                                                     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
```

```
          4,(EA(21),SXG),(EA(41),SXF)
        C
  6      80 GO TO (100,800),K
        C - - - - - - - - - - - - - - - - - - - -PRELIM - - - - - - - - - - -
 14     100 CALL READ (
          154H0X KR,KAL/ SCR,SCT,R*REF,T*REF,N,M/ (R*)/ (T*)   S
          1 ,-2,KE)
 17         CALL READ(0,6,E1)
 22         CALL READ(0,KE,XPR)
 25         CALL READ(0,KE,XPT)
 32     110 KR=KE(1)
 34     120 KAL(5)=KE(2)
 36     130 DO 150 I=1,KR
 40     140 XPR(I)=XPR(I)*E1(1)
 43     150 XPT(I)=XPT(I)*E1(2)
        C 160
 46     170 DO 200 I=1,KR
 50     180 DO 200 J=1,KR
 52     190 XPG(I,J)=(XPR(I)+XPR(J))/2.0
 60     200 XPF(I,J)= SQRT (XPT(I)*XPT(J))
        C 208
 75     210 XMT(11)=E1(3)
 77     220 XMT(12)=E1(4)
101     230 XMT(13)=E1(5)
103     240 XMT(14)=E1(6)
105     250 IF (KAL(5)-9) 300,260,300
107     260 DO 270 I=1,KR
115     270 XPG(I)=E1(3)*CONT(5)*XPR(I)**3
121     300 GO TO 6000
        C---------------------------------- MAIN ---------------------------
122     800 KE=KAL(5)+1
124     802 KEM(4)=KEM(4)+1
        C                          CHECK FOR KIASTOWSKY-WILSON
126     804 IF (KAL(5)-9) 810,806,810
130     806 CALL GEP(1)
134     808 CALL FKW(2)
        C
140     809 GO TO 1100
        C
141     810 GO TO (1000,2000,3000,4000,4000),KE
        C-------------------------------------------------------------------
        C 999                      NO MIX (ZERO)
        C 998
152     1000 GO TO (1020,6000,1100),L
        C1010                                NO MIX-ONE
161     1020 CALL GEP(1)
165     1030 DO 1040 I=1,KR
172     1040 XMU(I)=GM(5)
174     1050 GO TO 6000
        C1098                                NO MIX-THREE
        C                                          MIXTURE=REF. FLUID
175     1100 XMT(1)=GM(15)
177     1110 XMT(2)=GM(4)
201     1120 XMT(3)=GM(17)
203     1130 XMT(4)=GM(20)
205     1140 XMT(5)=GM(5)
207     1150 XMT(6)=GM(11)
211     1160 XMT(7)=GM(10)
213     1170 XMT(8)=GM(9)
215     1180 GO TO 6000
```

```
      C-------------------------------------------------------------------------------- XIM      110
      C1099                          IDEAL MIXING (ONE)                                   XIM      111
      C1098                                                                               XIM      112
216    2000 GO TO (2020,6000,2200),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 AMU(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 2260 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
      C2099                          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    3320 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
```

```
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,XMU    (    20) ,XMT   (    30) ,EV     (    20)             XIMS      15
  3        DIMENSION BILK(15)                                            XIMS      16
  3        DIMENSION SXG(20),SXF(20),SHN(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),XMU    ) ,(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,MFOR 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),SHN),(EA(81),STN)           XIMS      32
       C                                                                 XIMS      33
       C  90                         CALCULATE BAR= T*,R* / MOD 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 LH)        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
```

