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IMPROVEMENTS IN THE CHART D ENERGY FLOW
HYDRODYNAMIC CODE V: 1972/73 MODIFICATIONS

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ABSTRACT

CHART D is a flexible code for computing coupled hydrodynamic motion and energy flow. Over the years which it has been considered a production program, the experiences of code users have suggested several modifications and model improvements. Many of these have been incorporated into CHART D and its support programs. Most are relatively minor but some represent major changes. These include the treatments of porous materials, artificial viscosity and additional equation of state options.

The theory sections in the present report are intended to supplement not replace previous CHART D literature. Revised and complete input instructions for CHART D and its support programs are given.

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I. INTRODUCTION

The CHART D energy flow-hydrodynamic code and its related support programs CKEOS, MASPLT and ZCHART are described in detail in three reports which were distributed in early 1972.¹⁻³ In this paper, the model modifications and corrections which have been included since that time are presented. This report is intended to supplement, not replace, its predecessors. The previous reports will be referred to as R1, R2 and R3 in the following material.

Section II of this paper relates to the material in R1, section III to R2 and sections IV and V to R3. Revised input instructions for CHART D, MASPLT and CKEOS are found in the appendices. Any input deck which functioned properly with the older versions of these codes should work with the revised programs and give the same results. All codes have the same or less machine storage requirements as the previous versions.

The redimensioning program ZCHART described in R3 has had only minor coding changes. The previous input instruction still apply so that no section is included in this report related to ZCHART.

The time-sharing PDPIO programs EOS and ZONER function as previously indicated.³ The changes described in section III of this report have been included in EOS.

Program listings are not included in this report since the card numbering system used in R1 and R3 has been retained. By use of the CDC 6600 update processor, the changes have been included as correction sets without renumbering. This is intended as an aid to CHART D users external to Sandia in keeping current program decks.

Two sections of this report are not directly related to CHART D. Appendices A and B concern pure hydrodynamic codes; here meaning those employing energy and density as independent variables. The programs WONDY,⁴ TOODY,⁵ PUFF⁶ and TOIL (DORF)⁷ are of this nature. The modified P - α model for distended materials discussed in section II.2 for CHART D is reformulated in terms suitable for the ρ - E codes in Appendix A.

The ANEOS package as detailed in R2 and section III is quite flexible and can easily be used by other codes. As an illustration to show how few modifications to existing decks are really required, an example for WONDY is included in Appendix B.

Many of the modifications presented here are the result of suggestions by code users. Acknowledgements will be given in the various sections to individuals.

II. CHART D PROGRAM MODIFICATIONS

Several changes and additions to the models used in the CHART D program are discussed in this section. None of these involve extensive coding modifications. However, in some problems, they can lead to a considerable variation in the computed results.

Please note that changes in the analytic equation of state section (ANEOS) of the program are given in section III. In section IV, some additional tests for the selection of input data are discussed.

II.1 Artificial Viscosity

As discussed in R1, the form of the artificial viscosity employed in CHART D is

$$Q = B_\ell C_S \frac{\partial \rho}{\partial t} + B_q^2 \rho \left(\frac{1}{\rho} \frac{\partial \rho}{\partial t} \right)^2, \text{ if } \frac{\partial \rho}{\partial t} > 0 \\ = 0, \text{ if } \frac{\partial \rho}{\partial t} \leq 0. \quad (II.1.1)$$

Several changes have been made in the way that (II.1.1) is implemented in the program. Previously the plane symmetry form of the conservation of mass relation,

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial V}{\partial X}, \quad (II.1.2)$$

was combined with (II.1.1) so that

$$Q_i^{j+\frac{1}{2}} = \frac{1}{2} \left\{ \rho_i^j + \rho_i^{j+1} \right\} \Delta V \left\{ \tilde{B}_q^2 \Delta V + \tilde{B}_\ell [C_S]_i^j \right\}, \quad (II.1.3)$$

where

$$\tilde{B}_q = B_q / \Delta X$$

and

$$\tilde{B}_\ell = B_\ell / \Delta X \quad (II.1.4)$$

were the input quantities with default values of 2.0 and 0.1.

In some cases involving cylindrical or spherical geometry, the use of (II.1.2) has caused difficulty. As a result (II.1.3) has been replaced by

$$Q_i^{j+\frac{1}{2}} = |S_K| \beta \left\{ \frac{2 \beta \tilde{B}_q^2}{(\rho_i^j + \rho_i^{j+1})} + \tilde{B}_l [C_S]_i^j \right\}, \text{ if } \beta > 0$$

(II.1.5)

$$= 0, \text{ if } \beta \leq 0$$

where

$$\beta = \frac{(x_i^{j+1} - x_{i+1}^{j+1} + x_i^j - x_{i+1}^j)(\rho_i^{j+1} - \rho_i^j)}{2 \Delta t} \quad (\text{II.1.6})$$

and the plane geometry difference form of (II.1.2) is used. S_K is discussed below. It is a material layer (not zone) input quantity and is normally equal to unity. For plane geometry (II.1.5) should give exactly the same results as (II.1.3). On the other hand for cylindrical and spherical symmetry (II.1.5) is superior.

The generation of rarefaction shocks is possible in some materials.

In any region of the equation of state surface where

$$\left(\frac{\partial^2 P}{\partial \rho^2} \right)_S < 0 \quad (\text{II.1.7})$$

these discontinuities in relief wave structure can be found. Fused silica ($P \lesssim 34$ kilobars) is an example. The same effect can occur in materials which do not satisfy (II.1.7) but exhibit discontinuities in the derivative

$\left(\frac{\partial P}{\partial \rho} \right)_S$ due to phase transitions. The 130 kilobar polymorphic phase change in iron can cause this phenomenon.

Unfortunately the standard methods of employing viscosities in hydrodynamic codes are not well suited to treat this problem. The rarefaction shock will properly form but will tend to overshoot since (II.1.1) provides

no damping during expansion ($\frac{\partial \rho}{\partial t} < 0$). The result is a wave shape of the correct form but with a noisy structure.

The difficulty can be corrected by employing the viscosity term in both the compression and expansion phases. The option provided is

$$Q_i^{j+\frac{1}{2}} = |S_K| \beta \left\{ \begin{array}{l} \frac{2\beta \tilde{B}_q^2}{(\rho_i^j + \rho_i^{j+\frac{1}{2}})} + \tilde{B}_\ell [c_s]_i^j \\ \end{array} \right\} \text{ if } \beta > 0$$

(II.1.8)

$$= |S_K| \beta \left\{ - \frac{2\beta \tilde{B}_q^2}{(\rho_i^j + \rho_i^{j+1})} + \tilde{B}_\ell [c_s]_i^j \right\} \text{ if } \beta < 0$$

with β given by (II.1.6). This form is selected in the code by a negative value of S_K .

S_K is a new layer input quantity. For normal materials, it should be unity (the default value). However, material with special or abnormal properties (as those discussed above) sometimes require a different value. Below approximately 34 kilobars fused silica forms a ramp compressional wave and a rarefaction shock. The normal viscosity treatment during compression tends to slightly distort the shape of the ramp. A value of $S_K = -\frac{1}{2}$ seems to work well for preserving the ramp and above mentioned rarefaction shock. For the iron phase change, $S_K = -1$ provides correct behavior.

On the other extreme, porous materials with the normal viscosity treatment sometimes yield somewhat noisy pulse shapes. Increasing S_K slightly (~2 to 5) will smooth the results satisfactorily. In general, anytime undesirable noise is present, increasing S_K will eliminate it.

II.2 Porous Materials

The porous material model employed in CHART D is a modified form of the $P - \alpha$ model developed by Herrmann.¹ It is assumed that the reader is familiar with section V in R1. The additions to the model presented here are, for the most part, the result of extensive calculations by L. Buxton⁸ as related to the experimental work by F. Perry.

Two additions were suggested by Buxton which apply to relatively slow-low level deposition response. The first concerns the behavior in the "elastic" region at constant volume. The second relates to the melting response. These modifications were coded as options so that the previous models are still available. In general, the new forms are probably better for slow depositions (in relation to relaxation times) while the older forms are better for rapid depositions. At sufficiently high energy levels, the different forms should give the same result.

II.2-1 Elastic Region

In the previous description, "elastic" changes in distention were given by the relation

$$d\alpha = \left(\frac{\partial \alpha}{\partial \rho_f} \right) d\rho_f \quad (\text{II.2.1})$$

where the subscript f indicates properties of the foam. Quantities with no subscripts refer to the solid component in the distended material. Under adiabatic loading conditions, it has been shown¹ that

$$\left(\frac{\partial \alpha}{\partial \rho_f} \right) = \frac{h^2(\alpha) - \alpha}{\rho_f} \quad (\text{II.2.2})$$

where

$$h(\alpha) = \left(\frac{C_{eo}}{C_{oo}} \right) \left\{ \frac{\alpha - 1}{\alpha_e - 1} \right\} + \left\{ \frac{\alpha_e - \alpha}{\alpha_e - 1} \right\} . \quad (\text{II.2.3})$$

When these relations are applied to the problem of constant volume heating, such as could be obtained by rapid deposition from an electron beam, several things should be noted. If the foam density does not change, then according to (II.2.1), the distention is constant. The porous material acts much like the full density solid material. In other words, the deposition is assumed sufficiently rapid so that the solid material does not have time to expand into the voids while the material is in an elastic state. It, of course, should be recalled that this description is used only below the point of initial yield (\mathcal{P}_e). The relevant time period is that required to heat the material to initial yield and not the total deposition time. For strong sources, these time periods can differ by orders of magnitude. If it is assumed that the solid material can be described by the Grüneisen relation

$$\Gamma_S = \frac{1}{\rho} \left(\frac{\partial P}{\partial E} \right)_\rho , \quad (\text{II.2.4})$$

the above response at constant volume can be expressed as

$$\Delta P = \rho \Gamma_S \Delta E \quad (\text{II.2.5})$$

below the elastic limit. If one tries to define an "effective" Grüneisen coefficient for the foam by the relation

$$\Delta P = \rho_f \Gamma_{eff} \Delta E , \quad (\text{II.2.6})$$

it follows that

$$\Gamma_{\text{eff}} = \frac{\rho \Gamma_S}{\rho_f} > \Gamma_S . \quad (\text{II.2.7})$$

Again, this applies only below the yield point.

For relatively weak sources and slow deposition times, the solid material may expand into the voids while the material is in an elastic state. This would result in the previous method overpredicting the stresses generated by the deposition. The effect would be most noticeable in material with insufficient deposition to reach the yield point.

A generalization of (II.2.1) can be written as

$$d\alpha = \left(\frac{\partial \alpha}{\partial \rho_f} \right)_S d\rho_f + \left(\frac{\partial \alpha}{\partial S} \right)_{\rho_f} dS , \quad (\text{II.2.8})$$

where S is the specific entropy. The first term in (II.2.8) is the same as (II.2.1), while the second describes the entropy changes due to the deposition when coupled to the expansion into the voids.

To evaluate the coefficient $\left(\frac{\partial \alpha}{\partial S} \right)_{\rho_f}$, consider the situation of constant volume heating ($d\rho_f = 0$). In this case

$$dS = \frac{1}{T} dE \quad (\text{II.2.9})$$

where dE is the energy introduced into the material. Eq. (II.2.8) is then written as

$$d\alpha = \frac{1}{T} \left(\frac{\partial \alpha}{\partial S} \right)_{\rho_f} dE . \quad (\text{II.2.10})$$

To shorten the notation, define

$$K(\rho_f, \rho, T) = \frac{1}{T} \left(\frac{\partial \alpha}{\partial S} \right)_{\rho_f} . \quad (\text{II.2.11})$$

The problem is to now evaluate this coefficient K in terms of the thermodynamic properties of the solid and one additional property of the distended material. The additional constant is the "effective" Grüneisen coefficient Γ_{eff} given by (II.2.6).

In the present situation, (II.2.10) is written as

$$d\rho = \rho_f K dE . \quad (\text{II.2.12})$$

The required thermodynamic relations can be obtained from the derivative chain rule. Considering just the solid material properties, it follows that

$$dE = \left(\frac{\partial E}{\partial \rho} \right)_T d\rho + \left(\frac{\partial E}{\partial T} \right)_\rho dT \quad (\text{II.2.13})$$

and

$$dP = \left(\frac{\partial P}{\partial \rho} \right)_T d\rho + \left(\frac{\partial P}{\partial T} \right)_\rho dT \quad (\text{II.2.14})$$

so that

$$dP = \frac{\left(\frac{\partial P}{\partial T} \right)_\rho}{\left(\frac{\partial E}{\partial T} \right)_\rho} dE + \left\{ \left(\frac{\partial P}{\partial \rho} \right)_T - \frac{\left(\frac{\partial P}{\partial T} \right)_\rho \left(\frac{\partial E}{\partial \rho} \right)_T}{\left(\frac{\partial E}{\partial T} \right)_\rho} \right\} d\rho . \quad (\text{II.2.15})$$

Substitution of (II.2.6) and (II.2.12) into this relation defines the coefficient K ,

$$K(\rho_f, \rho, T) = \frac{\Gamma_{\text{eff}} - \frac{1}{\rho_f} \frac{\left(\frac{\partial P}{\partial T}\right)_P}{\left(\frac{\partial E}{\partial T}\right)_P}}{\left(\frac{\partial P}{\partial \rho}\right)_T - \frac{\left(\frac{\partial P}{\partial T}\right)_P \left(\frac{\partial E}{\partial \rho}\right)_T}{\left(\frac{\partial E}{\partial T}\right)_P}} . \quad (\text{II.2.16})$$

This expression is not difficult to evaluate in CHART D even though it appears complex. All of the required derivatives are present in the previous calculation for other purposes except $\left(\frac{\partial E}{\partial \rho}\right)_T$. This term can be found from the thermodynamic relation

$$\left(\frac{\partial E}{\partial \rho}\right)_T = \frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T}\right)_P . \quad (\text{II.2.17})$$

It is possible to derive many interesting relations from (II.2.8). Here we shall consider one as an example, the heat capacity of the foam at constant foam density C_{V_f} . First, however, it is convenient to rewrite (II.2.16) in a slightly different form. The sound speed in the solid material is

$$c_s^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \frac{T \left(\frac{\partial P}{\partial T}\right)_P^2}{\rho^2 \left(\frac{\partial E}{\partial T}\right)_P^2} . \quad (\text{II.2.18})$$

The term in (II.2.16)

$$\left(\frac{\partial P}{\partial \rho}\right)_T - \frac{\left(\frac{\partial P}{\partial T}\right)_\rho \left(\frac{\partial E}{\partial \rho}\right)_T}{\left(\frac{\partial E}{\partial T}\right)_\rho} = \left(\frac{\partial P}{\partial \rho}\right)_T + \frac{T \left(\frac{\partial P}{\partial T}\right)_\rho^2}{\rho^2 \left(\frac{\partial E}{\partial T}\right)_\rho} - \frac{\left(\frac{\partial P}{\partial T}\right)_\rho P}{\rho^2 \left(\frac{\partial E}{\partial T}\right)_\rho} \quad (\text{II.2.19})$$

can be written as

$$c_s^2 - \frac{\left(\frac{\partial P}{\partial T}\right)_\rho P}{\rho^2 \left(\frac{\partial E}{\partial T}\right)_\rho} \quad (\text{II.2.20})$$

from consideration of (II.2.18). It then follows that

$$K = \frac{\Gamma_{\text{eff}} - \frac{1}{\rho_f} \frac{\left(\frac{\partial P}{\partial T}\right)_\rho}{\left(\frac{\partial E}{\partial T}\right)_\rho}}{c_s^2 - \frac{P \left(\frac{\partial P}{\partial T}\right)_\rho}{\rho^2 \left(\frac{\partial E}{\partial T}\right)_\rho}} \quad . \quad (\text{II.2.21})$$

From (II.2.13), it can be seen that the heat capacity of the foam is

$$c_{v_f} = \left(\frac{\partial E}{\partial T}\right)_{\rho_f} = c_{v_s} + \left(\frac{\partial E}{\partial \rho}\right)_T \left(\frac{\partial \rho}{\partial T}\right)_{\rho_f} = c_{v_s} + \rho_f K \left(\frac{\partial E}{\partial \rho}\right)_T c_{v_f} , \quad (\text{II.2.22})$$

or

$$c_{v_f} = \frac{c_{v_s}}{1 - \rho_f K \left(\frac{\partial E}{\partial \rho}\right)_T} \quad (\text{II.2.23})$$

where C_{V_f} is the heat capacity of the solid. In most situations this yields

$$C_{V_f} \geq C_{V_s} \quad (\text{II.2.24})$$

as one might expect.

To further demonstrate the properties of these relations, let us assume that the solid material can be described by the Grüneisen relation (II.2.5), here written as

$$\left(\frac{\partial P}{\partial T}\right)_\rho = \rho \Gamma_s \left(\frac{\partial E}{\partial T}\right)_\rho \quad (\text{II.2.25})$$

It is clear that

$$K = \frac{\Gamma_{\text{eff}} - \frac{\rho}{\rho_f} \Gamma_s}{C_s^2 - \frac{\Gamma_s P}{\rho}} \quad (\text{II.2.26})$$

and

$$\left(\frac{\partial E}{\partial \rho}\right)_T = \frac{P}{\rho^2} - \frac{C_{V_s} T}{\rho} \quad (\text{II.2.27})$$

These two relations can be substituted into (II.2.23) with the result that

$$C_{V_f} = C_{V_s} \left\{ 1 - \left(\rho \Gamma_s - \rho_f \Gamma_{\text{eff}} \right) \left[\frac{C_{V_s} T - P/\rho}{\rho C_s^2 - \Gamma_s P} \right] \right\}^{-1} \quad (\text{II.2.28})$$

Since

$$\rho \Gamma_s \geq \rho_f \Gamma_{\text{eff}} \quad (\text{II.2.29})$$

for most distended materials, (II.2.24) follows at low pressures. Note that the results of the previous CHART D model are obtained by setting $\rho \Gamma_s = \rho_f \Gamma_{\text{eff}}$.

In practice, the above relations are applied in CHART D as

$$d\alpha = \left\{ \frac{h^2 - \alpha}{\rho_f} \right\} d\rho_f + K \dot{\mathcal{S}} dt \quad (\text{II.2.30})$$

where h is given by (II.2.3) and K by (II.2.16). $\dot{\mathcal{S}}$ is the energy source strength (see section VIII in R1) and t is the time. The finite difference form corresponding to (5.18) in R1 is

$$\alpha_n = \alpha_0 + \frac{2(\rho_n - \rho_0)}{(\rho_n + \rho_0)} \left\{ h^2(\alpha_0) - \alpha_0 \right\} + K(\alpha_0) \dot{\mathcal{S}} \Delta t . \quad (\text{II.2.31})$$

If the source strength $\dot{\mathcal{S}}$ is zero, this result is identical to the previous expression.