```
 50     500 DO 550 I=1,KR
 62     510 DO 530 J=1,KR
 64     520 SXF(I)=FMX(J+1)*XPF(I,J)*XPG(I,J)**BILK(14)    +SXF(I)
 77     530 SXG(I)=FMX(J+1)*XPF(I,J)*XPG(I,J)**BILK(15)      +SXG(I)
113     540 EV(11)=FMX(I+1)*SXF(I)+EV(11)
116     550 EV(12)=FMX(I+1)*SXG(I)+EV(12)
123     600 E3=1.0/(BILK(14)-BILK(15))
126     610 E4=BILK(14)*E3
130     620 E5=BILK(15)*E3
132     630 TSTAT=EV(12)**E4/EV(11)**E5
142     640 RSTAT=(EV(11)/EV(12))**E3
      C                                   REJOIN-CALC. VSTA
147     700 VSTAT=CONT(5)*RSTAT**3
      C 800
      C 810                        CALC MUS IF K=1
152    1000 IF (K)1010,1500,1010
      C
153    1010 CALL GEP(2)
      C1090                               I-BRANCH- CS OR 1-FLUID
      C                                                LH
156    1100 GO TO (1500,1150,1200,1300),KW
166    1150 DO 1160 I=1,KR
175    1160 XMU(I)=GM(5)
          1       +GM(4)*(2.0*(SXF(I)/XMT(12)-1.0)-(TSTAT/TSTA-1.0))
          2       +3.0*GM(10)*(2.0*(SXG(I)/XMT(11)-1.0)-(RSTAT/RSTA -1.0))
216    1170 GO TO 1500
      C1190                                            CS
217    1200  DO 1220 I=1,KR
221    1210 STN(I)=2.0*(SXF(I)/TSTAT-1.0)
224    1220 SRN(I)=2.0*(SXG(I)/RSTAT-1.0)
234    1230 GO TO 1400
      C1290                                            ONE-FLUID
235    1300 DO 1320 I=1,KR
237    1310 STN(I)= -2.0-2.0*E3*(BILK(15)*SXF(I)/EV(11)
          1           -BILK(14)*SXG(I)/EV(12))
251    1320 SRN(I)= 2.0*E3*(SXF(I)/EV(11)-SXG(I)/EV(12))
      C1390                               REJOIN FOR MU CALC.
261    1400 DO 1410 I=1,KR
270    1410 XMU(I)=XMT(5)+3.0*XMT(7)*SRN(I)+XMT(2)*STN(I)
277    1500 RETURN
300         END


            SUBROUTINE EQP
      C                       EQ PRELIMINARY
      C          REVISION  1 ERROR IN STATEMENT 520
      C              LOOP GOES TO KS, NOT 10
      C                  W.F.  3/60
      C
      C     EQP

  1         COMMON Z(4000)
  1         DIMENSION
           1 EPAL  (     20,      6),EPA    (            20),EPA1   (             20)
           2,EPC   (             10),EPW    (            10),FLAB   (     12,      8)
           3,KAL   (             20),KIM    (            10),KON    (      6,     10)
  1         DIMENSION KEPA(20),KEPA1(20),KEPAL(20,6),KEPC(10)
  1         DIMENSION KE1(12),L(12)
  1         EQUIVALENCE
           1 (Z( 1210),EPAL  ) ,(Z( 1190),EPA   ) ,(Z( 1330),EPA1  )
```

```
           2,(Z( 1350),EPC    ) ,(Z( 1360),EPQ    ) ,(Z( 3100),FLAB  )        EQP      19
           3,(Z( 1600),KAL    ) ,(Z( 1680),KIM    ) ,(Z( 1690),KON   )        EQP      20
      C                                                                       EQP      21
  1          EQUIVALENCE (KIM(2),KS),(KIM(3),KC)                              EQP      22
           2            ,(EPA,KEPA),(EPA1,KEPA1),(EPAL,KEPAL)                 EQP      23
           3            ,(EPC,KEPC)                                           EQP      24
      C                                                                       EQP      25
  1          EQUIVALENCE (FLAB(49),L)                                         EQP      26
      C                                                                       EQP      27
      C                                                                       EQP      28
  1       80 KAL(6)=1                                                         EQP      29
  2      100 CALL READ (                                                      EQP      30
           1   30H0X    C,S,P,-,PP,PHI / CAP Q  $                             EQP      31
           2 ,-6,KEPC)                                                        EQP      32
  5          CALL READ(0,KEPC,EPG)                                            EQP      33
 10      110 KC=KEPC(1)                                                       EQP      34
 12      120 KS=KEPC(2)                                                       EQP      35
 14      130 READ(10,140 )             (KE1(I),I=1,12)                        EQP      36
         140 FORMAT (12A6)                                                    EQP      37
 22      150 DO 160 I=1,KS                                                    EQP      38
 24      160 READ(10,170 )             L(I),(KEPAL(I,J),J=1,KC)               EQP      39
         170 FORMAT (A6,11I6)                                                 EQP      40
 46      180 READ(10,200 )             (KEPA(I),I=1,KS)                       EQP      41
 55      190 READ(10,200 )             (KEPA1(I),I=1,KS)                      EQP      42
         200 FORMAT (12I6)                                                    EQP      43
      C                                                                       EQP      44
 64      300 WRITE(9,310 )              (KE1(I),I=1,KS)                       EQP      45
         310 FORMAT (6H0      ,12A6/)                                         EQP      46
 73      320 DO 330 I=1,KS                                                    EQP      47
 75      330 WRITE(9,340 )              L(I),(KEPAL(I,J),J=1,KC)              EQP      48
           1                 ,KEPA(I),KEPA1(I)                                EQP      49
         340 FORMAT (6H       ,A6,11I6)                                       EQP      50
      C 490                                                                   EQP      51
124      500 DO 510 I=1,10                                                    EQP      52
131      510 EPC(I)=KEPC(I)                                                   EQP      53
133      520  DO 530 I=1,KS                                                   EQP      54
135      530 EPA(I)=KEPA(I)                                                   EQP      55
140      540 EPA1(I)=KEPA1(I)                                                 EQP      56
144      550 DO 570 I=1,KS                                                    EQP      57
146      560 DO 570 J=1,KC                                                    EQP      58
156      570 EPAL(I,J)=KEPAL(I,J)                                             EQP      59
163      580 KAL(6)=1                                                         EQP      60
      C 590                                                                   EQP      61
164      600 CALL EQPS(KON(1,8),EPC,EPQ,EPAL,EPAL(1,2),EPA,EPA1)              EQP      62
      C 690                                                                   EQP      63
174     1000 RETURN                                                           EQP      64
      C                                                                       EQP      65
175          END                                                              EQP      66