The value of Γ_{eff} is required as a new input parameter. If no value is defined, the older form of the calculation is used. Note that this means that for the newer model to be employed, it is required that $\Gamma_{\text{eff}} > 0$.

A rough estimate of Γ_{eff} can be obtained from the Budiansky model.⁹ This model fits the slowness assumptions discussed after eq. (II.2.3). From this work, it can be shown that

$$\Gamma_{\text{eff}} = \left(\frac{c_{eo}}{c_{oo}} \right)^2 \Gamma_s = h^2(\alpha_e) \Gamma_s , \quad (\text{II.2.32})$$

where the quantities are the same as in eq. (II.2.3).

The development in this section is slightly different from Herrmann's model as employed for example in WONDY⁴ and TOODY.⁵ In the elastic region, they use the relation

$$d\alpha = \left(\frac{\partial \alpha}{\partial P} \right) dP \quad (\text{II.2.33})$$

instead of (II.2.1). As discussed in R1, the two methods give the same result under adiabatic loading conditions. In appendix A, the expression corresponding to (II.2.8) is developed. It is shown that (II.2.32) is a result of (II.2.33).

II.2-2 Temperature Dependence of the Crushing Relations

As discussed in R1, the crush pressure \mathcal{P}_k is assumed to have the form

$$\mathcal{P}_k = \mathcal{P}_k^* (\alpha) K , \quad (\text{II.2.34})$$

where K is dependent only on the energy or temperature. Two expressions for the functional form of K were available in the previous coding and controlled by the input parameter k_o' . Below the melting point, the options available were

$$K \equiv 1 , \quad \text{if } k_o' > 0 , \quad (\text{II.2.35})$$

and for

$$-2 \leq k_o' \leq -1 \quad (\text{II.2.36})$$

$$K(E) = 1 - \left\{ \frac{E/\varepsilon_m - \delta}{1-\delta} \right\}^{-k_o'} , \quad \frac{E}{\varepsilon_m} > \delta . \quad (\text{II.2.37})$$

$$= 1 , \quad \frac{E}{\varepsilon_m} \leq \delta , \quad (\text{II.2.38})$$

where \mathcal{E}_m is the energy of completed melt and δ is a constant ($\delta = \frac{1}{2}$ was set in an internal code data statement). With either option, there is a cut off at the melting temperature so that

$$K = 0 , \text{ if } T \geq T_m . \quad (\text{II.2.39})$$

The detailed calculations of Buxton with regard to the electron beam measurements of Perry have suggested that, for this set of experimental conditions, the form of (II.2.37) is sufficient to match the data if the energy of incipient melt is employed instead of the energy of completed melt.⁸ From a coding point of view, it is easier to add an option involving the melt temperature instead of the incipient melt energy. For all practical purposes, it is the same and the required variables are already available in the storage arrays. Hence, the additional option for

$$-12 \leq k'_o \leq -11 , \quad (\text{II.2.40})$$

$$K(T) = 1 - \left\{ \frac{T/T_m - \delta}{1-\delta} \right\}^{-k'_o - 10} , \quad \frac{T}{T_m} > \delta \quad (\text{II.2.41})$$

$$= 1 , \quad \frac{T}{T_m} \leq \delta \quad (\text{II.2.42})$$

has been added. Eq. (II.2.39) is used as a cut off on these relations.

The parameter δ has also been made an input quantity with a default value of $\frac{1}{2}$.

II.3 Fracture in Partially Melted Materials

The fracture models were included in the CHART D coding long before equations of state with melt transitions were available. When these transitions were added, the storage was such as to allow partially melted material to support tensions of sizable magnitude before fracture. This causes problems since there is a discontinuity in sound speed at the melt-solid interface and multiple reflections could occur. The proper treatment of this phenomena is not clear at the present time. As a result, an option has been added to suppress tensions in partially melted states. This is done by zeroing the material strength at incipient melt energy. It should be noted that paths of constant energy coincide with isentropes near zero pressure due to the first law of thermodynamics. This means that the fracture strength vanishes at the entropy of incipient melt.

The previous model is still available in addition to the newer one.

II.4 Energy Flow Flux Limiter

The energy flow flux limiter employed in CHART D is

$$\eta_i \leq \frac{c \left\{ \rho_i E_i + \rho_{i-1} E_{i-1} \right\}}{2 T_i^4 \left| 1 - \left(\frac{T_{i-1}}{T_i} \right)^4 \right|} \quad (\text{II.4.1})$$

where η_i is defined by (3.25) in R1. In essence, this relation simply says that energy cannot be moved faster than the velocity of light. More exactly the maximum flux is

$$F_m = c \mathcal{E} \quad (\text{II.4.2})$$

where ϵ is the energy density. If this energy is due mainly to the radiation field,

$$\epsilon = \frac{4\sigma T^4}{c} \quad (\text{II.4.3})$$

then

$$F_m = 4\sigma T^4 \quad (\text{II.4.4})$$

Some code users have objected to this relation in that they feel that (II.4.4) overpredicts the allowable energy flux by a factor of four.¹⁰

They believe that the maximum flux should be limited by

$$F_{\max} = \sigma T^4 \quad (\text{II.4.5})$$

which is the maximum emission flux from the surface of a blackbody radiator.

To account for these possibilities, eq. (II.4.1) has been modified to the form

$$\eta_i \leq \frac{f c \left\{ \rho_i E_i + \rho_{i-1} E_{i-1} \right\}}{2 T_i^4 \left| 1 - \left(\frac{T_{i-1}}{T_i} \right)^4 \right|} \quad (\text{II.4.6})$$

where $f = 1$ or $1/4$. Unity leads to (II.4.3) while the latter value yields (II.4.5).

The expression for η represents three energy flow phenomena; radiation, plasma and phonon conduction. An example to demonstrate the relative importance of these processes is given in section III.2. This somewhat complicates the choice of a flux limiter. The author prefers (II.4.1) due to studies of numerical transport calculations but can see merits in the other value.

The flux limiter switch NRADCK (on input card 3) can be used to vary the value of f . The options now available are

$$\begin{aligned} \text{NRADCK} &> 0 ; f = \infty \text{ (no flux limiter)} \\ &= 0 ; f = 1 \\ &< 0 ; f = \frac{1}{4} \end{aligned} \quad (\text{II.4.7})$$

II.5 Additional Edit Capability

Two additional edit features have been added to CHART D at the request of several users.¹⁰⁻¹¹ The first is part of the standard edit and is simply a breakdown of the total energy in the problem. The internal and kinetic energy in each material layer are computed and printed at the end of the standard edit information.

The other new feature allows the user to observe the properties of a given zone at much more frequent intervals than is possible with the standard edit due to the length of the printed output. Additional input parameters for this feature are included on CHART D input card number 2.

III. ANEOS PACKAGE MODIFICATIONS

Several modifications to the previously available options and some new options have been added to the analytic equation of state package (ANEOS) as described in R2. These are detailed in this section of the report. Some tests of the ANEOS package input parameters are discussed in section IV as related to the program CKEOS.

The ANEOS package can easily be used in other hydrodynamic codes. In appendix B, a very simple procedure of coding is given to demonstrate one method. WONDY IV is employed as an example.⁴

III.1 Debye Solids

A Debye - Grüneisen model is employed for solid materials under ANEOS options 0, 1, 3 and 4. In the development followed in R2, a high temperature approximation was used with the Debye relations to increase the computational speed of the subroutines. This has caused some difficulty in comparison with very fine experimental data.¹² Slight deviations in the thermodynamic functions can shift phase region boundaries (melt transition) so that the intersection with isentropes moves an undesirable amount.

As a result, the option has been added to include the Debye function in the thermodynamic properties if it is desired. Use of this feature will slow the code by 5 to 10%. The older approximate form is still available and suitable for most problems.

Under this option, the nuclear free energy is written as

$$F_n = N_o kT \left\{ 3 \ln \left(1 - e^{-\theta/T} \right) - D(\theta/T) + \frac{3}{2} \ln (1+\psi) \right\} . \quad (\text{III.1.1})$$

All terms are as defined in section IV-3 in R2. Eq. (II.1.1) corresponds to (4.18) in R2. The other required thermodynamic relations are

$$P_n = \rho N_0 kT \left\{ 3\Gamma D(\theta/T) - (3\Gamma - 1) \frac{\psi}{1+\psi} \right\} \quad (\text{III.1.2})$$

$$E_n = N_0 kT \left\{ 3D(\theta/T) - \frac{3\psi}{2(1+\psi)} \right\} \quad (\text{III.1.3})$$

$$S_n = -N_0 k \left\{ 3\ln\left(1-e^{-\theta/T}\right) - 4D(\theta/T) + \frac{3}{2} \left[\frac{\psi}{1+\psi} + \ln(1+\psi) \right] \right\} \quad (\text{III.1.4})$$

$$C_{V_n} = \frac{E_n}{T} + N_0 k \left\{ 9 \left[D(\theta/T) - \frac{\theta/T}{e^{\theta/T} - 1} \right] - \frac{3}{2} \frac{\psi}{(1+\psi)^2} \right\} \quad (\text{III.1.5})$$

$$\frac{\partial P_n}{\partial T} = \frac{P_n}{T} + \rho N_0 k \left\{ 9\Gamma \left[D(\theta/T) - \frac{\theta/T}{e^{\theta/T} - 1} \right] - \frac{(3\Gamma-1)\psi}{(1+\psi)^2} \right\} \quad (\text{III.1.6})$$

$$\begin{aligned} \frac{\partial P_n}{\partial \rho} &= \frac{P_n}{\rho} + N_0 kT \left\{ 3\rho \left[D(\theta/T) - \frac{\psi}{1+\psi} \right] \frac{\partial \Gamma}{\partial \rho} \right. \\ &\quad \left. + 9\Gamma^2 \left[\frac{\theta/T}{e^{\theta/T} - 1} - D(\theta/T) \right] + \frac{2\psi(3\Gamma-1)^2}{3(1+\psi)^2} \right\} . \end{aligned} \quad (\text{III.1.7})$$

A new subroutine ANDEBY has been added to the ANEOS package to evaluate the Debye integral

$$D(X) = \frac{3}{X^3} \int_0^X \frac{y^3 dy}{e^y - 1} . \quad (\text{III.1.8})$$

To guard against round off errors, expressions for

$$3 \left\{ D(X) - \frac{X}{e^X - 1} \right\} \quad (\text{III.1.9})$$

and

$$\ln(1 - e^{-X}) \quad (\text{III.1.10})$$

are also determined by this subroutine.

The new option is switched on in the code by inputting $-\theta_o$ instead of θ_o in variable number 8 in the ANEOS input cards. A positive value of θ_o will lead to the subroutine using the high temperature approximation as previously coded.

III.2 Rosseland Mean Opacity

The expression employed in the ANEOS calculation for the Rosseland mean opacity as given in R2 is

$$K_r = \frac{10^{11} \rho Z \bar{Z}^2}{\bar{A}^2 T^{7/2}} + \frac{0.4 Z_m}{\bar{A}} . \quad (\text{III.2.1})$$

This relation was developed from material found in Russian literature.¹³

Unfortunately, it now appears that somewhere in this development, a factor

of 2 error was included (for electron spin states). The correct form should be

$$K_r = \frac{5 \times 10^{10} \rho \bar{Z} \bar{Z}^2}{\bar{A}^2 T^{7/2}} + \frac{0.4 Z_m}{\bar{A}} . \quad (\text{III.2.2})$$

III.2-1 Relative Importance of Terms in the Effective Opacity

It has been shown that it is possible to treat hot electron conduction and phonon conduction with the expressions developed for the radiation diffusion relations.^{1,2} An effective Rosseland opacity is defined by the expression

$$\frac{1}{K_{\text{eff}}} = \frac{1}{K_r} + \frac{1}{K_H} + \frac{1}{K_L} \quad (\text{III.2.3})$$

where

$$K_H = \frac{16 \sigma T^3}{3 \rho H} , \quad (\text{III.2.4})$$

and

$$K_L = \frac{16 \sigma T^3}{3 \rho L} . \quad (\text{III.2.5})$$

H and L are respectively the conductivities associated with phonon and plasma conduction and σ is the Stefan-Boltzmann constant. The phonon term is important only at low temperatures. The purpose of the present section is to demonstrate the relative importance of the K_r and K_L terms.

In figures III-1 and III-2, the functions K_r , K_L and K_{eff} are shown for copper at two densities. As for the functions K_r and K_L , the more important flow phenomena is the one with the smaller value of K. For

example at $\rho = 8.94$ and $T = 30$ ev, electron energy flow is approximately ten times as large as radiation energy flow. The two effects are of equal importance at the point of intersection of the curves. Figure III-3 shows the density-temperature relation where the two phenomena are the same magnitude. At high temperatures and low densities radiation flow is dominant, while plasma conduction is stronger at high densities and lower temperatures. This curve was calculated using the ANEOS package relations.

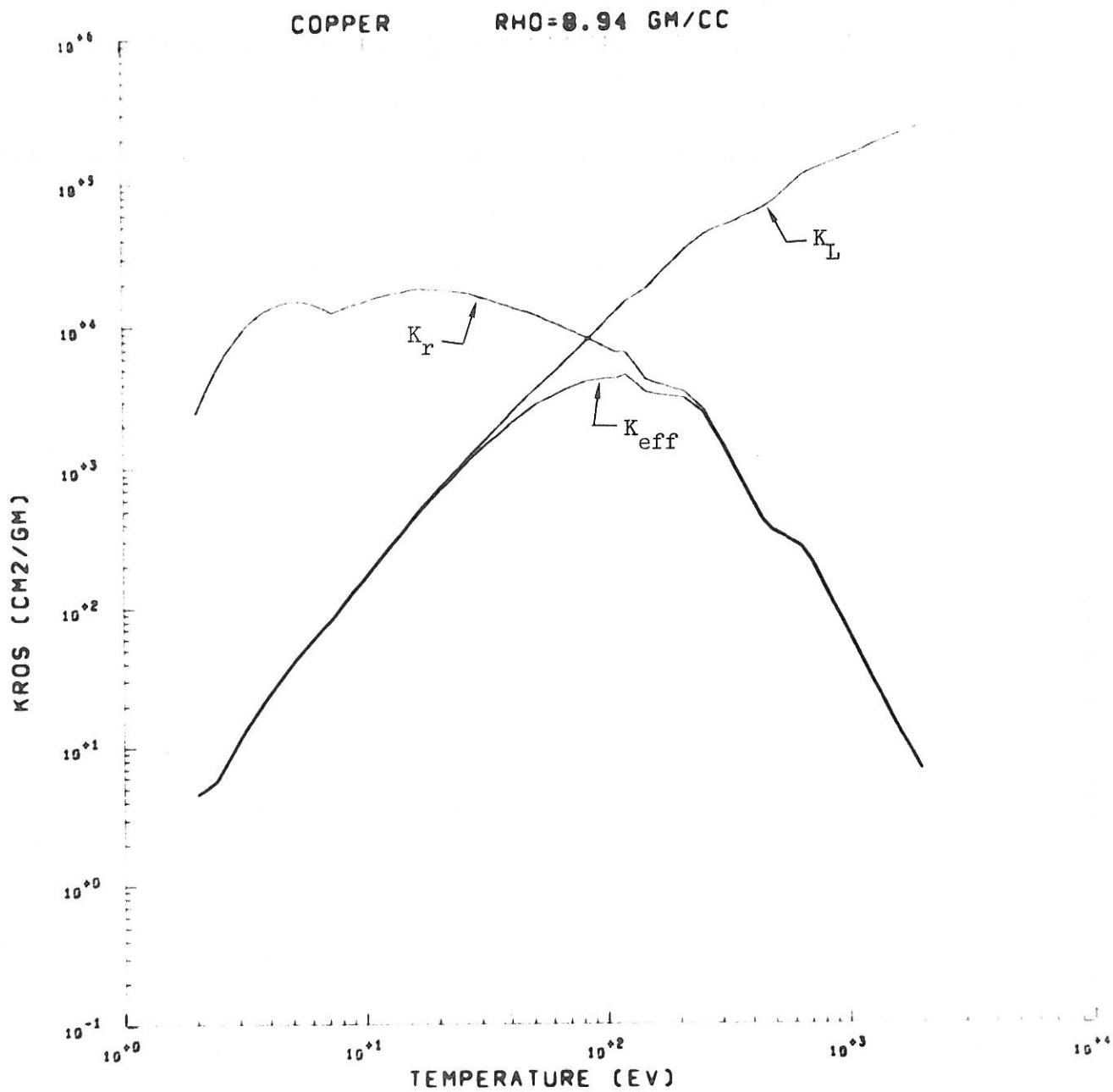


Figure III-1. Opacities of Copper for $\rho = 8.94 \text{ gm/cc.}$

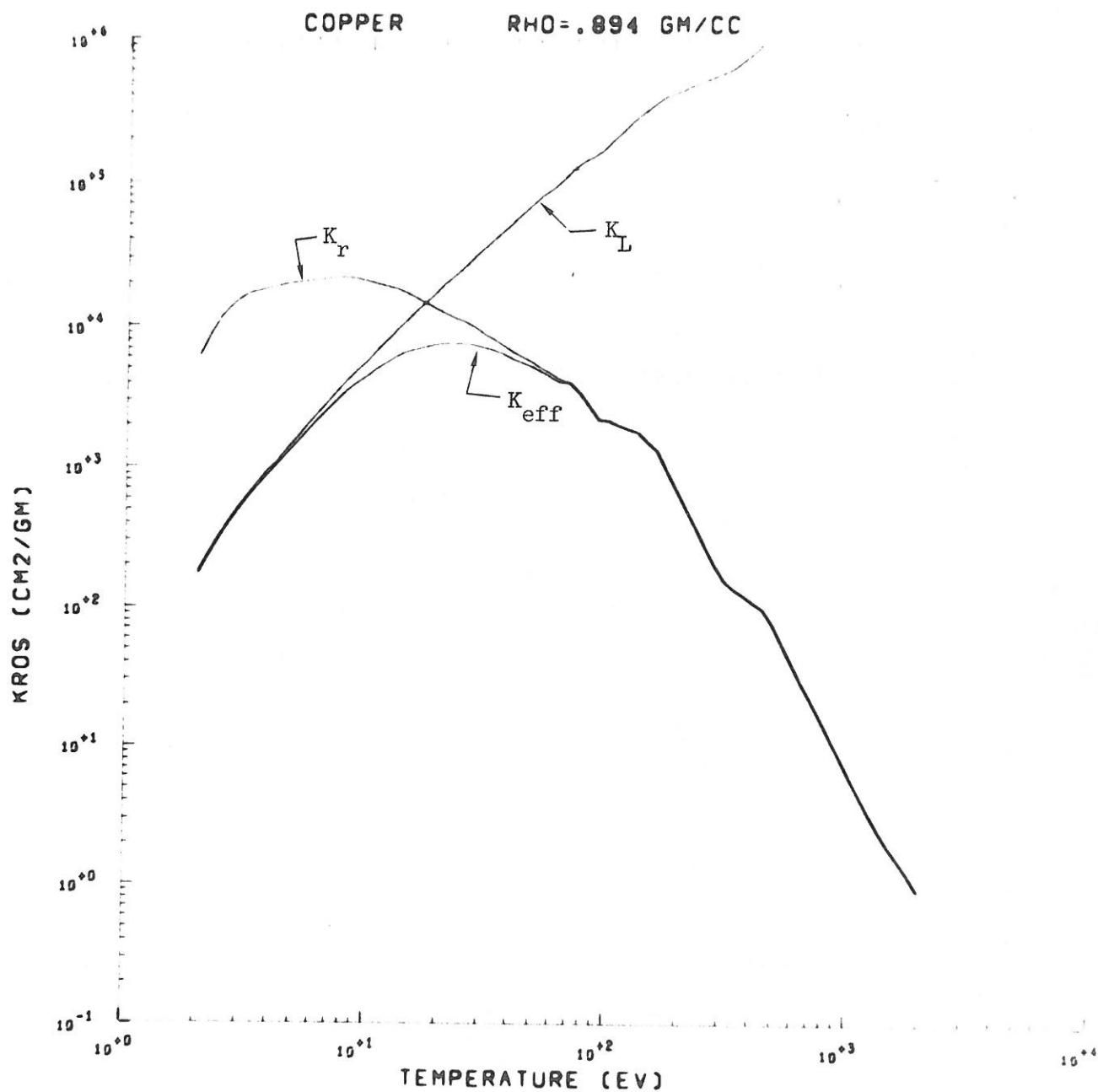


Figure III-2. Opacities of Copper for $\rho = .894 \text{ gm/cc.}$

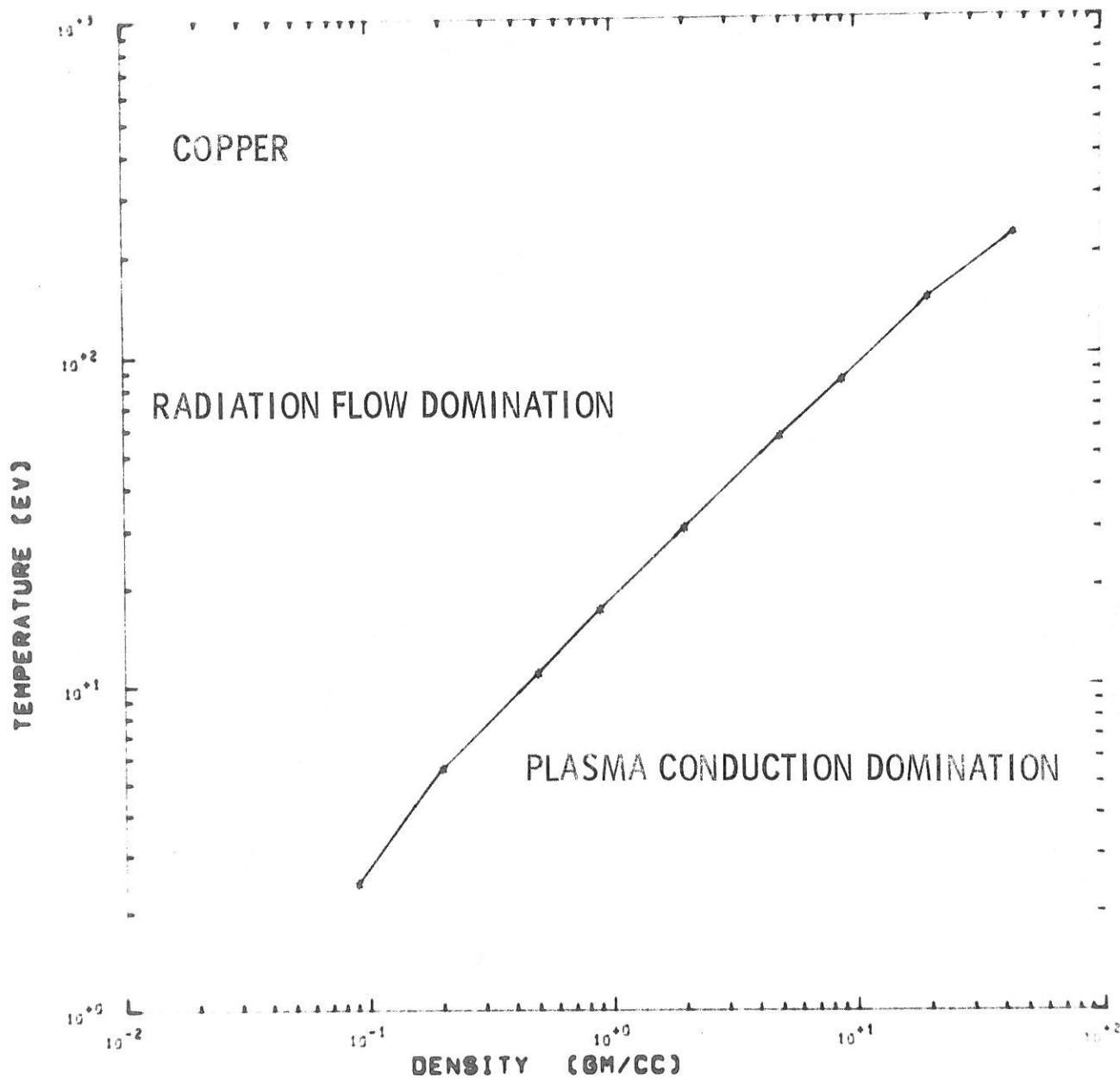


Figure III-3. Relative importance of energy flow phenomena in Copper.

III.3 Melt Transition Input Parameters

Complete details concerning the numerical treatment of the melt transition are given in section V of R2. An additional input option has been added to aid in the use of this feature.

The two required parameters concerning the melt are H_f , the heat of fusion, and one which determines the density of the liquid phase at zero pressure. Two optional forms were available for the latter. Either ρ_l/ρ_s (ratio of liquid to solid density) or ρ_l were acceptable.

In some cases, a third optional form would be more useful.¹² The Clapeyron-Clausius relation is

$$\frac{dP}{dT} = \frac{H_f}{T\Delta V}, \quad (\text{III.3.1})$$

where

$$\Delta V = V_l - V_s = \frac{1}{\rho_l} - \frac{1}{\rho_s}, \quad (\text{III.3.2})$$

and $\frac{dP}{dT}$ determines the change in pressure at melt with temperature. It is now possible to input the value of ΔV so that experimental data for $\frac{dP}{dT}$ can be fitted exactly even while other EOS parameters are being adjusted.

III.4 Additional Equation of State Forms

Three more equation of state options have been made available as part of the ANEOS package. All are relatively simple when compared to the previously available forms and, from a thermodynamic point of view, are a step backwards. However, in some problems, the increased computational speed is worth the loss of information.

The first form is designed for use when large masses of low temperature solid materials are present and is similar to the solid EOS employed in the WONDY code.⁴ The second is an ideal gas included mainly to aid in comparison with other hydrodynamic codes. The last is a modified form of the JWL EOS developed at LLL for the description of detonation products.¹⁴⁻¹⁵

III.4-1 Type-1 Equation of State, Low Temperature Solids

This form of equation of state is designed to be used for low temperature solids. Where it is valid, it has the advantage of increased computational speed when compared to other optional forms.

Consider a Helmholtz free energy of

$$F(\rho, T) = E_c(\rho) - \rho_o \Gamma_o C_v T / \rho - C_v T \ln(T/T_o) , \quad (\text{III.4.1})$$

where the notation is the same as used in R2. The subscript o represents a reference point. The heat capacity C_v and the product of the density and Grüneisen coefficient are assumed constant in this model. From this relation it follows that

$$P(\rho, T) = \rho^2 \frac{\partial F}{\partial \rho} = P_c + \rho_o \Gamma_o C_v T , \quad (\text{III.4.2})$$

$$E(\rho, T) = -T^2 \frac{\partial F}{\partial T} \left(\frac{F}{T} \right) = E_c + C_v T , \quad (\text{III.4.3})$$

$$S(\rho, T) = - \frac{\partial F}{\partial T} = C_v \left\{ \rho_o \Gamma_o / \rho + \ln(T/T_o) + 1 \right\} , \quad (\text{III.4.4})$$

where

$$P_c(\rho) = \rho^2 \frac{dE_c}{d\rho} . \quad (\text{III.4.5})$$

These relations should describe the material along the Hugoniot. If the subscript H represents the functions on the Hugoniot from the reference state, (III.4.2) and (III.4.3) can be written as

$$P_H = P_c + \rho_o \Gamma_o C_v T_H \quad (\text{III.4.6})$$

and

$$E_H = E_c + C_v T_H . \quad (\text{III.4.7})$$

By combining the above relations, the result is

$$P(\rho, T) = P_H(\rho) + \rho_o \Gamma_o C_v \left\{ T - T_H(\rho) \right\} \quad (\text{III.4.8})$$

and

$$E(\rho, T) = E_H(\rho) + C_v \left\{ T - T_H(\rho) \right\} . \quad (\text{III.4.9})$$

It is also well known that

$$E_H = \frac{P_H \eta}{2\rho_0} + E_0 , \quad (\text{III.4.10})$$

with

$$\eta = 1 - \rho_0/\rho \quad (\text{III.4.11})$$

and the assumption

$$P_H(\rho_0) = 0 . \quad (\text{III.4.12})$$

E_0 is the reference point energy and can be arbitrarily defined. Here we use

$$E_0 = C_v T_0 . \quad (\text{III.4.13})$$

We shall attempt to employ the relations (III.4.8) to (III.4.11) with fits to experiment Hugoniot data to describe the material. If P_H is a known function of density, the difficulty is to determine the function $T_H(\rho)$. Substitution of these relations with $T = 0$ in (III.4.5) yields

$$\rho_0 C_v \frac{dT_H}{d\eta} - \rho_0 \Gamma_0 C_v T_H = \frac{\eta}{2} \frac{dP_H}{d\eta} - \frac{1}{2} P_H , \quad (\text{III.4.14})$$

which must be solved for T_H . The result is

$$T_H = T_0 e^{\Gamma_0 \eta} + \frac{\Gamma_0 \eta}{2C_v \rho_0} \int_0^\eta e^{-\Gamma_0 \eta} \eta^2 \frac{d}{d\eta} \left\{ \frac{P_H}{\eta} \right\} d\eta . \quad (\text{III.4.15})$$

Unfortunately, the commonly used forms for experimental Hugoniot data do not yield expressions in the integral which can be evaluated simply. While the

integral can be done exactly in terms of incomplete Gamma functions, the approach employed here is to use an approximate form which has the correct limiting values and derivatives.

$$T_H \approx T_o e^{\Gamma_o \eta} + \frac{\eta^3}{4C_v \rho_o} \frac{d}{d\eta} \left\{ \frac{P_H}{\eta} \right\} . \quad (\text{III.4.16})$$

Note that from both (III.4.14) and (III.4.16), it follows that

$$\left. \frac{dT_H}{d\eta} \right|_{\rho_o} = \Gamma_o T_o \quad (\text{III.4.17})$$

and

$$\left. \frac{d^2 T_H}{d\eta^2} \right|_{\rho_o} = \Gamma_o^2 T_o \quad (\text{III.4.18})$$

The use of the approximate expression for T_H makes the relations thermodynamically inconsistent. Another way of viewing the situation is that T is no longer the absolute temperature but a closely related parameter in the equation of state. At a later point in this section, we will consider the implications with regard to (III.4.4).

Two expressions are available for the function P_H . It is often observed that experimental Hugoniot data may be represented over a limited range of pressures in the form

$$U_s = S_o + S_1 U_m \quad (\text{III.4.19})$$

where U_s and U_m are the shock and material velocities associated with the shock. S_o and S_1 are experimentally determined constants. Since

$$P_H = \rho_o U_m U_s \quad (\text{III.4.20})$$

and

$$U_m = \eta U_s \quad (\text{III.4.21})$$

it follows that

$$P_H = \rho_o s_o^2 \eta / (1 - s_1 \eta)^2 \quad (\text{III.4.22})$$

For some materials (III.4.19) cannot be employed, so the relation

$$P_H = \rho_o s_o^2 \eta \left(1 + K_1 \eta + K_2 \eta^2 + K_3 \eta^3 + K_4 \eta^4 \right) = \rho_o \eta U_s^2 \quad (\text{III.4.23})$$

is provided where K_1, K_2, K_3 and K_4 are input parameters.

These expressions yield acceptable results for compressed states

$\rho \geq \rho_o$, $\eta \geq 0$. However, difficulties are encountered for expanded states.

First consider (III.4.22) in the limit of zero density ($\eta \rightarrow -\infty$),

$$P_H \rightarrow \frac{\rho_o s_o^2}{\eta s_1^2} \rightarrow 0 \quad , \quad (\text{III.4.24})$$

$$E_H \rightarrow \frac{s_o^2}{2s_1^2} + E_o \quad , \quad (\text{III.4.25})$$

and, unfortunately,

$$T_H \rightarrow - \frac{s_o^2}{2c_v s_1^2} \quad , \quad (\text{III.4.26})$$

The negative temperature is clearly unacceptable. While this EOS option is not designed for use at low densities, this can cause problems for slightly expanded states in the solid phase and elevated temperature. Another approach is required.

Let the subscript s represent the isentrope through the reference point. From (III.4.4) it follows that

$$T_s = T_o e^{\Gamma_o \eta} . \quad (\text{III.4.27})$$

We now assume that the energy along this isentrope E_s can be represented by (III.4.10),

$$E_s \approx E_H = \frac{P_H \eta}{2\rho_o} + E_o . \quad (\text{III.4.28})$$

The pressure along the isentrope is not P_H , since P_s must satisfy the relation

$$P_s = \rho_o \frac{dE_s}{d\eta} . \quad (\text{III.4.29})$$

The result is

$$P_s = P_H / (1 - s_1 \eta) , \quad (\text{III.4.30})$$

where P_H is given by (III.4.22). In place of (III.4.8) and (III.4.9), we now use the relations

$$P(\rho, T) = P_s(\rho) + \rho_o \Gamma_o C_v \left\{ T - T_s(\rho) \right\} \quad (\text{III.4.31})$$

and

$$E(\rho, T) = E_s(\rho) + C_v \left\{ T - T_s(\rho) \right\} , \quad (\text{III.4.32})$$

for $\rho < \rho_o$. The above relations possess sufficient continuity at $\rho = \rho_o$.

The power series relation for P_H given by (III.4.23) is not well behaved for $\eta < 0$. As a result the form given by (III.4.22) is also used in place of (III.4.23) for negative η . The value of S_L employed can be supplied as an input parameter or defaulted to unity. Note that the effective sublimation energy given by this model is found from (III.4.25).

Again it should be stressed that these relations are not designed to be used at low densities. The expressions for $\rho < \rho_o$ are defined so as to ensure reasonable behavior up to the melting point. Eq. (III.4.16) is sometimes unreasonable in this area.

The specific entropy is found from (III.4.4). Due to the use of the approximate expression for T_H for $\rho > \rho_o$, the calculated values of S are not exactly correct. Within this limitation the equation of state is acceptable though inconsistent. The formulation is of course consistant for $\rho \leq \rho_o$.

The heat capacity C_V can be specified as an input parameter or defaulted to the value

$$C_V = 3 N_o k \quad (\text{III.4.33})$$

where k is Boltzmann's constant and N_o is the number of atoms per unit mass. It should be recalled that in CHART D, C_V must have the units of ergs/(gm ev).

The atomic numbers and fractions of the elements in the material are required as input data. They are used only to determine N_o in (III.4.33). No electronic calculation is attempted . As a result there is no way to calculate a Rosseland opacity or plasma conduction coefficient. Since this

option is designed to be used only at low temperatures where neither is important, the effective opacity for these two effects is set to a large number (10^5). Phonon conductivity can be included as with previous options [section VII-2 in R2].

Either a melt temperature T_m or a melt "energy" \mathcal{E}_m is required as an input parameter. If \mathcal{E}_m is defined, then T_m is computed by the approximate relation

$$T_m = \frac{\mathcal{E}_m}{C_v} + T_o \quad . \quad (\text{III.4.34})$$

This form is used because the solution of the exact relation is not worth the storage that would be required. As previously stated, this EOS option is not suggested for materials in the region of melt and above. However, if it is used in this area, then the modification to the fracture calculation discussed in section II.3 should also be employed.

III.4-2 Type-2 Equation of State, Ideal Gas

This equation of state option is a constant heat capacity ideal gas. Note that it is not the same as ANEOS option +2 as defined in R2.

The Helmholtz free energy is written as

$$F(\rho, T) = C_v T \left\{ 1 - \ln \left[\frac{T}{T_o} \left(\frac{\rho_o}{\rho} \right)^{\gamma-1} \right] \right\} . \quad (\text{III.4.35})$$

The heat capacity C_v and the ratio of specific heats γ are constants. The subscript o represents a reference point. It then follows that

$$P(\rho, T) = \rho^2 \frac{\partial F}{\partial \rho} = (\gamma - 1) \rho C_v T , \quad (III.4.36)$$

$$E(\rho, T) = -T^2 \frac{\partial}{\partial T} \left(\frac{F}{T} \right) = C_v T , \quad (III.4.37)$$

and

$$S(\rho, T) = - \frac{\partial F}{\partial T} = C_v \ln \left[\frac{T}{T_o} \left(\frac{\rho_o}{\rho} \right)^{\gamma-1} \right] . \quad (III.4.38)$$

The heat capacity can be specified as an input parameter or defaulted to the value

$$C_v = \frac{3}{2} N_o k \quad (III.4.39)$$

in the same manner as eq. (III.4.33). The form assumed for the effective Rosseland opacity is

$$\kappa_r(T) = K_1 / (1 + T/K_2)^3 + 0.2 \quad (III.4.40)$$

with K_1 and K_2 as input parameters.

III.4-3 Type-3 Equation of State, Generalized JWL Form for High Explosives

The method of treating high explosives in CHART D is discussed in R1 and section IV of this paper. The equations of state for such materials can be represented quite well by either the tabular or analytic (options 3 or 4) forms. There is, however, a difficulty in fitting the thermodynamic information to the available experimental data, in that it is quite time consuming. Most experimental data is related to dynamic, not thermodynamic, properties. Thermodynamic parameters must be adjusted through a long series of hydrodynamic code runs.

Investigators at other laboratories have had similar difficulties. A large amount of effort has gone into these studies. As a result, to aid CHART D users in obtaining instant EOS data for burning high explosives, an option has been added for a generalized form of the Jones-Wilkins-Lee (JWL) EOS developed at LLL.¹⁴⁻¹⁵ This form is suitable only for burning high explosive materials and related expansions. It is not intended for detailed response of the unburned solid nor use at very high temperatures. If these areas are important, other EOS options must be employed.