             SUBROUTINE EQM                                                   EQM       2
      C            EQUILIBRIUM COMPOSITION AND STATE AT T,P                   EQM       3
      C    INPUT                                                              EQM       4
      C      P,T=THER(1),(3). IMPLICIT FOR GEP VIA XIM-XIMS                   EQM       5
      C      SM - STATE OF SOLID                                              EQM       6
      C      IMG - IDEAL STATE                                                EQM       7
      C    OUTPUT                                                             EQM       8
      C      XI=EMX - (GAS) MOLE FRACTIONS                                    EQM       9
      C      XMT - GAS (MIXTURE) STATE                                        EQM      10
      C    VARIABLES                                                          EQM      11
```

```
      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),EV(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-FOR(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-RSTAT)-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



  24        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(  460),CONT  ) ,(Z( 1010),EMG   ) ,(Z( 1030),EMN   )          COUT
         2,(Z( 1170),EMX   ) ,(Z(  680),EV    ) ,(Z( 1390),FN    )          COUT
         3,(Z( 1370),FMU   ) ,(Z( 1530),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),U),(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(2),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),HGID),(TMS(4),SGID),(TMS(6),HHGID)            COUT
         1            ,(TMS(7),HSID),(TMS(9),SSID),(TMS(12),HHSID)          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*(HGID+XMT(3))+XS*(HSID+SM(3))                         COUT
 25    60 THER(20)=XG*(SGID+XMT(6))+XS*(SSID+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=BN*R*THER(20)                                                       COUT        63
 63      172 THER(14)=EV*(XG*(HMGID+XMI(3))+XS*(HMSID+SM(3)))                     COUT        64
 72      190 THER(2)=V/V0                                                          COUT        65
 74      200 Q=-HN*CALMB*(XG*HFG+XS*HFS)+HO+BN*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 FMU(I)=EMG(I)+E1                                                      COUT        74
135      270 FMU(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                                                                       POUT     34
  3      10 GO TO (100,180,300),K                                             POUT     35
      C   96                              LABELS                              POUT     36
      C   98                                                                  POUT     37
 12     100 WRITE(9,7100)                                                     POUT     38
 17     120 WRITE(9,7120)                                                     POUT     39
 24     140 WRITE(9,7130)                                                     POUT     40
 30         IF(N.EQ.0) GO TO 400                                              POUT     41
      C          --- SKIP PUNCH                                               POUT     42
 32     142 IF (KAL(11)) 400,150,400                                          POUT     43
      C                                                                       POUT     44
 33     150 WRITE(9,7150)               ((FLAB(J,I),J=1,12),I=1,4)            POUT     45
 50     160 WRITE(9,7160)                                                     POUT     46
 55     162 WRITE(9,7162)               (FLAB(I,5),I=1,KS)                    POUT     47
 65     164 WRITE(9,7164)                                                     POUT     48
 72     170 GO TO 400                                                         POUT     49
      C 176                               REG.PRINT                           POUT     50
      C 178                                                                   POUT     51
 73     180 KEN(9)=KEN(9)+1                                                   POUT     52
 75     200 WRITE(9,7200)               KEN(9)                                POUT     53
           1            , (THER(I),I=1,5),HE(1),THER(7)                       POUT     54
           2            , THER(8),THER(9),THER(13),(EMN(I),I=1,3),EMN(7)      POUT     55
124     230 WRITE(9,7210)               THER(15),THER(16),                    POUT     56
           1THER(20),THER(21),(FN(I),I=1,3),XMT(1),XMT(2),                    POUT     57
           2XMT(6),XMT(7),(FN(I),I=4,6),GM(15),GM(4),GM(11),                  POUT     58
           3GM(10),(FN(I),I=7,9),SM(1),SM(2),SM(6),SM(7),(FN(I),I=10,12)      POUT     59
           4 , (XMT(I+15 ), I=1,3)                                            POUT     60
210     240 CALL DOUT (4HPOUT,1)                                              POUT     61
213         IF(N.EQ.0) GO TO 400                                              POUT     62
      C          --- SKIP PUNCH                                               POUT     63
215     242 IF (KAL(11)) 400,250,400                                          POUT     64
      C                                                                       POUT     65
216     250 WRITE(9,7250)                                                     POUT     66
           1,HF(1),THER(1),THER(2),THER(3),THER(4),THER(5)                    POUT     67
           2,THER(8),THER(9),XMT(16),XMT(18),XMT(17),THER(7)                  POUT     68
           3,EMN(2),EMN(1),EMN(3),SM(1),XMT(1),THER(15)                       POUT     69
           4,(FN(I),I=1,12)                                                   POUT     70
271     260 GO TO 400                                                         POUT     71
      C 296                               DIFF. PRINT                         POUT     72
      C 298                                                                   POUT     73
272     300 WRITE(9,7300)               (THER(I),I=22,25)                     POUT     74
301     310 CALL DOUT (4HPOUT,2)                                              POUT     75
304         IF(N.EQ.0) GO TO 400                                              POUT     76
      C          ---SKIP PUNCH                                                POUT     77
306     312 IF (KAL(11)) 400,320,400                                          POUT     78
      C                                                                       POUT     79
307     320 WRITE(9,7320)                                                     POUT     80
           1THER(22),THER(23),THER(24),THER(25),THER(27)                      POUT     81
326     400 RETURN                                                            POUT     82
       7100 FORMAT (1H0,7X,13HOUTPUT LABELS//12X,1H1,6X,                      POUT     83
           11HP,14X,4HV/V0,11X,1HT,14X,1HU,14X,1HD,14X,3HRHO,12X,4HGCAL       POUT     84
           2/12X,1H2,6X,1HV,14X,1HE,14X,1HS,14X,2HNG,13X,2HNS,13X,1HN,14X     POUT     85
           36HSUPSAT )                                                        POUT     86
      C                                                                       POUT     87
       7120 FORMAT (12X,1H3,6X,1HV,14X,4HE/RT,11X,3HS/R,12X,5HPV/RT,          POUT     88
           110X,2HN1,13X,2HN2, 3X,2HN3 / 12X,1H4,6X,11HDU. FOR GAS,           POUT     89
           249X,6HN4,N5,N6/12X,1H5,6X,12HDU. FOR REF.,48X,8HN7,N8,N9          POUT     90
           3/12X,1H6,6X,13HDU. FOR SOLID,47X,11HN10,N11,N12 )                 POUT     91
      C                                                                       POUT     92
       7130 FORMAT (12X,1H7,6X,5HRBAR*,10X,5HTBAR*,10X,5HVBAR*,10X            POUT     93
```

```
        1           ,5HGAMMA,10X,5HALPHA,10X,4HBETA,11X,1HC )       POUT      94
      C                                                             POUT      95
      C                                                             POUT      96
       7200 FORMAT (1H0,6HPOINT I2,3X                               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,4HHBAR 8X,4HVBAR 8X,4HTBAR 8X,1HQ   POUT     110
        3/4H$ 3 2HS 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$J 1PE11.4 ,5E12.4 / (1H$ 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 FROUT,              MESC      11
      C           USING MES FOR FUNCTION CALCULATION                MESC      12
      C                                                             MESC      13
      C                                                             MESC      14
      C                               ALL USE SAME FROUT 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
  6         EQUIVALENCE (THER(8),V),(THER(13),S),(THER(9),E)              MESC
  6         EQUIVALENCE (THER(3),T)                                       MESC
       C                                                                  MESC
  6       4 KEN(14)=0                                                     MESC
  7       6 KEN(8)=KEN(8)+1                                               MESC
 11       8 KEN(16)=KEN(16)+1                                             MESC
 13      10 IF (KG-1) 30,15,30                                            MESC
 15      15 T=ASUC(1)                                                     MESC
 16      20 CALL MES                                                      MESC
 21      25 GO TO 200                                                     MESC
 22      30 KCM(1)=0                                                      MESC
 23      35 CM(4)=T                                                       MESC
 25      40 CM(2)=T*FOB( 9)                                               MESC
 27      45 CALL FROOTT (CM,KON(3,8))                                     MESC
 34      46 KEXIT=KCM(2)                                                  MESC
 36      50 GO TO (200,80,70,60), KEXIT                                   MESC
 46      60 CALL DBUG (4HMESC,1)                                          MESC
 53      62 GO TO 200                                                     MESC
 54      70 CALL DBUG (4HMESC,2)                                          MESC
 61      72 GO TO 200                                                     MESC
 62      80 T=CM(2)                                                       MESC
 64         CALL MES                                                      MESC
 65         I=KG-1                                                        MESC
 70         GO TO (90,100,110),I                                          MESC
 76      90 CM(3)=V-ASUC(3)                                               MESC
100      95 GO TO 120                                                     MESC
101     100 CM(3)=(( EXP((S/ASUC(4))*ALOG(ASUC(1))))/ASUC(1))-1.          MESC
116     105 GO TO 120                                                     MESC
117     110 CM(3)=E-ASUC(5)                                               MESC
121     120 CALL DOUT (4HMESC,1)                                          MESC
126     125 GO TO 45                                                      MESC
       C                                           CALC. ISE INTEGRAL PDV MESC
127     200 IF (KG-3) 220,210,220                                         MESC
131     210 THER(4)=(HE(8)-THER(9))/CONT(4)                               MESC
       C                                                                  MESC
134     220 CALL DOUT (4HMESC,2)                                          MESC
141     300 RETURN                                                        MESC
142         END                                                           MESC