The JWL equation of state is

$$P = A_L \left(1 - \frac{\omega}{\mu R_{1L}} \right) e^{-\mu R_{1L}} + B_L \left(1 - \frac{\omega}{\mu R_{2L}} \right) e^{-\mu R_{2L}} + \frac{\omega E_v}{\mu} , \quad (\text{III.4.41})$$

where

$$\mu = \frac{\rho_0}{\rho} . \quad (\text{III.4.42})$$

ρ_0 is the density of the undetonated explosive, E_v is the energy per unit reference volume, and A_L , B_L , R_{1L} , R_{2L} and ω are material constants. The equation of an isentrope can easily be shown to be

$$P_s = A_L e^{-\mu R_{1L}} + B_L e^{-\mu R_{2L}} + C_L \mu^{-(\omega+1)} , \quad (\text{III.4.43})$$

where the value of C_L determines the entropy value. Tables of the constants for many explosive compounds are available.¹⁵ The value of C_L listed corresponds to the isentrope through the Chapman - Jouguet state.

For the present purpose, it is convenient to rewrite these relations in terms of density instead of μ and, since the LLL tabulations employ

megabar, etc., units, redefine the material constants. The new expressions are

$$P = A \left(1 - \frac{\omega\rho}{R_1} \right) e^{-R_1/\rho} + B \left(1 - \frac{\omega\rho}{R_2} \right) e^{-R_2/\rho} + \omega \rho E \quad (\text{III.4.44})$$

and

$$P_s = A e^{-R_1/\rho} + B e^{-R_2/\rho} + C \rho^{\omega+1}, \quad (\text{III.4.45})$$

where

$$A = 10^{12} A_L, \quad (\text{III.4.46})$$

$$B = 10^{12} B_L, \quad (\text{III.4.47})$$

$$C = C_L \rho_o^{-(\omega+1)}, \quad (\text{III.4.48})$$

$$R_1 = \rho_o R_{1L}, \quad (\text{III.4.49})$$

$$R_2 = \rho_o R_{2L}. \quad (\text{III.4.50})$$

The following development will employ the coefficients on the left-hand side of these equations. Please note, however, that the input parameters in the ANEOS package are those on the right, i.e., those in the LLL tables.¹⁵

To employ this EOS in CHART D, it must be generalized to a form with temperature and density as independent variables and hopefully be complete and self-consistent. Such a form is

$$F(\rho, T) = E_c(\rho) - C_v T \ln \left[\frac{T}{T_o} \left(\frac{\rho_o}{\rho} \right)^\omega \right], \quad (\text{III.4.51})$$

where F is the Helmholtz free energy, C_V is the heat capacity assumed constant, and E_c is the zero temperature compressional energy

$$E_c(\rho) = \frac{A}{R_1} e^{-R_1/\rho} + \frac{B}{R_2} e^{-R_2/\rho} - \frac{\rho^\omega}{\omega \rho_{oo}^{\omega+1}} \left\{ A e^{-R_1/\rho_{oo}} + B e^{-R_2/\rho_{oo}} \right\} + E_{oo} \quad (\text{III.4.52})$$

The density ρ_{oo} and energy E_{oo} are considered below as is the proof that (III.4.44) and (III.4.45) follow from (III.4.51).

The required thermodynamic functions can be obtained from the usual relations

$$P(\rho, T) = P_c(\rho) + \omega \rho C_V T , \quad (\text{III.4.53})$$

$$E(\rho, T) = E_c(\rho) + C_V T , \quad (\text{III.4.45})$$

$$S(\rho, T) = C_V \left\{ 1 + \ln \left[\frac{T}{T_o} \left(\frac{\rho_o}{\rho} \right)^\omega \right] \right\} , \quad (\text{III.4.55})$$

and

$$P_c(\rho) = \rho^2 \frac{dE_c}{d\rho} \quad (\text{III.4.56})$$

$$= A e^{-R_1/\rho} + B e^{-R_2/\rho} - \left(\frac{\rho}{\rho_{oo}} \right)^{\omega+1} \left\{ A e^{-R_1/\rho_{oo}} + B e^{-R_2/\rho_{oo}} \right\} .$$

As with the other EOS options ρ_{oo} is the density at zero temperature and pressure. The normal reference point of the unburned explosive is at ρ_o , T_o . The density ρ_{oo} is determined by the condition that

$$P(\rho_o, T_o) = 0 , \quad (\text{III.4.57})$$

or

$$\left\{ A e^{-R_1/\rho_{oo}} + B e^{-R_2/\rho_{oo}} \right\} \rho_{oo}^{-(\omega+1)} = \quad (III.4.58)$$

$$\left\{ A e^{-R_1/\rho_o} + B e^{-R_2/\rho_o} + \omega \rho_o C_v T_o \right\} \rho_o^{-(\omega+1)} .$$

Assuming that T_o is small, this relation can easily be solved by an iterative procedure since ρ_{oo} is only slightly greater than ρ_o due to thermal expansion. E_{oo} is then defined so that

$$E(\rho_{oo}, 0) = E_c(\rho_{oo}) = 0 \quad . \quad (III.4.59)$$

The heat capacity C_v can be specified as an input parameter or defaulted to the value

$$C_v = 3 N_o k \quad (III.4.60)$$

as discussed in relation to eq. (III.4.33). It should be clear that the temperature at the burn front can be adjusted by changing the value of C_v .

Either a melt temperature T_m or a melt energy \mathcal{E}_m is required as an input parameter even though they have no effect on the equation of state. In most cases, a value of T_m slightly greater than T_o is sufficient. The relation between \mathcal{E}_m and T_m is given by (III.4.34).

The only remaining problem in defining the EOS is specification of the Rosseland opacity and conductivities. The form given by (III.4.40) is assumed for K_r . Phonon conduction is treated as in section VII-2 in R2. No plasma conduction expression is included.

It is now shown that these relations can be reduced to the JWL expressions. Substitution of (III.4.54) into (III.4.53) yields

$$P = P_c + \omega \rho (E - E_c) . \quad (\text{III.4.61})$$

Then employing (III.4.52) and (III.4.56), it follows that

$$P = A \left(1 - \frac{\omega \rho}{R_1} \right) e^{-R_1/\rho} + B \left(1 - \frac{\omega \rho}{R_2} \right) e^{-R_2/\rho} + \omega \rho (E - E_{\infty}) , \quad (\text{III.4.62})$$

which is the desired result. The shift in the zero point of energy given by E_{∞} is necessary since CHART D requires nonnegative energy values. The reference point energy in (III.4.44), defined by $P(\rho_0, E) = 0$ is a large negative number.

It follows from (III.4.55) that an isentrope is determined so that

$$T \rho^{-\omega} \equiv \delta = \text{constant} . \quad (\text{III.4.63})$$

Substitution of this relation into (III.4.53) and (III.4.56) demonstrates that (III.4.45) is the result with

$$C = \omega C_v \delta - \left(A e^{-R_1/\rho_{\infty}} + B e^{-R_2/\rho_{\infty}} \right) \rho_{\infty}^{-(\omega+1)} . \quad (\text{III.4.64})$$

In CHART D and CKEOS, this EOS is treated in the same manner as other HE forms. The Chapman - Jouguet pressure P_{cJ} and detonation wave velocity D are defined as input parameters. The density behind the detonation front is

$$\rho_{cJ} = \rho_0 / \left(1 - P_{cJ}/\rho_0 D^2 \right) \quad (\text{III.4.65})$$

and the temperature is defined by the relation

$$P(\rho_{cJ}, T_{cJ}) = P_{cJ} . \quad (\text{III.4.66})$$

The Q value is then

$$Q = E(\rho_{cJ}, T_{cJ}) - E(\rho_o, T_o) - \frac{1}{2} P_{cJ} \left\{ \frac{1}{\rho_o} - \frac{1}{\rho_{cJ}} \right\} \quad (\text{III.4.67})$$

and the maximum energy available for conversion to kinetic energy and internal energy in other materials besides the explosive products is (see section IV.2)

$$\epsilon_{HE} = Q - \left\{ E_\infty - E(\rho_o, T_o) \right\} , \quad (\text{III.4.68})$$

where E_∞ is the internal energy of the expanded detonation products. If the material expands adiabatically to zero density and temperature, then $E_\infty = E_{oo}$. This assumption is employed in the Livermore tabulation of the energy output parameter EO .¹⁵ In terms of the present notation

$$EO = \rho_o \left\{ Q - E_{oo} + E(\rho_o, T_o) \right\} . \quad (\text{III.4.69})$$

Unfortunately this somewhat overpredicts the useful energy output because the detonation products fail to expand to such extend in reasonable time periods. In the CKEOS calculation discussed in section IV.2, a higher final density is assumed with the result that $E_\infty > E_{oo}$.

III.5 Tension Suppression Above

The Melt Temperature in EOS Types 0 and 1

The method of calculation described in section V-6 of R2 is used in ANEOS options 0 and 1. No liquid-vapor mixed-phase construction was attempted and tensions were suppressed above the melt temperature. This tension suppression feature has now been removed since it sometimes caused thermodynamic problems at other points in CHART D (it could lead to negative temperatures). In practice the same effect that was desired can be realized using the fracture calculation and the features described in section II.3.

IV. CKEOS PROGRAM MODIFICATIONS

CKEOS is a test program to aid in the selection of input data for CHART D and the ANEOS package. Both tabular and analytic equations of state can be considered as discussed in R3. Three changes have been made in the coding in addition to those discussed in section III. The first is an isentrope calculation which requires no explanation here. The second computation will suggest values of input parameters for the ANEOS package data to move the critical point to a desired location. The last considers the details of burning high explosives.

IV.1 Adjustment of Critical Points

Some of the procedure for adjustment of the location of the critical point under ANEOS options 3 and 4 is given in appendix E of R2. A computation has now been added to CKEOS to suggest values for the ANEOS input parameters C_{53} and C_{54} to move the critical point to any desired location. Unfortunately the suggested values are not guaranteed to work in all cases due to the problem discussed on page 37 in R2. For most materials this is not a problem.

The critical point is defined by the relations

$$\left(\frac{\partial P}{\partial \rho}\right)_T = \left(\frac{\partial^2 P}{\partial \rho^2}\right)_T = 0 . \quad (\text{IV.1.1})$$

The adjustable term in the zero temperature pressure function is (section III-2 in R2)

$$P = C_{53} \eta^2 \left\{1 - \frac{\eta}{C_{54}}\right\}^3 \left\{\frac{\eta}{C_{54}} - 0.2\right\} \quad (\text{IV.1.2})$$

where

$$\eta = \frac{\rho}{\rho_{\infty}} \leq C_{54} . \quad (\text{IV.1.3})$$

In effect this term modifies the shape of the interatomic potential function without changing its strength.

The method used here calculates the derivatives in (IV.1.1) with $C_{53} = 0$ and then sets the appropriate derivatives of (IV.1.2) to the negative of the computed values. The resulting two equations with the two unknowns C_{53} and C_{54} can be solved by an iterative procedure.

Several tests can easily be applied to these computed parameters. It follows from (IV.1.3) that

$$C_{54} > \frac{\rho_c}{\rho_{\infty}} \quad (\text{IV.1.4})$$

where ρ_c is the desired critical density. The properties of liquid phase at zero pressure melt are used to determine the liquid equation of state. Therefore, for this calculation, the condition

$$\frac{\rho_{lm}}{\rho_{\infty}} > C_{54} \quad (\text{IV.1.5})$$

must be imposed even though it is not a normal requirement. It also follows that the computed pressure using these parameters must be positive at the desired critical point. A negative pressure is a clear indication of the multiple critical point structure pictured on page 37 of R2. If any of these tests fail, the code prints a message to that effect. On the other hand, if the tests are satisfied, the new parameters should be submitted to CKEOS in the normal manner for a final check.

IV.2 Evaluation of Equations of State for High Explosives

Unfortunately much of the experimental data relating to the detonation of high explosives is concerning the dynamic response and not the thermodynamic properties. The only way to determine the best equation of state for a given material is by computer experimentation with the hydrodynamic code. There is, however, one thermodynamic parameter which is normally available. It is ϵ_{HE} , the maximum energy available for conversion to kinetic energy and internal energy of other materials in the calculation (due to shock heating).

As discussed in R1, Q is the chemical energy released per unit mass at the burn front. In other words, Q is the energy that must be added to the material at the burn front by the CHART D energy source subroutines. The value of Q is

$$Q = E_{cJ} - E_o - \frac{1}{2} \left(P_{cJ} + P_o \right) \left(\frac{1}{\rho_o} - \frac{1}{\rho_{cJ}} \right) \quad (\text{IV.2.1})$$

where the subscript o represents the reference point of the undetonated material and cJ represents the Chapman - Jouguet point. ϵ_{HE} is then found from the energy conservation law to be

$$\epsilon_{HE} = Q + E_o - E_\infty , \quad (\text{IV.2.2})$$

with E_∞ the internal energy of the expanded detonation products.

A calculation has been added to CKEOS to determine ϵ_{HE} and the conversion factor ϵ_{HE}/Q . The value of E_∞ is found by considering the release isentrope from the Chapman - Jouguet point. The final density is determined so that the pressure is one atmosphere.

V. MASPLT PROGRAM MODIFICATIONS

MASPLT is an all purpose plot program for CHART D.³ The major change in this program is the addition of the capability of producing plots which present several different functions per frame. Up to four ordinate variables can be plotted against a common abscissa variable. No detailed explanation is required. S. Gasser of the Sandia computing group has greatly aided in the system's problems.

The new input instructions are found in appendix D.

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APPENDIX A

MODIFICATIONS TO HERRMANN'S POROUS MATERIAL MODEL FOR A VARIABLE EFFECTIVE GRÜNEISEN COEFFICIENT

APPENDIX A

Modifications to Herrmann's Porous Material Model for a Variable Effective Grüneisen Coefficient

The differences in the elastic region calculations between the CHART D model and Herrmann's model^{16,17} as employed in WONDY,⁴ TOODY⁵ and other codes are discussed in R1. The modification presented in section II.2-1 can be formulated in terms of Herrmann's model. His model does have an effective Grüneisen coefficient; however, it is determined by the elastic wave velocity and cannot be varied independently.

It is assumed that the reader has covered the material in section II.2-1. The same reasoning concerning relaxation time, etc., applies to the following developments.

Under Herrmann's formulation, changes within the elastic region are described using the relation

$$d\alpha = \left(\frac{\partial \alpha}{\partial P} \right)_S dP . \quad (A.1)$$

where

$$\left(\frac{\partial \alpha}{\partial P} \right)_S = \frac{\alpha}{K_0} \left\{ 1 - \frac{\alpha}{h^2} \right\} , \quad (A.2)$$

$$K_0 = \rho C_s^2 \quad (A.3)$$

and h is given by (II.2.3). As before quantities with no subscript refer to the solid material in the foam.

The modified form of (A.1) corresponding to (II.2.30) is written as

$$d\alpha = \left(\frac{\partial \alpha}{\partial P} \right)_S dP + K_w \dot{S} dt \quad (A.4)$$

where the first term on the right hand side is as given above. $\dot{S} dt$ is the same as defined in section II.2-1. K_w is the function to be determined and, formally, is defined as

$$K_w = \frac{1}{T} \left(\frac{\partial \alpha}{\partial S} \right)_P . \quad (A.5)$$

By the same method from which (II.2.15) was calculated, it follows that

$$dP = \left(\frac{\partial P}{\partial E} \right)_\rho dE + \left\{ \left(\frac{\partial P}{\partial \rho} \right)_S - \left(\frac{\partial P}{\partial E} \right)_\rho \left(\frac{\partial E}{\partial \rho} \right)_S \right\} d\rho \quad (A.6)$$

where

$$c_s^2 = \left(\frac{\partial P}{\partial \rho} \right)_S \quad (A.7)$$

and

$$\frac{P}{\rho^2} = \left(\frac{\partial E}{\partial \rho} \right)_S . \quad (A.8)$$

Now considering a constant foam density ρ_f , it follows from (A.4) that

$$d\rho = \rho_f \left\{ \Phi dP + K_w dE \right\} , \quad (A.9)$$

using the notation

$$\Phi = \left(\frac{\partial \alpha}{\partial P} \right)_S \quad (A.10)$$

and

$$dE = \dot{P} dt \quad . \quad (A.11)$$

Substitution of this result and

$$dP = \rho_f \Gamma_{eff} dE \quad (A.12)$$

into (A.6) leads to the conclusion that

$$K_w = - \rho_f \Gamma_{eff} \Phi + \frac{\Gamma_{eff} - \frac{1}{\rho_f} \left(\frac{\partial P}{\partial E} \right)_P}{\rho_f \left\{ C_s^2 - \frac{P}{\rho} \left(\frac{\partial P}{\partial E} \right)_P \right\}} \quad . \quad (A.13)$$

Let us now assume that the solid material can be described by the Grüneisen relation here written as,

$$\left(\frac{\partial P}{\partial E} \right)_P = \rho \Gamma_s \quad (A.14)$$

the above relation becomes

$$K_w = - \rho_f \Gamma_{eff} \Phi + \frac{\Gamma_{eff} - \frac{\rho}{\rho_f} \Gamma_s}{C_s^2 - \frac{\Gamma_s P}{\rho}} \quad . \quad (A.15)$$

Note that if we consider loading from the reference state ($P = 0$) where

$$\Phi = \frac{1}{\rho_f C_s^2} \left\{ 1 - \frac{\rho C_s^2}{\rho_f C_e^2} \right\} \quad (A.16)$$

it is then clear that

$$K_w = \frac{\rho}{\rho_f} \left\{ \frac{\Gamma_{eff}}{c_e^2} - \frac{\Gamma_s}{c_s^2} \right\} . \quad (A.17)$$

If $K_w = 0$ (Herrmann's original model), it follows that

$$\Gamma_{eff} = \left(\frac{c_e}{c_s} \right)^2 \Gamma_s \quad (A.18)$$

as suggested at the end of section II.2-1.

APPENDIX B
A SIMPLE METHOD OF EMPLOYING THE
ANEOS PACKAGE IN OTHER HYDRODYNAMIC CODES

APPENDIX B

A Simple Method of Employing the ANEOS Package in Other Hydrodynamic Codes

The ANEOS equation of state package is constructed as a self-contained unit which can be employed with other codes requiring thermodynamic information. The basic coding requirements are given in section IX of R2. The purpose of this appendix is to demonstrate a very simple method which requires a minimum of new coding while retaining complete generality.

To illustrate how simple a procedure can be used, an example for WONDY IV⁴ is given. Admittedly each program must be treated in a slightly different manner but the general logic is the same. The same method should work for any Lagrangian code employing ρ -E independent variables. Eulerian codes will need a more complex coupling subroutine due to "mixed" cells but the ANEOS package itself and the existing hydrodynamic code modifications should be no more complex than with Lagrangian codes.