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

```
  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)/FOB(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 FOB(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 - R+ =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)R+
      C                               (8)R-
      C              E2               SAVE NC
      C
      C       GAMM

  5           COMMON Z(4000)
  6           DIMENSION
            1 DER    (    10) ,EMN    (    20) ,FOB    (    60)
            2,RF     (    10) ,KAL    (    20) ,THER   (    50)
            3,SUCG   (    20)
  6           EQUIVALENCE
            1 (Z( 1000),DER    ) ,(Z( 1030),EMN    ) ,(Z( 1410),FOB    )
            2,(Z( 1590),RF     ) ,(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
  6       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
126     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(4)*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                                                TED     2
   C                                                                    TED     3
   C      DETONATION HUGONIOT CONTROL                                   TED     4
   C            CALCULATE DET. HUG. POINTS AT P VALUES                  TED     5
   C            FOUND IN PT ARRAY                                       TED     6
   C                                                                    TED     7
   C    INPUT                                                           TED     8
   C      KAL(1), KAL(2) - DIFF SWITCHES                                TED     9
   C      PT - PRESSURE TABLES                                          TED    10
   C    OUTPUT                                                          TED    11
   C      PRINTED POINT OUTPUT                                          TED    12
   C----------                                                          TED    13
   C                                                                    TED    14
   C      REVISION 1.LEAVE P CORRECT ON EXIT                            TED    15
   C                  FOR RESTART OPTION                                TED    16
   C                        W. F. 3/1/62                                TED    17
   C                                                                    TED    18
   C      TED                                                           TED    19
                                                                        TED    20
 1        COMMON Z(4000)                                                TED    21
 1        DIMENSION                                                     TED    22
         1 KAL    (    20) ,PT     (    50)                             TED    23
         2, THER (50)                                                   TED    24
 1        EQUIVALENCE                                                   TED    25
         1 (Z( 1600),KAL    ) ,(Z( 1750),PT     )                       TED    26
         2 , (Z(1920),THER)                                             TED    27
   C                                                                    TED    28
 1        EQUIVALENCE (THER(1),P)                                       TED    29
   C                                                                    TED    30
   C                                          SET TGUESS ON FIRST ENTRY TED    31
 1     12 CALL POUT(1)                                                  TED    32
 3     20 I=1                                                           TED    33
 4     30 IF(PT(I)) 200,200,40                                          TED    34
 6     40 P=PT(I)                                                       TED    35
10     50 I=I+1                                                         TED    36
12     60 CALL HUG                                                      TED    37
13     70 CALL POUT(2)                                                  TED    38
15     80 IF (KAL(1)+KAL(2)) 100,30,100                                 TED    39
17    100 CALL GAMM (KAL(1),KAL(2))                                     TED    40
22    150 CALL POUT(3)                                                  TED    41
24    180 GO TO 30                                                      TED    42
25    200 RETURN                                                        TED    43
   C                                                                    TED    44
26        END                                                           TED    45

          SUBROUTINE CJ                                                 CJ      2
   C                                                                    CJ      3
   C      CALCULATE CJ LOCUS AT VALUES OF RHO ZERO                      CJ      4
   C            IN ROT TABLE                                            CJ      5
   C                                                                    CJ      6
   C            ITERATE ON P ALONG HUGONIOT UNTIL                       CJ      7
   C            CJ CONDITION IS SATISFIED                               CJ      8
   C    INPUT                                                           CJ      9
   C      KAL(1), KAL(2) - DIFF SWITCHES                                CJ     10
   C      ROT - INITIAL-DENSITY TABLE                                   CJ     11
   C    OUTPUT                                                          CJ     12
   C      PRINTED POINT OUTPUT                                          CJ     13
   C----------                                                          CJ     14
```

```
     C                         CONST. V DET. P CALCD FROMQ,GAMMA               CJ        15
     C                         W. F. 11/21/61                                  CJ        16
     C                                                                         CJ        17
     C                    REVISION 2. SAVE INITIAL E FOR INTEGRAL PDV          CJ        18
     C                         W. F. 1/3/62                                    CJ        19
     C                                                                         CJ        20
     C                                                                         CJ        21
     C      CJ                                                                 CJ        22
                                                                               CJ        23
  1         COMMON Z(4000)                                                     CJ        24
  1         DIMENSION                                                          CJ        25
           1 CAR    (     10,      8),HE     (            10),KAL    (      20) CJ        26
           2,KON    (      6,     10),ROT    (            20),THER   (      50) CJ        27
           3,KEN(60)                                                           CJ        28
  1         DIMENSION CC(10),KCC(2)                                            CJ        29
  1         EQUIVALENCE                                                        CJ        30
           1 (Z(   920),CAR    ) ,(Z( 1590),HE     ) ,(Z( 1600),KAL    )       CJ        31
           2,(Z( 1690),KON     ) ,(Z( 1800),ROT    ) ,(Z( 1920),THER   )       CJ        32
           3,(Z(1620),KEN)                                                     CJ        33
     C                                                                         CJ        34
     C                                                                         CJ        35
  1         EQUIVALENCE (CAR(1),CC),(CC(8),KCC)                                CJ        36
  1         EQUIVALENCE (HE(6),V0),(HE(2),P0),(HE(1),RHO)                      CJ        37
  1         EQUIVALENCE (THER(1),P),(THER(22),GAM),(THER(26),GAM0)             CJ        38