The flow of logic in a hydrodynamic code is quite complex and no attempt will be made here to reproduce it. Normally the last step in a cycle calculation is the solution, for each cell or zone, of the conservation of energy expression. In Lagrangian form, this can be expressed as

$$\frac{dE}{dt} = -(P+Q) \frac{dV}{dt} + \dot{R} + \dot{K} \quad (\text{B.1})$$

where

E = specific internal energy

P = pressure

Q = viscosity

$V = \frac{1}{\rho}$ = specific volume

t = time

and $\dot{R} + \dot{K}$ is a general term describing a collection of things required to make (B.1) correct. These terms might for example relate to elasticity, porosity or heat conduction. R is to be treated in an explicit fashion, K implicitly.

It will be assumed that K depends only on the local material properties or rates. Effects which have nonlocal spatial dependences (such as implicit energy flows) must be treated in a more complex fashion as found in section III of R1. In the WONDY example to follow, the K term is not required but it is carried in this development for generality.

The finite difference form of this relation is written as

$$E_n = E_o - \left\{ \frac{1}{2} (P_n + P_o) + Q \right\} \Delta V + \dot{R} \Delta t + K_n - K_o , \quad (B.2)$$

where the subscript n represents the new cell quantities (those to be calculated) and o represents the old or previously known values. At this point in the calculation

$$\Delta V = V_n - V_o = \frac{1}{\rho_n} - \frac{1}{\rho_o} \quad (B.3)$$

has been determined. The three quantities E_n , P_n and K_n are the only unknowns.

Thermodynamically the three unknowns cannot be independent for an equilibrium state. Since the density ρ_n is known, only one other variable is required to completely determine the thermodynamic state. As in CHART D, the temperature T is now introduced so that

$$E_n = E(T_n, \rho_n) \quad (B.4)$$

$$P_n = P(T_n, \rho_n) \quad (B.5)$$

$$K_n = K(T_n, \rho_n \dots) \quad (B.6)$$

where ... can mean rate dependent terms, etc. The problem is now to determine the new cell temperature T_n which satisfies (B.2) through (B.4) to (B.6). This can be done as in CHART D by an iteration with a safety backup procedure.¹ Starting from a guess at T_n , corrections are computed from the relation

$$\Delta T_n = - \frac{E(T_n^\ell, \rho_n) - c_1 + c_2 P(T_n^\ell, \rho_n) - K(T_n^\ell, \rho_n)}{\left\{ \frac{\partial E}{\partial T} + c_2 \frac{\partial P}{\partial T} - \frac{\partial K}{\partial T} \right\}} \Bigg|_{T_n^\ell, \rho_n} \quad (B.7)$$

$$= T_n^{\ell+1} - T_n^\ell$$

where

$$C_1 = E_o - \left\{ \frac{1}{2} P_o + Q \right\} \Delta V + R \Delta t - K_o , \quad (B.8)$$

$$C_2 = \frac{1}{2} \Delta V \quad (B.9)$$

and T_n^{ℓ} is the current value of the temperature at the end of the ℓ^{th} iteration. The iteration is continued until some predefined convergence is obtained. The condition

$$\left| \Delta T_n \right| \leq 10^{-6} T_n^{\ell} \quad (B.10)$$

is used. As a backup, the slow but dependable upper-lower bound procedure can be provided.

Now consider the program WONDY IV. WONDY is of course a dynamic code in which improvements are continually being added. The version considered here is as published in appendix B of reference 4; however, the modifications given here should work in nearly any version.

In WONDY, the solution of (B.2) is coded in the (STAT) subroutines. Here only the normal solid-vapor sections (HVEP - STAT1) are considered. The treatment of distended materials (STAT6) is slightly more complex but could be handled in the same manner.

The method of coding requires a minimum of coding changes in both WONDY and the ANEOS package. A special subroutine THEOS is provided to couple the two. All linkage is through this subroutine. The cell storage in WONDY is not altered. The cell temperature is not retained. The initial guess at the cell temperature is taken as the last calculated

value (normally that for the adjacent cell). If it is desired to save additional cell quantities for printout or other purposes, the modifications will be obvious.

Unfortunately the exact details of coding are difficult to explain. There are three functions for the subroutine THEOS to perform. The general nature of these three steps is given. All further details can be found in the listing of THEOS.

Step 1. Initialization of the ANEOS package. This is done after defining the material layers in WONDY. THEOS sorts through the layers, decides which use the ANEOS package and checks for the same EOS in different layers. The ANEOS package subroutine ANEOS2 is called to read input cards and complete the initialization. The absolute reference point energy is saved so that the normal WONDY reference energy of zero can be used in the WONDY calculations.

Step 2. Initialization of WONDY material layer variables from the EOS data. The statement 190 deals with this function.

Step 3. The normal cycle cell energy balance, i.e., solution of (B.2). If it is desired to return additional EOS data to WONDY, the variables could be set after statement 180.

Now let us return to WONDY. The changes in the WONDY input instructions are given below. The STATEL input variable number 35 is not used for the normal WONDY EOS. The variable is now used as an input flag to indicate that the ANEOS package is to provide the EOS. A blank or zero value indicates a normal WONDY EOS form, anything else indicates an ANEOS material.

As previously stated the coding modifications to WONDY are referenced to the listing in appendix B of reference 4. The changes correspond to the above three steps.

```

SUBROUTINE THEOS(RHON,RHO0,ENERGY,PRESS,Q,REST,CS,LAYER)      THE 1
C
C THIS SUBROUTINE COUPLES ANEOS PACKAGE TO REST OF HYDROCODE.   THE 2
C COMMON /BIG/ IS USED ONLY TO END OF INITIALIZATION. AFTER    THE 3
C INITIALIZATION THIS STORAGE CAN BE USED FOR SOMETHING ELSE.   THE 4
C                                                               THE 5
C                                                               THE 6
C COMMON /BIG/ DUMMY(5600)
COMMON /ANES/ ACK(1080),ZZS(100),COT(100),FNI(100),RCT(21),TCT(21)THE 8
1,RSOL(1000),RVAP(1000),TTWO(1000),SAVER(92),CMLT(8),ZB(92),DZR(40)THE 9
2,BOLTS,FIP(4370),LOCSS(21),LOCKP(21),LOCKPL(21)           THE 10
DIMENSION LAY(21),NEOS(20),EREF(20)                         THE 11
EQUIVALENCE (NEOS(1),EREF(1))                                THE 12
DATA T,TLOW,TUP,TREF/0.,0.01,100.,0.02567785/                 THE 13
DATA CKJEMP,LAY/1.E-6,21*0/                                  THE 14
TF(LAYER) 10,10,100                                         THE 15
C START INITIALIZATION                                     THE 16
10 N=-LAYER                                              THE 17
READ 20,(NEOS(I),I=1,N)                                    THE 18
20 FORMAT(16I5)                                            THE 19
PRINT 30,(I,NEOS(I),I=1,N)                                THE 20
30 FORMAT(23H1THERMODYNAMIC EOS DATA,/, (7H0LAYER(,I2,14F) = EOS NUMBER)THE 21
1R,I6))
L=1                                                       THE 22
DO 40 I=1,N                                              THE 23
IF(NEOS(I).EQ.0.) GO TO 40                               THE 24
LAY(I)=NEOS(I)                                           THE 25
GO TO 50                                                 THE 26
40 CONTINUE                                              THE 27
40 CONTINUE                                              THE 28
C NO THERMODYNAMIC EOS REQUESTED                         THE 29
RETURN                                                 THE 30
50 DO 70 I=1,N                                           THE 31
IF(NEOS(I).EQ.0.) GO TO 70                               THE 32
DO 60 K=1,L                                              THE 33
IF(LAY(K).EQ.NEOS(I)) GO TO 70                           THE 34
60 CONTINUE                                              THE 35
L=L+1                                                   THE 36
LAY(L)=NEOS(I)                                           THE 37
70 CONTINUE                                              THE 38
PRINT 80,L                                              THE 39
80 FORMAT(//,29H EOS DATA MUST BE ENTERED FOR,15,10H MATERIALS)THE 40
C READ INPUT DATA                                         THE 41
CALL ANEOS2(1,L,0,LAY)                                   THE 42
C SAVE REFERENCE POINT ENERGY AND EOS NUMBER             THE 43
DO 90 I=1,N                                              THE 44
LAY(I)=K=-NEOS(I)                                         THE 45
EREF(I)=0.                                               THE 46
IF(K.EQ.0) GO TO 90                                      THE 47
L=LOCSS(K)                                              THE 48
CALL ANEOS(ACK(L+12)*ACK(L+11),P,EREF(I),S,CV,DPT,DPR,FK,C1,KPA,K)THE 49
90 CONTINUE                                              THE 50
RETURN                                                 THE 51
C END INITIALIZATION                                     THE 52

```

```

C ENERGY BALANCE THE 53
C   IF(T.LE.TLOW) T=TREF THE 54
K=LAY(LAYER) THE 55
F=ENERGY+EREF(LAYER) THE 56
IF(RHON.LE.0.) GO TO 190 THE 57
IF(RHO0.LE.0.) GO TO 210 THE 58
IF(E.LE.0.) GO TO 210 THE 59
DVOL=(RHOO-RHON)/(RHOO*RHON) THE 60
C1=F-(.5*PRESS+Q)*DVOL+REST THE 61
THE 62
L=0 THE 63
C2=.5*D VOL THE 64
CALL ANEOS(T,RHON,P,E,S,CV,DPT,DPR,FK,CS,KPA,K) THE 65
E=E-C1+P*C2 THE 66
FD=CV+DPT*C2 THE 67
IF(FD).LT.130.130.120 THE 68
THE 69
120 FD=-F/ED
F=ABS(ED)
IF(F.LE.CKTEMP*T) GO TO 180 THE 70
IF(F.GT.0.5*T) ED=0.5*T*F/ED THE 71
L=L+1 THE 72
IF(L.GT.50) GO TO 130 THE 73
T=T+FD THE 74
IF(T-.001).LT.130.130.110 THE 75
THE 76
130 T=TREF THE 77
T1=TLOW THE 78
T2=TUP THE 79
THE 80
140 CALL ANEOS(T,RHON,P,E,S,CV,DPT,DPR,FK,CS,KPA,K) THE 81
IF(T2-T1.LE.CKTEMP*T) GO TO 180 THE 82
F=F-C1+P*C2 THE 83
IF(F).LT.150.180.160 THE 84
THE 85
150 T1=T
GO TO 170 THE 86
160 T2=T
THE 87
170 T=.5*(T1+T2)
GO TO 140 THE 88
THE 89
C THERMODYNAMIC STATE DETERMINED THE 90
180 ENERGY=F-EREF(LAYER) THE 91
PRESS=P THE 92
IF(T.GT.TUP) T=TREF THE 93
RETURN THE 94
190 IF(RHOC.NE.-77.777) GO TO 210 THE 95
C RETURN REFERENCE DENSITY THE 96
L=LOC SV(K) THE 97
RHON=RHO0=ACK(L+11) THE 98
GO TO 100 THE 99
200 FORMAT(19H1ILLEGAL THEOS CALL,I7,/,7E15.6) THE 100
210 PRINT 200,LAYER,RHON,RHO0,ENERGY,PRESS,Q,REST,E THE 101
END THE 102

```

Step 1. Initialization of the ANEOS package. Note that most of the coding is to see if the ANEOS package is used. * I ... means insert after

```
*I WON.138
C     $$$$$$$$$$ ANEOS PACKAGE MODIFICATION $$$$$$$$$$S
C     TEST TO SEE IF ANEOS PACKAGE IS USED
DO 1901 IC=1,NOP
IF(STATE(IC).NE.1.) GO TO 1901
IF(IC.EQ.35,IC).NE.0.) GO TO 1902
1901 CONTINUE
C     NO ANEOS DATA REQUESTED
      GO TO 1903
C     INITIALZATION OF ANEOS PACKAGE
C     READ ALL INPUT DATA
1902 IC=NOP
      CALL THEOS(RN,R,E,P,Q,GN,C,IC)
1903 CONTINUE
C     $$$$$$$$$$ ANEOS PACKAGE MODIFICATION $$$$$$$$$$S
```

Step 2. Initialization of WONDY material layer variables from the EOS. Note that the input value of the stress deviator is retained.

```
*1 WOK.172
C      ##### ANEOS PACKAGE MODIFICATION #####
C      SET REFERENCE AND INITIAL PLATE VARIABLES FROM ANEOS PACKAGE


---


C      IF(STATE(PLATE).NE.1.) GO TO 1904
IF(CES(35,PLATE).EQ.0.) GO TO 1904
E=P=Q=N=0.
C      REFERENCE SOUND SPEED AND DENSITY
RN=R=-77.777
CALL THEOS(RN,R,E,P,Q,QN,CES(2,PLATE),PLATE)
CFS(1,PLATE)=R


---


C      INITIAL PRESSURE AND STRESS
E=EZERO(PLATE)
IF(RZER0(PLATE).GT.0.) RN=RZERO(PLATE)
R=RN
CALL THEOS(RN,R,E,P,Q,QN,C,PLATE)
SZERO(PLATE)=SZERO(PLATE)+P-PZERO(PLATE)
PZERO(PLATE)=P


---


C      NEXT STATEMENT FOR ZERO DIVID IN STATE1 SETUP ONLY
CES(16,PLATE)=-5.4321
1904 CONTINUE
C      ##### ANEOS PACKAGE MODIFICATION #####

```

Step 3. The normal cycle cell energy balance, i.e., solution of
(B.2). *D ... means delete ... and insert following cards in its place.

*D ST1.143
C \$\$\$\$\$\$\$\$\$\$\$\$\$\$ ANEOS PACKAGE MODIFICATION \$\$\$\$\$\$\$\$\$\$\$\$\$\$
C 7131 IF (CES(35,PLATE).NE.0.) GO TO 7190
MU=RN/CES(35,PLATE)-1.0
C \$\$\$\$\$\$\$\$\$\$\$\$\$\$ ANEOS PACKAGE MODIFICATION \$\$\$\$\$\$\$\$\$\$\$\$\$\$

*I ST1.219
C \$\$\$\$\$\$\$\$\$\$ ANEOS PACKAGE MODIFICATION \$\$\$\$\$\$\$\$\$\$
C ANEOS EVALUATION
C 7190 FP1=DELETE+QDEP
FP2=.5*(Q+QN)
PN=P
EN=E
CALL THEOS(RN,R,EN,PN,FP2,FP1,CN,PLATE)
SN=PN-TX
IF (NUY.NE.0) CN=CN*SQRT(KCONST(PLATE))
GO TO 7157
C \$\$\$\$\$\$\$\$\$\$ ANEOS PACKAGE MODIFICATION \$\$\$\$\$\$\$\$\$\$

To set up a card deck to use this coding, the above modifications should be made in WONDY and the subroutine THEOS and the ANEOS package added. The ANEOS package is cards CHD 3984 to CHD 6732 in the listing in appendix of R1. Note that if the ANEOS package is not referenced by any layer, it and THEOS need not be loaded.

There is one thing about the above procedure which, in most cases, should be changed for extensive calculations. The storage in COMMON /BIG/ is used by the ANEOS package only through the initialization phase (step 1). After that point, the storage is available for other uses. In WONDY, the main cell storage arrays in blank COMMON could use this space as they are not referenced until after step 1 is complete. This would require changing all blank COMMON in WONDY to COMMON /BIG/ but would reduce the central memory requirements by 5600₁₀ in execution phase. This task is straightforward and will not be reproduced here.

The input data deck changes for WONDY are as follows. For a STAT1 material with ANEOS properties, the WONDY layer EOS parameters 1 to 5, 7 to 21 and 34 are not used. Variables 6, 22 to 33 are defined in the normal manner. Variable 35 is anything except zero. Note that step 2 above will supply values for variables 1, 2 and 16.

For a STAT1 material with the older form of EOS, all variables are defined in the normal WONDY manner except variable 35 must be zero.

The inputs to the ANEOS package are present only if at least one layer uses the package. The cards follow the end of file card after the 1 to 20 WONDY input cards. Due to an odd quirk of coding, the printed output of the ANEOS package comes out before any WONDY output.

ANEOS Card 1. Format (16I5)

There is one input card to THEOS with one input variable for each material layer in the WONDY calculation. Zero is used for any layer not using the ANEOS package. For any layer using ANEOS, an EOS indicator from -1 to -20 is entered which must be related to the ANEOS equation of state number as on card 1 in appendix F. Each different material should use a different indicator. Different layers with the same equation of state should have the same indicator. The input order is the same as the layer numbering in WONDY.

ANEOS Card Set 2.

There is one set of cards for each different equation of state referenced on card 1. The card sets are as given in appendix F and are the same as CHART D input card set 12.

As an example, consider the eight layer problem.

layer number							
1	2	3	4	5	6	7	8
ANEOS Aluminum	Other Form	ANEOS Beryllium	ANEOS Iron	Other Form	ANEOS Aluminum	ANEOS Iron	Other Form
-1	0	-17	-9	0	-1	-9	0
-1	6 4		Aluminum				
-17	8 4		Beryllium				
-9	5 4		Iron				

The ANEOS inputs might be as follows. Note references are to the built in library data as given in appendix C of R2.

-1	0	-17	-9	0	-1	-9	0
-1	6 4		Aluminum				
-17	8 4		Beryllium				
-9	5 4		Iron				

APPENDIX C
REVISED CKEOS INPUT INSTRUCTIONS

APPENDIX C

Revised CKEOS Input Instructions

CKEOS Input Instructions

CKEOS requires 160000₈ central memory locations on the CDC 6600 with the FTN compiler. Remember that the SCORS package¹⁸ is employed and that the master EOS file must be requested on unit 12 for tabular data.

See R3 for more details. A ★ represents a change on a card from the form given in R3.

Card 1 Format (3I10,4E10.3,A10)

(1-10) NEOS = EOS number; -1 to -20 for analytic and > 0 for tabular. This variable has the same meaning as IES, variable 7, card 11.1 in appendix E.

(11-20) NPLS = number of constant density plots on each graph (see card 6). Normally a large number.

(21-30) IOVER = switch to control constant density calculations.
 > 0, input data on cards 4, 5 and 6.
 = 0 and NEOS > 0, tabular mesh points determine mesh.
 Skip cards 4, 5 and 6
 = 0 and NEOS < 0, code sets IOVER = 1
 < 0, no constant density calculation, skip cards 4,
 5 and 6.

(31-40) T_{min} = minimum temperature for 3-D plot.

(41-50) T_{max} = maximum temperature for 3-D plot.

(51-60) ρ_{min} = minimum density for 3-D plot.

(61-70) ρ_{max} = maximum density for 3-D plot.

(71-80) Any BCD information used for plot identification.

Note: If any of T_{min} , T_{max} , ρ_{min} , $\rho_{max} \leq 0$, no 3-D plots are produced. If the plot is generated, a 60 x 60 mesh is used with equal log spacing.

Card 2Format (8E10.3) ★

Produces one and two-wave Hugoniots and isentropes.