  1         EQUIVALENCE (THER(8),V)                                            CJ        39
  1         EQUIVALENCE (THER(6),Q)                                            CJ        40
  1       6 KEN(15)=0                                                          CJ        41
  2       8 KEN(16)=0                                                          CJ        42
     C   10 Q+Q+E                                INPUT, OUTPUT LABEL           CJ        43
  3      30         CALL POUT(1)                                               CJ        44
  5      40         I=1                                                        CJ        45
     C   50 M1+E                                 SET UP FROOTT                 CJ        46
  6      60         RHO=ROT(I)                                                 CJ        47
 10      65         HE(1)=RHO                                                  CJ        48
 12      70         V0=1./RHO                                                  CJ        49
 14      72 IF(P) 80,74,80                                                     CJ        50
 15      74 P=0.3                                                              CJ        51
 17      80 CC(4)=P                                                            CJ        52
 21     100         KCC(1)=0                                                   CJ        53
     C  110 Q(G2,G3,G4,G5)                       FROOTT                        CJ        54
 22     120         CALL FROOTT(CC,KON (1,8))                                  CJ        55
 25     130         KEXIT=KCC(2)                                               CJ        56
 27     140         GO TO (365,200,180,160), KEXIT                             CJ        57
     C  150 M5+Q                                 FROOT ERROR EXIT 1            CJ        58
 37     160 CALL DBUG (2HCJ,1)                                                 CJ        59
 42     170 GO TO 365                                                          CJ        60
 43     180 CALL DBUG (2HCJ,1)                                                 CJ        61
 46     190 GO TO 365                                                          CJ        62
 47     200 IF (KON(1,8)) 260,204,260                                          CJ        63
 50     204 IF (KCC(1)-2) 260,210,260                                          CJ        64
 52     210 E1=GAM                                                             CJ        65
 54     220 IF(GAM)240,230,240                                                 CJ        66
 55     230 E1=GAM0                                                            CJ        67
 57     240 E2=V0*E1/(E1+1.0-P0/P)                                             CJ        68
 64     250 CC(2)=P*(V/E2)**E1                                                 CJ        69
     C                                                                         CJ        70
 72     260 IF (KCC(1)-2)280,280,262                                           CJ        71
 75     262 E1=GAM                                                             CJ        72
 77     264 IF(GAM)268,266,268                                                 CJ        73
100     266 E1=GAM0                                                            CJ        74
```

```
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 350 H2+Q+G+Q                                  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
151    390        CALL POUT(2)                                                 CJ        95
153    420 CALL GAMM(KAL(1),KAL(2))                                            CJ        96
156    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 MESO - ACON=0                                    CON       14
      C       2. ERR - ACON=1 - SKIP THRU NEXT REND 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 REND 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),FOB     (       6,      10),HE      (               10) CON
         4,KAL     (                 20),KIM     (               10),KON     (        6,     10) CON
         5,PT      (                 50),ROT     (               20),SUC     (               20) CON
         6, THER(60)                                                            CON
 3        EQUIVALENCE                                                           CON
         1 (Z(  400),BS     ) ,(Z(  420),CAR     ) ,(Z(  460),CONT   )          CON
         2,(Z( 1030),EMN    ) ,(Z( 1170),EMX     ) ,(Z( 1390),FN     )          CON
         3,(Z( 3100),FLAB   ) ,(Z( 1410),FOB     ) ,(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(2),BPAS),(BS(36),BEND)                                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),MELAB)                         CON
 3        EQUIVALENCE (FLAB(25),CURLAB),(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),MELAB(12),CURLAB(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=0.                                                            CON
16     80 CALL FIO (3HRIT,13H(2A6,6A10,A8) ,  9, E, 0)                          CON
23     90 CALL FIO (3HWOT,14H(/1X6A6, 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
    C8348                                                                       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=21,2900
131      210  CONT(I)=0.0
133          CALL HEAD1(F(3))
135          CALL HEAD(9LBEGIN RUN)
      C
140      250 DO 252 I=1,96
145      252 FLAM(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 REAP(
            1501HDIFF, 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 KAL(I)=KE(I)
172      308 CONTINUE
174      310 GO TO 80
      C 398                                                   FOM
175      400 CALL REAP(
            10L*.  FROOT EPS(CC,CH,CN,CO,CS,C)/ RATIOS/ DP,DT,EPSIN,OUT/ FROOT
            2 BOUNDS*
            2  ,36,F(3))
201      410 DO 420 I=1,5
211      420 CAR(1,I)=FOM(I)
214      430 GO TO 80
215      500 GO TO 80
      C 598                                                   DIP
216      600 KON(7)=1
217      610 CALL DIP1
221      620 GO TO 80
      C 698                                                   DIS
222      700 CALL REAP (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 REAP (0,-1,KE)
244      820 KON(KE,8)=1
246      830 CALL REAP (0,3,CAR(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(I)=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                                                TED                    CON       176
366    1700 CALL HEAD(14LTED - HUGONIOT)                                          CON       177
370         CALL READ (11H  P-TABLE $, 0, PT)                                     CON       178
      C                                                                           CON       179
374    1710 CALL TED                                                              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(9))                                                           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
420         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
```

```
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 JOB CON     250
526    3600 CONTINUE                                                     CON     251
526         CALL HEADE (7HJOBEND$   )                                    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
```

```
     C      NOTES -
     C      1. CHANGES WHEN INCORPORATED INTO REVIVED MES
     C         (MARKED KERSHNER 3/17/76)
     C        A. MAKE AVECT LOCAL, FILLED FROM ARGS EPA, EPA1,
     C           IN EQPS
     C        B. EMOL(2) REPLACED BY EMOL(7), IN EQMS
     C*************************************************************************

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