(1-10) RHG = initial density for Hugoniot calculation.

If RHG < 0, calculation is skipped.

(11-20) THG = initial temperature.

If THG < 0, code sets THG = .02567785.

(21-30) RORUS = initial density for two-wave Hugoniot. If
RORUS ≤ 0, calculation is skipped.

(31-40) PORUS = elastic yield stress.

(41-50) CORUS = elastic wave velocity.

NOTE: A single-wave solution is computed using only RHG and THG. If the two-wave calculation is desired, RHG should define the initial solid material density and RORUS the initial foam density for porous materials, i.e.,

$$\frac{\text{RHG}}{\text{RORUS}} = \text{distention ratio.}$$

The two-wave calculation is good only for pressures in excess of initial yield.

(51-60) ρ_{crit} } Used only for ANEOS package. If entered, code will(61-70) T_{crit} } attempt to suggest values of C_{53} and C_{54} to move the critical point to this region. (See section IV.1).

(71-80) CICE = switch for isentrope calculation. If CICE ≤ 0, no calculation. If CICE > 0, insert card set 7.

No plots are produced by these sections.

Card 3

Present only for analytic equations of state (NEOS < 0 on card 1). Insert the standard ANEOS data card set described in Appendix F.

Card 4

Format (2I5,4E10.3)

Present only if IOVER > 0 on card 1.

(1-5) NTUP = defines the number of test temperatures in card 5.

(6-10) NRHUP = number of test densities in card 6.

Note: The next 4 variables are used only for testing high explosives; otherwise leave blank. See Section X in R1 and Section IV.2.

(11-20) TOHE = initial temperature before start of burn. If $TOHE \leq 0$, code sets $TOHE = .02567785$.

(21-30) ROHE = initial density.

(31-40) DHE = detonation velocity.

(41-50) QHE = chemical energy release per unit mass or - Chapman-Jouquet detonation pressures (same as variable 6, card 13.6 in Appendix D).

Card 5

Format (E20.10)

Present only if IOVER > 0 on card 1.

There are two possible forms depending on NTUP on card 4.

If $NTUP > 0$, input NTUP ordered temperatures.

If $NTUP < 0$, input 2 temperatures. The code will put in $|NTUP|$ values between them equally spaced on log scale.

Card 6

Format (E20.10)

Present only if IOVER > 0 on card 1.

Input NRHUP ordered densities.

Card 7

Format (4E10.3, I10) *

Present only if CICE > 0 on card 2.

Insert one of the following cards for each desired isentrope. No plots are produced.

(1-10)

ρ_{SREF} }
 T_{SREF} } used to determine entropy.

(11-20)

ρ_{min} = lowest density calculated

(31-40)

ρ_{max} = highest density calculated.

(41-50)

N = numbers of density intervals between ρ_{min} and
 ρ_{max} to be calculated.

When finished with the isentrope calculation,
insert a blank card to stop.

Insert a blank card to stop or return to card 1
for another EOS.

APPENDIX D

REVISED MASPLT INPUT INSTRUCTIONS

APPENDIX D

Revised MASPLT Input Instructions

MASPLT Input Instructions

MASPLT requires 100000_8 central memory locations on the CDC 6600 with the FTN compiler. Remember that the SCORS package ¹⁸ is employed. See R3 for more details. A ★ represents a change on a card from the form given in R3.

Table of Variable Selection Code for
Parameters 1 and 2 on Card 1 and Card 12

N(1),N(2)	Variable	Standard Unit
1	I = zone or boundary number	--
2	position (boundary)	cm
3	position (zone center)	cm
4	velocity (boundary)	cm/sec
5	velocity (zone center)	cm/sec
6	temperature	eV
7	density	gm/cc
8	pressure	dynes/cm ²
9	stress X	dynes/cm ²
10	pressure + artificial viscosity	dynes/cm ²
11	stress X + artificial viscosity	dynes/cm ²
12	X stress deviator	dynes/cm ²
13	stress Y	dynes/cm ²
14	stress Z	dynes/cm ²
15	Z stress deviator	dynes/cm ²
16	specific entropy	ergs/gm eV
17	specific internal energy	ergs/gm
18	distention ratio	--
19	momentum summed from front*	taps
20	mass depth from front*	gm
21	solid density (distention ratio x density)	gm/cc

* for plane geometry problems only

★

Card 1	Format (16I5)
(1-5)	N(1) = X (abscissa) variable code (see Table). Not used if N(16) = 1.
(6-10)	N(2) = Y (ordinate) variable code (see Table). <u>or</u> -1, -2 for plots with several curves on each frame. Code will attempt to save Y mesh from one frame to the next if -2, will not save if -1. Use with N(4) = N(5) = N(6) = N(7) = N(16) = 0. YMIN and YMAX on card 8.1 are not used. Add card 12 data. Not used if N(16) = 1.
(11-15)	N(3) = 0 for hard-copy output. = 1 for output on tape unit 39.
(16-20)	N(4) = 0 plot frequency determined by record number. = 1 plot frequency determined by time inputs. See card set 8. Not used if N(16) = 1.
(21-25)	N(5) = 0 for linear X scale. = 1 for log X scale.
(26-30)	N(6) = 0 for linear Y scale. = 1 for log Y scale.
(31-35)	N(7) = 0 no plot grid is shown in graph. = 1 plot grid is shown on graph.
(36-40)	N(8) determines number of title and The End frames. If N(8) > 0, N(8) is the number of frames of each. If N(8) = 0, no title or The End frames. If $-1000 \leq N(8) < 0$, no The End frames but $-N(8)$ title frames. If $N(8) < -1000$, no title frames but $-(N(8) + 1000)$ The End frames.
	The options with $N(8) \leq 0$ are useful in making continuous movies from several data tapes.
(41-45)	N(9) = number of frames of each plot except the first in a given interval.
(46-50)	N(10) = number of frames of the first plot in a given interval. This is useful in freezing the action in a movie to adjust to scale changes.

(51-55) $N(11) = 0$. Join points with lines.
 = 1. Do not join points with lines.
 = 2. Join points with lines except across spalls.
 (2 not available if $N(2) = -1$ or -2).
(56-60) $N(12) = 0$ for small size frame. This must be used for movies
 or any 16 mm plot because of frame overlap.
 = 1 for large size frame. Plot grid is always shown.
(61-65) $N(13) =$ number of data packages in card 8.
 If $N(16) = 0$ then $0 < N(13) \leq 10$.
 If $N(16) = 1$ then $N(13) = 0$.
(66-70) $N(14) =$ number of plot symbols in card 6.
 $1 \leq N(14) \leq 50$.
(71-75) $N(15) =$ input tape number (1, 2, 3, or 4).
(76-80) $N(16) = 0$ for plot of variables at a given time.
 = 1 for a single plot of variable as a function of time
 or with time as a parameter. User must supply
 subroutine TIMEVA. An example is given in the code
 listing in R3.

Card 2 Format (3A10)
(1-30) Input label 1 (for first title frame, should be
 centered).

Card 3 Format (3A10)
(1-30) Input label 2 (for first title frame, should be
 centered).

Card 4 Format (3A10)
(1-30) Input label 3 (for second title frame, should be
 centered).

Card 5 Format (3A10)
(1-30) Input label 4 (for second title frame, should be
 centered).

Card 6

Format (8(I5,A1,4X))

There are N(14) sets of the following variables.

I = 1,N(14).

Variable odd - NBDY(I) = last point to be plotted
with the symbol NSD(I).

Variable even - NSD(I) = plot symbol (can be blank).

Note: NBDY(N(14)) is set to the last point to be
plotted.

Card 7

Format (5E10.3)

(1-10) SCALX = a scale factor for the X variable when N(16) = 0.

SCALX is used to change units.

If SCALX = 0, code sets SCALX = 1.

If N(16) = 1, SCALX can be used as an input parameter
to TIMEVA.

(11-20) SCALY = same as SCALX except for the Y variable.

(21-30) DLABX = 0 - for MASPLT to supply X label.

= 1 - input X label in card set 8 or 9 (must be used
if N(16) = 1 or SCALX ≠ 0 or 1).

(31-40) DLABY = same as DLABX except for Y label.

(41-50) EXTR = the number of data points pairs to be read in card
set 10. $0 \leq EXTR \leq 90$.

Note: all should be zero if N(2) = -1, -2.

Card Set 8	Present only if N(16) = 0. There are N(13) sets of these cards. I = 1, N(13).
Card 8.1	Format (2I10,6E10.3)
(1-10)	ICY(I) = tape record number to start plotting with dump frequency ICYD(I). Not used if N(4) = 1.
(11-20)	ICYD(I) = tape record frequency for plots between record ICY(I) and ICY(I+1). Not used if N(4) = 1.
(21-30)	TM(I) = time to start plotting at time intervals of TMD(I). Not used if N(4) = 0.
(31-40)	TMD(I) = time interval for plots between time TM(I) and TM(I+1). Not used if N(4) = 0.
(41-50)	XMIN(I) = smallest X value to be plotted in this interval.
(51-60)	XMAX(I) = largest X value to be plotted in this interval.
(61-70)	YMIN(I) = same as XMIN(I) except for Y.
(71-80)	YMAX(I) = same as XMAX(I) except for Y.
<u>Notes:</u> Points outside of minimum-maximum range are dropped. If N(13) > 1, plotting will start at first record \geq ICY(1) and stop when record number $>$ ICY(N(13)) if N(4) = 0 or start at first time \geq TM(1) and stop when time $>$ TM(N(13)) if N(4) = 1. In the case that N(13) = 1, the program will plot until the tape end of file.	
Card 8.2	Format (5A10)
(1-50)	Present only if DLABX = 1 (card 7). X label for this interval. Should be centered.
Card 8.3	Format (5A10)
(1-50)	Present only if DLABY = 1 (card 7). Y label for this interval. Should be centered.

Card Set 9

Present only if N(16) = 1.

Card 9.1

Format (2I10,6E10.3)

(1-10) Blank
(11-20) Blank
(21-30) TSTART = time to begin plot.
(31-40) TSTOP = time to stop plot.
(41-50) XMIN(1) = same as on card 8.1.
(51-60) XMAX(1) = same as on card 8.1.
(61-70) YMIN(1) = same as on card 8.1.
(71-80) YMAX(1) = same as on card 8.1.

Note: Only tape dumps between TSTART and TSTOP are employed.

Card 9.2

Same as 8.2 (must be present).

Card 9.3

Same as 8.3 (must be present).

Card Set 10

Format (2E10.3)

Present only if EXTR > 0 (card 7).

There are EXTRA sets of the following variables.

I = 1,EXTR

(1-10) EXTRX(I)
(11-20) EXTRY(I)

This set of variables is plotted on each frame
with lines connecting the points.

Card 11

Format (8A10)

Present only if N(16) = 1.

(1-80) Top label for graph. Only 1-50 are used for small
size frame.

Card 12

Format (4I5)



Present only if N(2) = -1,-2.

(1-5)

MULT(1) Y variable code for 1st curve.

(6-10)

MULT(2) Y variable code for 2nd curve.

(11-15)

MULT(3) Y variable code for 3rd curve.

(16-20)

MULT(4) Y variable code for 4th curve.

} See
Table

For only 3 curves per frame, MULT(4) = 0.

For only 2 curves per frame, MULT(4) = MULT(3) = 0.

For only 1 curve per frame, MULT(4) = MULT(3) = MULT(2) = 0

If more plots are desired, go back to card 1.

If finished, insert a blank card to stop.

APPENDIX E

REVISED CHART D INPUT INSTRUCTIONS

APPENDIX E

Revised CHART D Input Instructions

CHART D requires 200000_8 central memory locations plus a variable amount of extended core on the CDC 6600 with the FTN compiler. See R1 for more details. An * refers to R1. A ★ represents a change on a card from the form given in R1.

Card 1	Format (13A6)	
	78-column problem identification - any BCD information. If the problem is a restart, this name must agree exactly with the name on the restart tape.	
Card 2	Format (6I5, 3E10.3, 2I5)	★
Variable 1. (1-5)	ITIMEL - Computer time limit in seconds. Shortly before this allotted time is used, the code writes a restart tape dump, edits last cycle, and terminates. If ITIMEL = 0, the job card time limit is used. If ITIMEL < 0, the problem will generate and stop on cycle 0.	
Variable 2. (6-10)	NG - A switch to signify whether the problem is to be generated or restarted. If NG ≥ 0, generate the problem from the following data cards. If NG < 0, restart. The code reads -NG tape dumps before restarting.	
Variable 3. (11-15)	NDUMP - The time interval in seconds of computer time between writing restart tape dumps. If NDUMP = 0, the code sets NDUMP = 9999 (2.75 hours).	
Variable 4. (16-20)	IS - A switch to select restart output tape. If IS ≤ 0, restart output on tape 10 (standard). If IS > 0, restart output on tape 11 (optional). Under the latter option, tape 10 information past the restart point is not destroyed.	
Variable 5. (21-25)	IS1 - A switch to select extra binary edit output on tape 2. If IS1 ≤ 0, tape 2 edit is not written. If IS1 > 0, tape 2 edit is written. See note on page 105 in R1.	

Variable 6. NEDREJ - A switch to force edits whenever a fracture or
 (26-30) rejoin takes place. If NEDREJ = 0, no extra edit following
 fracture or rejoin. If NEDREJ > 0, standard edit following
 fracture or rejoin. If NEDREJ < 0, one line edit following
 fracture or rejoin.

Variable 7. FRACDT - Fraction of Courant stability used to calculate
 (31-40) sound speed time step. (Normally 0.8, in no case greater
 than 1). If FRACDT \leq 0, FRACDT = 0.8.

Variable 8. DTINCR - Factor used to increase time step from one cycle
 (41-50) to the next (normally \sim 1.05). If DTINCR \leq 0, DTINCR = 1.05.

Variable 9. TEND - The end of problem time. If TEND \leq 0, TEND is set
 (51-60) to very large number and run is terminated on ITIMEL variable.

Variable 10. NEXZON - Indicator for special edit of zone quantities.
 (61-65)

- If NEXZON = 0, no special edit.
- If $1 \leq NEXZON \leq$ number of zones, special edit for
 the $NEXZON^{\text{th}}$ zone.
- If $-100 \leq NEXZON \leq -1$, special edit for the 1^{st}
 zone in the $(-NEXZON)^{\text{th}}$ layer.
- If $NEXZON < -100$, special edit for the last zone in
 the $(-NEXZON -100)^{\text{th}}$ layer.

Variable 11. NEXFRE - Cycle frequency of special edits for zone determined
 (66-70) by NEXZON.

 * If the problem is being restarted, the preceding
 * cards are the only data cards required.

Card 3	Format (16I5)
Variable 1. (1-5)	<p>IGM - A geometry switch.</p> <p>If IGM = 1, plane geometry.</p> <p>If IGM = 2, cylindrical geometry.</p> <p>If IGM = 3, spherical geometry.</p>
Variable 2. (6-10)	NRZC - The number of different zoning regions (see card set 11). There is no limit on the size of NRZC.
Variable 3. (11-15)	<p>NMTRLS - The number of material layers in the problem. A material is counted more than once if there is another material between the various pieces (see card set 11).</p> <p>NMTRLS \leq NRZC. NMTRLS \leq 20.</p>
Variable 4. (16-20)	NPRIN - The number of edit (print out) frequency intervals (see card set 5). $1 \leq$ NPRIN \leq 24.
Variable 5. (21-25)	NDTMAX - The number of maximum input Δt intervals (see card set 6). $0 \leq$ NDTMAX \leq 24. If NDTMAX \leq 0, the maximum Δt is set to a very large number.
Variable 6. (26-30)	NDTMINN - The number of minimum input Δt intervals (see card set 7). $0 \leq$ NDTMINN \leq 24. If NDTMINN \leq 0, the minimum Δt is zero.
Variable 7. (31-35)	NBPRES - The number of points in the boundary pressure histories (see card set 9). NBPRES \leq 24. If NBPRES \leq 0, there are no boundary pressures.
Variable 8. (36-40)	NOSOUR - A switch for internal energy sources. If NOSOUR \leq 0, there are no internal sources. If NOSOUR $>$ 0, there are internal sources and NOSOUR is the type of input information (see card set 13). NOSOUR = 1, 2, 3, 4, 5, and 6 are possible.
Variable 9. (41-45)	<p>IBS - A switch to determine if boundary NZP (smallest X) is free to move or fixed in space.</p> <p>If IBS = 0, boundary NZP is free.</p> <p>If IBS = 1, boundary NZP is fixed ($V \equiv 0$).</p>
Variable 10. (46-50)	<p>OBS - A switch to determine if boundary l (largest X) is free to move or fixed in space.</p> <p>If OBS = 0, boundary l is free.</p> <p>If OBS = 1, boundary l is fixed ($V \equiv 0$).</p>

Variable 11. NSPALL - A switch for fracture calculations.
(51-55) If NSPALL < 0, no material fracture is allowed.
If NSPALL = 0, material fracturing is allowed.
If NSPALL > 0, voids will be zoned into the initial configuration with card set 15. The latter may only be used for plane geometry.
If ~~NSPALL~~ < 0 and type 7 zoning (see card set 11) is used, this input is ignored.

Variable 12. NACTION - The number of regions with initially active zones (see card set 14).
(56-60) If NACTION = 0, only zones with sources or moving boundaries are active on cycle 1.

Variable 13. NORAD - A radiation switch.
(61-65) If NORAD = 0, no radiation diffusion is calculated.
If NORAD = 1, implicit radiation diffusion.
If NORAD = 2, explicit radiation diffusion.
If NORAD = 3, approximate implicit radiation diffusion.
If NORAD = 4, the code attempts to use faster of 1, 2, 3. The hydrodynamic calculation can be suppressed with options 1 through 4 by using the negative of the option number.

Variable 14. NTHIST - The number of points in the boundary temperatures histories (see card set 10).
(66-70) NTHIST \leq 24. (Ignored if NORAD = 0.)
If NTHIST \leq 0, there are no boundary temperatures.

Variable 15. NRADCK - A switch for the radiation flux limiter. (Ignored if NORAD = 0.)
(71-75) If NRADCK = 0, the limiter is used (normal option).
If NRADCK > 0, the limiter is not used.
If NRADCK = -1, the limiter is used but with $\frac{1}{4}$ maximum flux of NORAD = 0. (See section II.4.)

Variable 16. MOVIE - The number of movie frame frequency intervals.
(76-80) (See card set 8.) Movie \leq 9.
If MOVIE = 0, no movie tape is produced.
If MOVIE > 1, movie tape is produced on unit 3.