```
232         4 QBAR(J)=XNUMAT(ND+1,J)/SUMQ                                  EQPS      67
234           DO 5 I=1,ND                                                  EQPS      68
241           XNU(I)=0.0                                                   EQPS      69
243           DO 5 J=1,NCMP                                                EQPS      70
252         5 XNU(I)=XNU(I)+XNUMAT(I,J)                                    EQPS      71
      C PRINT NU-MATRIX AND QBAR                                           EQPS      72
263           WRITE(9,6)(QBAR(J),J=1,NCMP)                                 EQPS      73
271           WRITE(9,7)(XNUMAT(1,J),J=1,NC)                               EQPS      74
            6 FORMAT(1H0,5X,4HQBAR,5X,  6E15.7)                            EQPS      75
            7 FORMAT(1H0,5X,6HNU MAT,3X,  6E15.7)                          EQPS      76
            8 FORMAT(10X,I3,2X,  6E15.7)                                   EQPS      77
317           IF(ND.LE.1)GO TO 90                                          EQPS      78
321           DO 9 I=2,ND                                                  EQPS      79
323         9 WRITE(9,8)I,(XNUMAT(I,J),J=1,NC)                             EQPS      80
352           GO TO (10,15),NPHI1                                          EQPS      81
360        90 IF(NPHI.EQ.1.AND.NP.EQ.1)GO TO 11                            EQPS      82
367        10 RETURN                                                       EQPS      83
370        11 NP=0                                                         EQPS      84
370           KV=2                                                         EQPS      85
372           GO TO 14                                                     EQPS      86
373        15 GO TO (16,10),KFLAG                                          EQPS      87
401        16 DO 17 I=1,ND                                                 EQPS      88
403           XNUS(I)=XNU(I)                                               EQPS      89
405           DO 17 J=1,NC                                                 EQPS      90
415        17 XNUMATS(I,J)=XNUMAT(I,J)                                     EQPS      91
425           XNUS(ND1)=NP                                                 EQPS      92
430           DO 18 I=1,NS                                                 EQPS      93
435        18 NAVECS(I)=NAVEC(I)                                           EQPS      94
437           SUMQS=SUMQ                                                   EQPS      95
440           DO 19 J=1,NC                                                 EQPS      96
451        19 QBARS(J)=QBAR(J)                                             EQPS      97
453           KFLAG=2                                                      EQPS      98
454           GO TO (20,21),NPS                                            EQPS      99
465        20 NP=0                                                         EQPS     100
465           KV=2                                                         EQPS     101
467           GO TO 22                                                     EQPS     102
470        21 NP=1                                                         EQPS     103
470           KV=1                                                         EQPS     104
472        22 XNU(ND1)=NP                                                  EQPS     105
475           GO TO 14                                                     EQPS     106
475        30 NP=CSP(5)                                                    EQPS     107
475           NPS=NP+1                                                     EQPS     108
501           GO TO (31,33),NPS                                            EQPS     109
506        31 NP=1                                                         EQPS     110
506           KV=1                                                         EQPS     111
510        32 KFLAG=1                                                      EQPS     112
511           GO TO 14                                                     EQPS     113
512        33 NP=0                                                         EQPS     114
512           KV=2                                                         EQPS     115
514           GO TO 32                                                     EQPS     116
515           END                                                          EQPS     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  EMCL(2) REPLACED BY EMCL(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
231         EMOL(2)=XC*EMOL(1)
      C RESTORE MOLE FRACTION ORDER
234      81 DO 9 I=1,NS
243         NAV=NAVEC(I)
243       9 XCOMP(I)=RXCOMP(NAV)
247         IF(NPHI.EQ.1)GO TO 22
      C EXIT WITH COMPUTED EQUILIBRIUM COMPOSITION
253      10 RETURN
      C
      C ENTRY TO CALCULATE CORRECTIONS TO MOLE FRACTIONS
254      11 DO 13 J=1,NCMP
256         SUMF=0.0
257         DO 12 I=1,NO
272      12 SUMF=SUMF+(XNUMAT(I,J)-GBAR(J)*(XNU(I)-1.0))*RXCOMP(I+NC)
303      13 F(J)=GBAR(J)-RXCOMP(J)-SUMF
311         DO 14 J=1,NCMP
313         DO 14 JP=1,NCMP
314         A(J,JP)=0.0
317         IF(J.EQ.JP)A(J,JP)=RXCOMP(J)
322         DO 14 I=1,NO
340      14 A(J,JP)=A(J,JP)+(XNUMAT(I,J)-GBAR(J)*(XNU(I)-1.0))*RXCOMP(I+NC)*
           1XNUMAT(I,JP)
357         CALL LSS(NCMP,1,6,A,F,DET)
363         IF (DET.EQ.0.0)GO TO 20
367         DO 17 J=1,NCMP
370         RXCOMP(J)=RXCOMP(J)*(1.0+F(J))
373         IF(RXCOMP(J).LT.EPSILON)RXCOMP(J)=EPSILON
377      17 CONTINUE
402         ITERCO=ITERCO+1
403         GO TO 3
404      20 CALL DBUG(1)
406         GO TO 1000
      C TEST FOR PREVIOUS SOLUTION FOR PHI = 1
411      22 IF(NPHFLAG.EQ.2)GO TO 10
414         IF(NP.EQ.1)GO TO 40
      C SATURATION TEST FOR 1-PHASE SOLUTION
      C SELECT NON-ZERO ELEMENT OF 2-PHASE NU
416         DO 50 I=1,NO
417         IF(XNUMATS(I,NC).NE.0.0)GO TO 51
422      50 CONTINUE
424         CALL DBUG(2)
      C LOCATED SPECIES FORMED FROM SOLID
430      51 ISP=I
432         DO 52 I=1,NS
437         NAV=NAVECS(I)
437         RXCOMP(NAV)=XCOMP(I)
437      52 RFDAG(NAV)=FDAG(I)
444         ZLNKI=-RFDAG(ISP+NC)
447         DO 53 J=1,NC
462      53 ZLNKI=ZLNKI+XNUMATS(ISP,J)*RFDAG(J)
465         XLNS=ALOG(RXCOMP(ISP+NC))-ZLNKI
472         NCM1=NC-1
474         DO 54 J=1,NCM1
500      54 XLNS=XLNS-XNUMATS(ISP,J)*ALOG(RXCOMP(J))
514         EMOL(7)=XLNS
      C**************************************************
      C   EMOL(7) SET 2/10/76
      C**************************************************
      C TEST FOR SUPERSATURATION
```

```
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
546           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,ND1                                                  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(ND1)                                                    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
  44          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
 24          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 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 30,(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. Tc, pc 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. $-\ (\partial\ \ell n\ p/\partial\ \ell n\ v)_T$
7. C_p/R
8. $(\partial\ \ell n\ v/\partial\ \ell n\ T)_p$

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).

☆ U.S. GOVERNMENT PRINTING OFFICE: 1976—777-018/30