Card 4

Format (8E10.3)

Variable 1. (1-10)	BL - The constant in the linear viscosity term (normally 0.1).
Variable 2. (11-20)	BQ - The constant in the quadratic viscosity term (normally 2.0). Note: Both BL and BQ should not be zero. If $BL + BQ = 0$, code sets $BL = 0.1$ and $BQ = 2.0$.
Variable 3. (21-30)	XM2(1) - Temporary storage for the fictitious outer boundary mass (boundary 1) (normally 0).
Variable 4. (31-40)	XM2(2) - Temporary storage for the fictitious inner boundary mass (boundary NZP) (normally 0).
Variable 5. (41-50)	SCRADF - A scale factor for the front surface boundary temperature. (Ignored if NORAD = 0.) If $SCRADF > 0$, the incident flux is scaled by SCRADF. If $SCRADF = 0$, the code sets $SCRADF = 1$. If $SCRADF < 0$, no radiation is allowed to pass through the front surface in either direction, i.e., $FLUX(1) = 0$.
Variable 6. (51-60)	SCRADB - A scale factor for the back surface boundary temperature. Inputs are the same as for Variable 5. (Ignored if NORAD = 0.) In cylindrical or spherical geometry, SCRADB is set = -1 when there is no central void. If there is a central void, and $SCRADB \geq 0$, any radiation passing into the void will be lost. $SCRADB < 0$ is the physically realistic choice.
Variable 7. (61-70)	TRADOFF - The earliest time at which the code will check to see if the radiation can be turned off (normally 0).
Variable 8. (71-80)	SWEP - Elastic-plastic switch. If $SWEP = 0$, no elastic-plastic calculation. If $SWEP = 1$, elastic-plastic calculation.

Card Set 5

Format (8E10.3) Edit (Print Out) Information

The times refer to problem times in seconds. There are NPRIN sets of these variables (see card 3).

Variable Odd. TIMEP (I) - The time at which edit intervals switch from DTIMEP (I-1) to DTIMEP (I).
[TIMEP (1) = 0, always.]

Variable Even. DTIMEP (I) - The interval between edits from TIMEP (I) to TIMEP (I+1).

For times > TIMEP (NPRIN), the last value of DTIMEP is used to the end of the problem.

Card Set 6

Format (8E10.3) Maximum Time Step Information

Present only if NDTMAX > 0 (see card 3).

There are NDTMAX sets of these variables.

Variable Odd. TIMES (I) - The time at which the maximum time step switches from DLTTMX (I-1) to DLTTMX (I).
[TIMES (1) = 0, always.]

Variable Even. DLTTMX (I) - The maximum time step allowed between TIMES(I) and TIMES (I+1).

For times > TIMES (NDTMAX), the last value of DLTTMX is used to the end of the problem.

Card Set 7

Format (8E10.3) Minimum Time Step Information

Present only if NDIMINN > 0 (see card 3).

There are NDIMINN sets of these variables.

Variable Odd. TDIMINN (I) - The time at which the minimum time step switches from DMINNN (I-1) to DMINN (I).
[TDIMINN (1) = 0, always.]

Variable Even. DMINNN (I) - The minimum time step allowed between TDIMINN (I) and TDIMINN (I+1). For times > TDIMINN (NDIMINN), the last value of DMINNN is used to the end of the problem. In case of any conflict, the minimum time step criterion is never violated.

Card Set 8 Format (8E10.3) Movie Frame Frequency

Present only if MOVIE > 0 (see card 3).

There are MOVIE sets of these variables.

Variable Odd. TMOV (I) - The time at which the movie edit frequency switches from DTMOV(I-1) to DTMOV(I).

[TMOV(1) = 0, always.]

Variable Even. DTMOV(I) - The movie edit frequency time interval from TMOV(I) to TMOV(I+1).

Note: The dumps are terminated when the time \geq TMOV (MOVIE).

MOVIE \geq 2 to function properly.

Card Set 9 Format (3E10.3) Boundary Pressure Information

Present only if NBPRES > 0 (see card 3).

There are NBPRES cards with:

Variable 1. TBPRES(I) - The time of the Ith boundary pressure (1-10) history point. [TBPRES(1) = 0, always.]

Variable 2. PINNER (I) - The boundary pressure at boundary NZP (11-20) (smallest X) at time TBPRES(I).

Variable 3. POUTER (I) - The boundary pressure at boundary 1 (21-30) (largest X) at time TBPRES(I).

The code does a linear interpolation in time between these points. For times $>$ TBPRES (NBPRES), the last boundary pressures are used to the end of the problem.

Card Set 10

Format (3E10.3) Boundary Temperature Information

Present only if NTHIST > 0 (see card 3).

There are NTHIST cards with:

Variable 1. TITH(I) - The time of the Ith boundary temperature history point. [TITH(1) = 0, always.]
(1-10)

Variable 2. TEINTH(I) - The boundary temperature at boundary NZP (smallest X) at time TITH(I).
(11-20)

Variable 3. TEOUTH(I) - The boundary temperature at boundary 1 (largest X) at time TITH(I).
(21-30)

The code does a linear interpolation in time between these points. For times > TITH(NTHIST), the last boundary temperatures are used to the end of the problem.

Card Set 11

Zoning the Problem

The problem is zoned with a series of different regions, each of which is zoned independently. These are NRZC zoning regions and NMTRLS material layers, with NRZC ≥ NMTRLS. There can be several regions per material layer but not more than one material in any region. The material boundaries must be a subset of the region boundaries.

Each region is zoned by first giving a set of region information cards and then by using one, and only one, of the seven types of zoning routines. The regions are considered in order, starting with the outermost (largest X) and working inward.

Material Boundary Card

Format (8E10.3)

Variables. XMATUP(I), I = 1, (NMTRLS + 1). These are the positions of the boundaries of the various materials, starting with the largest X first. In case Type 7 zoning (voids) is used, the lower boundary of the void is used if the void is between different materials.
A void is not counted as a material.

Next are NRZC sets of the following cards:

Region Information Card 1.

Format (I5, 5E10.3, I5)

This is always the first card for zoning a region with any of the seven types below.

Variable 1. ITYPE = 90 + number of the zoning type to be used for this
(1-5) region.

Variable 2. X_{up} - The upper boundary of the region being zoned. Except
(6-15) for the first region, this must always equal the lower boundary of the preceding region. X_{up} for the first region is the outer (first) boundary of the problem. For Type 6 zoning in the first region, this is ignored.

Variable 3. X_{low} - The lower boundary of the region. For the last region
(16-25) this denotes the inner (last) boundary of the problem. For Type 6 zoning in the last region, this is ignored.

Variable 4. ρ_o - The initial density to be used for each zone in this
(26-35) region. When Type 1 zoning is used, this density can be superseded for specified zones.

Variable 5. T_o - The initial temperature to be used for each zone in
(36-45) this region. When Type 1 zoning is used, this temperature can be superseded for specified zones.

If $T_o \leq 0$, code sets $T_o = 0.02567785$ ($298^\circ K$).

Variable 6. V_o - The initial velocity to be used for the upper boundary
(46-55) of each zone in this region. When Type 1 zoning is used, this velocity can be superseded for specified zones.

Variable 7. IES - The equation-of-state number for the material in this
(56-60) region.

IES > 0 for tabular EOS.

-20 ≤ IES ≤ -1 for analytic EOS (see card set 12).

For Type 7 zoning, variables 4 to 7 are ignored.



This is always the second card for zoning a region and contains the information for the elastic-plastic or distended material calculation. The eight input variables are named YIELD(I), I = 1, 8.

Use only one of the following forms.

I. Nonporous - hydrodynamic material and type 7 zoning.

All eight variables read and stored but not used.

II. Elastic-Plastic Material (see Section IV-2* and variable 8, card 4).

Variable 1. y_o
(1-10)

Variable 2. y_1
(11-20)

Variable 3. o . - Computed internally. The absolute melt energy
(21-30) (ϵ_m) as determined from the equation of state is stored
in this location. If a positive number is entered
here, it will override the internally computed value.

Variable 4. ρ_o - Reference density. If zero, the density is taken to
(31-40) be the same as ρ_o on region information card 1.

Variable 5. v_o - Reference Poisson's ratio.
(41-50)

Variable 6. α - Fraction of melt energy at which the material starts to
(51-60) lose strength (normally 0.8).
If $\alpha \leq 0$, code sets $\alpha = 0.8$.

Variable 7.
(61-70)

Variable 8.
(71-80)

}

Read and stored but not used.

III. Distended or Porous Material (see Section V-5* and Section II.2).

Variable 1. ρ_{so} - Normal solid density at the temperature given by
(1-10) T_o on region information card 1. This is used to calculate the initial distention ratio.

Variable 2. k_o' - A constant used in computing the temperature dependence
(11-20) of the crush strength. (See Section II.2).
If $k_o' = 0$, code sets $k_o' = -2$.

Variable 3. (-1.) This is a switch.
(21-30)

Variable 4. P_e - The elastic limit pressure of the material at full
(31-40) distention.

Variable 5. P_s - The elastic limit pressure as all voids vanish in the
(41-50) quadratic model,
or
(-a) - constant in the exponential model.

Variable 6. C_{eo} - Sound speed in the material at full distention. If
(51-60) no value is given, the normal solid sound speed is used.

Variable 7. Γ_{eff} - Effective Grüneisen coefficient for revised
(61-70) $P - \alpha$ model (see Section II.2).
If $\Gamma_{eff} \leq 0$, code uses older $P - \alpha$ model.

Variable 8. δ - Constant in Section II.2-2.
(71-80) If $\delta \leq 0$, code sets $\delta = \frac{1}{2}$.



This is always the third card for zoning a region and contains the information for the material fracture calculation. The eight input variables are named FRACT(I), I = 1, 8.

Use only one of the four following forms.

I. A blank card for type 7 zoning.

II. Stress Gradient Model (see Section VII for notation). *

Variable 1. σ_u - Ultimate tensile strength ($\sigma_u > 0$).
(1-10)

Variable 2. T_s - Strength vanishing temperature.
(11-20) If $T_s \leq 0$, code sets $T_s = 10$.

Variable 3. A.
(21-30)

Variable 4. B.
(31-40) If $B = 0$, code sets $B = 1$.

Variable 5. C.
(41-50) If $C = 0$, code sets $C = 1$.

Variable 6. σ_o - Static tensile strength ($\sigma_o > 0$).
(51-60) If $\sigma_o = 0$ code sets $\sigma_o = \sigma_u$.

Variable 7. Switch to suppress tensions in partially melted material.
(61-70) = 0, can have tensions above incipient melt.
= 1, cannot have tensions above incipient melt.
See Section (II.3).

Variable 8. Scale factor for Q in this layer.
(71-80) Default value is 1. If negative the viscosity is used in expansion as well as compression. See Section (II.1).
0 or 1 - normal materials
 ~ 4 or 5 - porous materials
 $-\frac{1}{2}$ - materials like fused silica

III. Cumulative Damage Model (see Section VII for notation).*

Variable 1. $K(0)$. (normally 0).
(1-10)

Variable 2. T_s - Strength vanishing temperature.
(11-20) If $T_s \leq 0$, code sets $T_s = 10$.

Variable 3. σ_o - Static tensile strength ($\sigma_o > 0$).
(21-30)

Variable 4. λ .
(31-40)

Variable 5. (-C) (must be negative).
(41-50)

Variable 6. K_s .
(51-60)

Variable 7.
(61-70)

Variable 8.
(71-80)

}

Same as option II.

IV. Tensile Strength Limit (see Section VII for notation).*

Variable 1. σ_s - Maximum tensile strength ($\sigma_s > 0$).
(1-10)

Variable 2. T_s - Strength vanishing temperature.
(11-20) If $T_s \leq 0$, code sets $T_s = 10$.

Variable 3. Blank
(21-30)

Variable 4. Blank
(31-40)

Variable 5. C.
(41-50) If $C = 0$, code sets $C = 1$.

Variable 6. Blank
(51-60)

Variable 7. }
(61-70) Same as option II.
Variable 8. }
(71-80)

Seven Zoning Options

Zoning Type 1 - ΔX (HAND) Zoning

First Data Card	Format (I5)
Variable 1. (1-5)	NDXC - The number of ΔX zoning cards used to zone this region.
Next NDXC Data Card	Format (I5, 4E10.3)
Variable 1. (1-5)	The number of zones desired with this ΔX .
Variable 2. (6-15)	The ΔX to be used for these zones.
Variable 3. (16-25)	ρ_o^* - Used as the temperature for these zones if $\rho_o^* > 0$; it overrides the specified region density. If $\rho_o^* = 0$, the specified region density is used.
Variable 4. (26-35)	T_o^* - Used as the temperature for these zones if $T_o^* > 0$; it overrides the specified region temperature. If $T_o^* = 0$, the specified region temperature is used.
Variable 5. (36-45)	V_o^* - Used as the velocity of the upper boundary for these zones if $V_o^* \neq 0$; it overrides the specified region velocity. If $V_o^* = 0$, the specified region velocity is used.

The sum of zone widths must equal the difference between the upper and lower region boundaries.

Zoning Type 2 - Specification of Both Region Boundary Zone Widths
(See Appendix B)*

Only Data Card	Format (3E10.3)
Variable 1. (1-10)	W_1 - Width of first zone in region (largest X). If $W_1 < 0$, width of first zone is $-W_1$ times the width of last zone in last region scaled for density. W_1 cannot be negative for the first region.
Variable 2. (11-20)	W_L - Width of last zone in region (smallest X).
Variable 3. (21-30)	Maximum fraction error allowed in ratio of adjacent zone masses (0.01 is 1 percent).

If the specified input is inconsistent with reality, the zoning will fail.

Zoning Type 3 - Increasing-Decreasing Mass Ratio (suggested only for plane geometry)

Only Data Card	Format (2E10.3)
Variable 1. (1-10)	W - Specifies the width of the first and last zones of the region. If $W = 0$, an error has occurred. If $W > 0$, W is the width of the first and last zones of the region. If $W < 0$, $-W$ times the width of the last zone of the last region is the new zone width for the first and last zones of this region. W cannot be negative in the first region. The zoning routine comes as close to this value as possible.
Variable 2. (11-20)	RATIO - The ratio of adjacent zone masses to be used in the upper (first) half of this region. $1/RATIO$ is the ratio of adjacent zone masses to be used in the lower (last) half of the region. RATIO may not be 1.

If $RATIO > 1$, this provides thin zones at the region boundaries and thick zones in the region center in order to conserve the number of zones. $RATIO < 1$ results in thicker zones at the boundaries than at the center. The zone widths are symmetric about the region center.

Zoning Type 4 - Specification of One Region Boundary Zone Width and Mass Ratio (See Appendix B)*

Only Data Card Format (4E10.3)

Variable 1. W_1 - Width of first zone in region (largest X).
(1-10) If $W_1 < 0$, width of first zone is RATIO times
the width of last zone in last region scaled for
density. W_1 cannot be negative for the first region.

Variable 2. W_ℓ - Width of last zone in region (smallest X).
(11-20)

Variable 3. RATIO - Adjacent zone mass ratio.
(21-30)

Variable 4. Maximum fraction error allowed.
(31-40)

Note: Either W_1 or W_ℓ must be zero. RATIO then applies to moving away
from the nonzero value.

Zoning Type 5 - Specifications of Mass Ratio and Number of Zones (See
Appendix B)*

Only Data Card Format (I5, E10.3)

Variable 1. Number of zones desired in region.
(1-5)

Variable 2. Mass ratio in increasing position direction.
(6-15)

Zoning Type 6 - Free Boundary (only for the first or last region)

Only Data Card Format (I5, 3E10.3)

Variable 1. ℓ - Number of zones desired in region.
(1-5)

Variable 2. RATIO - Mass ratio in direction away from interior
(6-15) of problem.

Variable 3. X_m - Maximum or minimum position.
(16-25)

Variable 4. Width of interior zone.
(26-35)

The region will be zoned away from the interior until either ℓ zones are used or a position of X_m is encountered. If $\ell \leq 0$, ℓ is ignored. If $X_m = 0$, X_m is ignored. A correction will be made to XMATUP(1) or XMATUP(NMTRLS + 1).

Zoning Type 7 - Voids

Used only on interior boundaries and cannot be used when a type 5 energy source is present. There are no data cards.

Card Set 12 - Analytic Equation-of-State Data

Any inputs for analytic equations of state go here. See Appendix F for format.

Card Set 13 - Internal Source Information

Present only if NOSOUR > 0 (see card 3). There are six types of internal sources. However, only one of the six can be used in a given problem. NOSOUR on card 3 determines the type. Type 1 is the hardest to input, but all other types are reduced to Type 1 for code use. See Section VIII-4* for notation.

Source Type 1 - Hand Input for Each Zone

Card 1 Format (I10)

Variable 1. NOSOUR - The last zone (largest zone number) in
(1-10) the problem to have a source.

All Other Cards Format (I5, 6E10.3)

Variable 1. I = Zone number.
(1-5)

Variable 2. τ_1 - For Zone I.
(6-15)

Variable 3. τ_2 - For Zone I.
(16-25)

Variable 4. τ_3 - For Zone I.
(26-35)

Variable 5. τ_4 - For Zone I.
(36-45)

Variable 6. $\dot{\mathcal{P}}_2$ - For Zone I.
(46-55)

Variable 7. $\dot{\mathcal{P}}_3$ - For Zone I.
(56-65)

Cards must be ordered by increasing zone number with the smallest number first. The reading is terminated when the zone number = NOSOUR. Zones with number < NOSOUR are not required to have a source and may be omitted from the sequence.

Source Type 2 - Input Total Energy per Zone

Card 1 is the same as the first Type 1 card.

All other Data Cards Format (I5, 3E10.3)

Variable 1. I = Zone number.
(1-5)

Variable 2. $\tau_1 = \tau_2$.
(6-15)

Variable 3. $\tau_3 = \tau_4$.
(16-25)

Variable 4. Zone energy (ergs).
(26-35)

Order requirement on zone input is the same as for Type 1.

$$\dot{\mathcal{S}}_2 = \dot{\mathcal{S}}_3 = \frac{\text{zone energy}}{(\tau_4 - \tau_1) M_i} .$$

Source Type 3 - Input Total Specific Energy per Zone

Same as Type 2, except Variable 4 is the zone specific energy (ergs/gm).

Source Type 4 - Source Region

Card 1 Format (I10)

Variable 1. KK - The number of source regions.
(1-10)

Next KK data Cards (one for each region) Format (5E10.3)

Variable 1. Right-hand boundary of source region (largest X).
(1-10)

Variable 2. Left-hand boundary of source region (smallest X).
(11-20)

Variable 3. Energy source strength, the total energy to be
 introduced between right and left boundaries.
(21-30)

Variable 4. $\tau_1 = \tau_2$.
(31-40)

Variable 5. $\tau_3 = \tau_4$.
(41-50)

The code will try to match X values with zone boundaries. If it is unable to do this, it will take the right-hand boundary at the first boundary to right of the region and the left-hand boundary at the first boundary to the left.

Caution note: on Type 4 when KK > 1: If some regions overlap, the code will lose some of the input energy, since all but the last source in any overlapped zone is dropped. This results in a diagnostic message.

Source Type 5 - Externally Generated Energy Profile (for plane geometry only)

Only Input Card Format (6E10.3, 2I5)

Variable 1. $F_o = \pm |$ total incident flux $|$.
(1-10) If $F_o \geq 0$ flux in ergs/cm².
 If $F_o < 0$ flux in cal/cm².

Variable 2. τ_1 .
(11-20)

Variable 3. τ_2 .
(21-30)

Variable 4. τ_3 .
(31-40)

Variable 5. τ_4 .
(41-50)

Variable 6. $\dot{\mathcal{P}}_2 / \dot{\mathcal{P}}_3$ (see Type 1, same for all zones).
(51-60)

Variable 7. A switch to select data input tape.
(61-65) If \neq 1, input tape unit is 7.
If = 1, input tape unit is 17 = card reader.

Variable 8. A switch for time retardation from front surface.
(66-70) If \neq 1, there is no time retardation.
If = 1, time retardation is included.

See Section VII-5.* If card input is indicated, insert cards discussed
in Appendix D* at this point.

Source Type 6 - HE Burn Format (8E10.3) (See Section X-2* and Section IV.2)

Variable 1. X_0 - Point of initiation of burn.
(1-10)

Variable 2. t_0 - Detonation time (start of burn).
(11-20)

Variable 3. X_R - Right-hand boundary (largest X) of burn region.
(21-30)

Variable 4. X_L - Left-hand boundary (smallest X) of burn region.
(31-40)

Variable 5. D - Detonation velocity.
(41-50)

Variable 6. Q - Chemical energy release per unit mass.
(51-60) or
 $(-P_{CJ})$ - Chapman-Jouguet pressure. The self-detonation
calculation is active only if P_{CJ} is defined.

Variable 7. N - Number of zones in the detonation front
(61-70) (normally ~ 3).

Variable 8. Switch = 1 if more HE burn region cards are to follow.
(71-80) Switch = 0 if no more cards are to follow.

Card Set 14 - Initial Zone Activation Format (8E10.3)

Present only if NACTION > 0 (see card 3).

There are NACTION sets of these variables.

Variable Odd. Lower boundary of active region.

Variable Even. Upper boundary of active region.

Card Set 15 - Rezone for Initial Voids with Type 5 Energy Source

Can be used only in plane geometry.

Present only if NSPALL > 0 (card 3).

Card 1 Format (I5)

Variable 1. JJJ - Number of breaks in materials.

(1-5)

Next JJJ Cards Format (I5, E15.7)

Variable 1. JJ - The material zone boundary number at the break.

(1-5)

Variable 2. The space between the parts of the material.

(6-20)

Initial space can only be made at an interior boundary, i.e.,

$2 \leq JJ \leq NMTRLS$.

APPENDIX F

ANEOS INPUT CARDS

APPENDIX F

ANEOS Input Cards

The input cards here perform the same function as those in Appendix A of R2 and Appendix I in R1. They form card set 12 in CHART D and card set 3 in CKEOS. Note that eight different options are now available.

References to an equation number or report section with an * refer to R2. Those without refer to this report. A ★ represents an input variable with new optional form.

Inputs for ANEOS options 0 to +4

Card 1	Format (I3, I5, I2, 5A10, 2E10.3)
Variable 1. (1-3)	Equation-of-state number (negative number). -1 to -20 always.
Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero. [†]
Variable 3. (9-10)	Used only with a library equation of state. This variable determines the type of analytic calculation (see variable 2, card 2 below). If out of range 0 to 4, or library information is only for a gas, this input is ignored.
Variable 4 - 8. (11-60)	Fifty-column identification label: any BCD information.
Variable 9. (61-70)	RHUG - The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).
Variable 10. (71-80)	THUG - The initial temperature for the Hugoniot calcu- lation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below).

*
* If a library equation of state is requested,*
* no further data cards are required.*

[†] See Appendix C in R2 for contents.

Cards 2,3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. (1-10)	The number of elements in this material.
Variable 2. (11-20)	Switch for type of equation of state. See R2 for these options.
	0. - Solid-gas without electronic terms and without detailed treatment of the liquid-vapor region.
	1. - Solid-gas with electronic terms but without detailed treatment of the liquid-vapor region.
	2. - Gas only with electronic terms.
	3. - Same as 0., but with a detailed treatment of the liquid-vapor region.
	4. - Same as 1., but with a detailed treatment of the liquid-vapor region.
Variable 3. (21-30)	ρ_0 - Reference density.
Variable 4. (31-40)	T_0 - Reference temperature. If $T_0 \leq 0$, code sets $T_0 = 0.02567785$ ev (298°K).
Variable 5. (41-50)	P_0 - Reference pressure (normally 0).
Variable 6. (51-60)	B_0 - Reference bulk modulus (positive number)[III-3] [*] , or $(-S_0)$ - Constant in linear Hugoniot shock-particle velocity relation (negative number)[VIII-1] [*] .
Variable 7. (61-70)	Γ_0 - Reference Grüneisen coefficient.

- Variable 8. $\pm \theta_0$ - Reference Debye temperature. ★
 (71-80) If $\theta_0 = 0$, code sets $\theta_0 = 0.025$.
 If $\theta_0 > 0$, use high temperature approximation as in R2.
 If $\theta_0 < 0$, calculate complete Debye functions
 See section III 1.
- Variable 9. T_T - Parameter [3.10].*
 (1-10) $T_T = -1$, Slater theory,
 $T_T = 0$, Dugdale and MacDonald theory,
 $T_T = 1$, free-volume theory,
 or
 S_1 - Constant in linear Hugoniot shock-particle
 velocity relation [VIII-1].*
- Input variable is defined in relation to variable 6.
- Variable 10. $3C_{24}$ - Three times the limiting value of the Grüneisen
 coefficient for large compressions, usually either
 2 or 0. When a value of 2 is used, $C_{24} = 2/3$
 [4.11].*
- Variable 11. E_s - Zero temperature separation energy [3.23].*
 (21-30)
- Variable 12. T_m - Melting temperature [V-5],*
 (31-40) or
 $(-E_m)$ - Energy to the melting point at zero pressure
 from the reference point [V-5].*
- Variable 13. C_{53} - Parameter for low density P_c modification to
 move critical point (normally zero)[3.33].*
- Variable 14. C_{54} - Parameter for low density P_c modification to
 move critical point (normally zero)[3.33].*
 If $C_{54} = 0$ and $C_{53} \neq 0$, codes sets $C_{54} = 0.95$.
- Variable 15. H_0 - Thermal conductivity coefficient. If zero,
 thermal conduction is not included. Note that the
 units of $H = H_0 T_{41}^C$ are ergs/(cm sec eV)[7.6].*

Variable 16. C_{41} - Temperature dependence of thermal conduction coefficient (see variable 15)[7.6].*

Variable 17. ρ_{\min} - Lowest allowed solid density, usually about 0.8 ρ_o . If zero or negative, code sets $\rho_{\min} = 0.8 \rho_o$ [V-3].*

Variable 18. Parameter D_1

Variable 19. Parameter D_2

Variable 20. Parameter D_3

Variable 21. Parameter D_4

Variable 22. Parameter D_5

Variable 23. H_f - Heat of fusion to determine melt transition parameters [V-1].*

If $H_f = 0$, no transition is included.

If $H_f < 0$, code sets $H_f = 1.117 \times 10^{12} T_m/A$ (ergs/gm), where A is the average atomic weight.

Note: Code will run slower if the melt transition is included. Use only when necessary and after testing.

Variable 24. ρ_l/ρ_s - Ratio of liquid to solid density at melt point *

or

($-\rho_l$) - Density of liquid at melt point.

or

$1 + \Delta V = 1 + V_l - V_s$ - Change in volume at melt plus one. Note: In the first option, the input number is between 0 and 1; in the second it is negative; and in the third greater than one.

If $H_f \neq 0$ and $\rho_l/\rho_s = 0$, code sets $\rho_l/\rho_s = 0.95$ [V-1].*

For a gaseous equation of state(type 2), variables 5 to 14 and 17 to 24 are read but not used.

Card 5

Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

I = 1, number of elements [VI].*

Variable Odd. Z(I) - Atomic number of element.

Variable Even. Unnormalized atomic number fraction of element
[COT(I)],
or
- (Unnormalized atomic weight fraction of element)
All elements should be defined in the same way.

Inputs for ANEOS Option -l

Card 1	Format (I3, I5, I2, 5A10, 2E10.3)
Variable 1. (1-3)	Equation-of-state number (negative number). -1 to -20 always.
Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero.
Variable 3. (9-10)	Used only with a library equation of state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -1 in this case.
Variable 4 - 8. (11-60)	Fifty-column identification label: any BCD information.
Variable 9. (61-70)	RHUG = The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).
Variable 10. (71-80)	THUG = The initial temperature for the Hugoniot calcu- lation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below). ***** * If a library equation of state is requested, * * no further data cards are required. * *****

Cards 2,3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. The number of elements in this material.
(1-10)

Variable 2. Switch for type of equation of state.
(11-20) Must be -1 for this option.

Variable 3. ρ_0 - Reference density.
(21-30)

Variable 4. T_0 - Reference temperature.
(31-40) If $T_0 \leq 0$, code sets $T_0 = 0.02567785$ eV ($298^\circ K$).

Variable 5. Blank.
(41-50)

Variable 6. S_0 - Reference point bulk sound speed.
(51-60)

Variable 7. Γ_0 - Reference Grüneisen coefficient.
(61-70)

Variable 8. Blank.
(71-80)

Variable 9. S_1 - Constant in linear Hugoniot shock-particle
(1-10) velocity relation for use of (III.4.22)
 or

(-100) - For power series representation of P_H
(III.4.23). Enter variables 18 to 21.

 or

($-S_1$ -100) - For power series representation with
 S_1 for low density (see Section III.4-1).

Variable 10. Blank.
(11-20)

Variable 11. (21-30)	C_v - Heat capacity. If $C_v \leq 0$, code sets $C_v = 3$ No k.
Variable 12. (31-40)	T_m - Melting temperature or $(-E_m)$ - Energy to the melting point at zero pressure from the reference point (see eq. III.4.34).
Variable 13. (41-50)	Blank.
Variable 14. (51-60)	Blank.
Variable 15. (61-70)	H_o - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = H_o T^{C_{41}}$ are ergs/(cm sec eV)[7.6].*
Variable 16. (71-80)	C_{41} - Temperature dependence of thermal conduction coefficient (see variable 15)[7.6].*
Variable 17. (1-10)	ρ_{min} - Lowest allowed solid density, usually about 0.8 ρ_o . If zero or negative, code sets $\rho_{min} = 0.8 \rho_o$ [V-3].*
Variable 18. (11-20)	K_1 .
Variable 19. (21-30)	K_2 .
Variable 20. (31-40)	K_3 .
Variable 21. (41-50)	K_4 .
Variable 22. (51-60)	Blank.
Variable 23. (61-70)	Blank.
Variable 24. (71-80)	Blank.

{ Constants in equation (III.4.23).
Enter only if variable 9 ≤ -100
Blank otherwise.

Card 5

Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable l, card 2.

I = l, number of elements.

Variable Odd. Z(I) - Atomic number of element.

Variable Even. Unnormalized atomic number fraction of element
[COT(I)],

or

-(Unnormalized atomic weight fraction of element.)

All elements should be defined in the same way.

Inputs for ANEOS Option-2

Card 1	Format (I3, I5, I2, 5A10, 2E10.3)
Variable 1. (1-3)	Equation-of-state number (negative number). -1 to -20 always.
Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero.
Variable 3. (9-10)	Used only with a library equation of state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -2 in this case.
Variable 4 - 8. (11-60)	Fifty-column identification label: any BCD information.
Variable 9. (61-70)	RHUG = The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).
Variable 10. (71-80)	THUG = The initial temperature for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below). ***** * If a library equation of state is requested,* * no further data cards are required.* *****

Cards 2,3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. The number of elements in this material.
(1-10)

Variable 2. Switch for type of equation of state.
(11-20) Must be -2 for this option.

Variable 3. ρ_0 - Reference density.
(21-30)

Variable 4. T_0 - Reference temperature.
(31-40) If $T_0 \leq 0$, code sets $T_0 = 0.02567785$ eV ($298^\circ K$).

Variable 5. K_1 - Constant in Rosseland opacity expression.
(41-50) Units are cm^2/gm .

Variable 6. Blank.
(51-60)

Variable 7. $(\gamma-1)$ - Specific heat ratio minus one.
(61-70)

Variable 8. K_2 - Constant in Rosseland opacity expression
(71-80) Units are eV.

If $K_2 \leq 0$, code sets $K_2 = .025$ eV.

Variable 9. Blank.
(1-10)

Variable 10. Blank.
(11-20)

Variable 11. C_v - Heat capacity.
(21-30) If $C_v \leq 0$, code sets $C_v = 3/2$ No k.

Variable 12. Blank.
(31-40)

Variable 13. Blank.
(41-50)

Variable 14. Blank.
(51-60)

Variable 15. Blank.
(61-70)

Variable 16. Blank.
(71-80)

Variable 17. Blank.
(1-10)

Variable 18. Blank.
(11-20)

Variable 19. Blank.
(21-30)

Variable 20. Blank.
(31-40)

Variable 21. Blank.
(41-50)

Variable 22. Blank.
(51-60)

Variable 23. Blank.
(61-70)

Variable 24. Blank.
(71-80)

Card 5 Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

I = 1, number of elements.

Variable Odd Z(I) - Atomic number of element.

Variable Even. Unnormalized atomic number fraction of element [COT(I)],

or

- (Unnormalized atomic weight fraction of element.)

All elements should be defined in the same way.

Inputs for ANEOS Option-3

Card 1	Format (I3, I5, I2, 5A10, 2E10.3)
Variable 1. (1-3)	Equation-of-state number (negative number). -1 to -20 always.
Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero.
Variable 3. (9-10)	Used only with a library equation of state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -3 in this case.
Variables 4 - 8. (11-60)	Fifty-column identification label: any BCD information.
Variables 9. (61-70)	RHUG = The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).
Variable 10. (71-80)	THUG = The initial temperature for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below).

```
*****  
* If a library equation of state is *  
* requested, no further data cards *  
* are required. *  
*****
```

Cards 2,3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. (1-10)	The number of elements in this material.
Variable 2. (11-20)	Switch for type of equation of state. Must be -3 for this option.
Variable 3. (21-30)	ρ_0 - Reference density.
Variable 4. (31-40)	T_0 - Reference temperature. If $T_0 \leq 0$, code sets $T_0 = 0.02567785$ eV ($298^\circ K$).
Variable 5. (41-50)	K_1 - Constant in Rosseland opacity expression. Units are cm^2/gm .
Variable 6. (51-60)	l. - Integer which must be entered but not used.
Variable 7. (61-70)	ω - LLL constant. (See variable 18 below.)
Variable 8. (71-80)	K_2 - Constant in Rosseland opacity expression. Units are eV. If $K_2 \leq 0$, code sets $K_2 = 0.25$ eV.
Variable 9. (1-10)	Blank.
Variable 10. (11-20)	Blank.
Variable 11. (21-30)	C_V - Heat capacity. If $C_V \leq 0$, code sets $C_V = 3$ No k.
Variable 12. (31-40)	T_m - Melting temperature. or $(-E_m)$ - Energy to the melting point at zero pressure from the reference point (see eq. III.4.34).

Variable 13. (41-50)	Blank.
Variable 14. (51-60)	Blank.
Variable 15. (61-70)	H_o - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = H_o T^{C_{41}}$ are ergs/(cm sec eV)[7.6].*
Variable 16. (71-80)	C_{41} - Temperature dependence of thermal conduction coefficient (see variable 15)[7.6].*
Variable 17. (1-10)	ρ_{min} - Lowest allowed solid density, usually about 0.8 ρ_o . If zero or negative, code sets $\rho_{min} = 0.8 \rho_o$ [V-3].*
Variable 18. (11-20)	A.
Variable 19. (21-30)	B.
Variable 20. (31-40)	R_1
Variable 21. (41-50)	R_2
Variable 22. (51-60)	Blank.
Variable 23. (61-70)	Blank.
Variable 24. (71-80)	Blank.

LLL Constants.
See reference 15.

Card 5

Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

I = 1, number of elements. See reference 14 for element table.

Variable Odd Z(I) - Atomic number of element.

Variable Even Unnormalized atomic number fraction of element [COT(I)],
or

-(Unnormalized atomic weight fraction of element.)

All elements should be defined in the same way.

Contents of the C Array for EOS Types -1, -2 and -3.

A summary of the contents of the C (internal storage) array for EOS types 0 to 4 is given in Appendix B of R2. The following is the corresponding information for the new options.

ANEOS -1	ANEOS -2	ANEOS -3
C.		
1. not used	not used	not used
2. --	--	--
3. E_o	γ	E_{oo}
4. c_v	c_v	c_v
5. $\rho_o \Gamma_o c_v$	$(\gamma-1)c_v$	R_1
6. error message counter	$\ln \left\{ T_o \rho_o^{(1-\gamma)} \right\}$	R_2
7. --	--	--
8. --	--	--
9. --	--	--
10. --	--	--

ANEOS -1	ANEOS -2	ANEOS -3
11. ρ_o	ρ_o	ρ_o
12. T_o	T_o	T_o
13. --	--	--
14. --	--	--
15. Γ_o	$\gamma - 1$	ω
16. --	--	--
17. --	--	--
18. T_m	--	T_m
19. --	--	ρ_{oo}
20. --	--	--
21. $\rho_o s_o^2$	$K_1 K_2^3$	$K_1 K_2^3$
22. constant in $(7.8)^*$	--	constant in $(7.8)^*$
23. ρ_{min}	not used	ρ_{min}
24. --	--	--
25. --	K_2	K_2
26. $Z_m [Eq.(6.5)]^*$	Z_m	Z_m
27. $N_o [Eq.(6.10)]^*$	N_o	N_o
28. Number of elements in material.	Number of elements	Number of elements
29. $\bar{A} [Eq.(6.2)]^*$	\bar{A}	\bar{A}
30. EOS type switch, -1	-2	-3
31. Internal storage location	Internal storage location	Internal storage location
32. s_o	--	A
33. s_1	--	B

ANEOS -1	ANEOS -2	ANEOS -3
34. --	--	--
35. T_m for error test.	--	$\left\{ Ae^{-R_1/\rho_{\infty}} + Be^{-R_2/\rho_{\infty}} \right\} \left(\omega \rho_{\infty}^{\omega+1} \right)$
36. $1/2 \rho_0$	--	--
37. --	--	--
38. --	--	--
39. --	--	--
40. --	--	--
41. Constant in (7.8)*	--	--
42. --	--	--
43. --	--	--
44. K_1	--	--
45. K_2	--	--
46. --	--	--
47. --	--	--
48. --	--	--
49. --	--	--
50. --	--	--
51. --	--	--
52. --	--	--
53. K_3	--	--
54. K_4	--	--