33 SANDIA REPORT SAND81-2581 • Unlimited Release • UC-34

New Features and Revised Input Instructions for Chart D

MASTER

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Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-76DP00789



SF2900Q(8-81)

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Printed in the United States of America Printed in the United States of America Available from National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road Springfield, VA 22161

NTIS price codes Printed copy: \$8.00 Microfiche copy: A01

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UC-34

SAND81-2581 UNLIMITED RELEASE PRINTED NOVEMBER 1981

SAND--81-2581

DE82 011684

NEW FEATURES AND REVISED INPUT INSTRUCTIONS FOR CHART D

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ABSTRACT

Recent improvements in the one-dimensional, Lagrangian, radiation-hydrodynamics code, CHART D, are described. They include transmitting boundaries, a generalized failure surface and improved editing capabilities.

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1. INTRODUCTION

Chart D is a one-dimensional, Lagrangian, radiation-hydro-dynamics code that has been in use for over ten years. Chart D has changed little in the past few years yet some new features have been added recently that are documented here for the first time. This report describes these new features and the revised input instructions. It does not document features already described in earlier reports [1,2,3].

Four new features have been added to Chart D; two improve the editing capability and two improve the physics. The user can now change the print and plot edit frequency when restarting a calculation. The user can also generate history records at Lagrangian locations in the mesh and these records can be processed with the CSQHIST program [4]. These histories can be easily compared to gauge records from experiments. A generalized failure surface has been included which should be better than the von Mises failure surface for modeling geologic materials [5]. A transmitting boundary condition has been added which approximates a semi-infinite material because it absorbs incident stress waves with little reflection. Without a transmitting boundary condition, incident stress waves will reflect off the mesh boundary and propagate back into the mesh. The only alternative to a transmitting boundary condition is to include enough material in the mesh so that reflected stress waves from the boundary do not propagate into the region of interest during the calculation. Each of these four items is discussed in a section

in the following body of the report. The input for Chart D, ANEOS, and MASPLT are described in Appendices A, B, and C. There are no changes in the ANEOS and MASPLT input instructions but they are included in this report for completeness. The Chart D input variables that have been changed are marked with a vertical line to the left of the description of the variable.

2. EDIT FREQUENCY CHANGES ACROSS A RESTART

Binary restart dumps may be written to a file at selected times and at the end of a calculation. Each dump contains all the material data and cell variables at a particular cycle. This data may be read off the file, used to initialize all the variables in Chart D, and the calculation may be continued. In the past, the user could not change the print or plot edit frequency from the values written in the restart dump. Recent modifications enable the user to change the edit frequency when restarting. This can be used to change the edit frequency during a long calculation. Alternatively, the user can complete the calculation generating a modest number of edits and then return to a time of interest, restart, and generate several print or plot edits during the time of interest.

3. HISTORY EDITS AT LAGRANGIAN POINTS

Chart D has been modified to write binary edit files suitable for input to CSQHIST, the history plot, print, and edit program used by CSQII and TOODY. Cell variables at Lagrangian locations and global quantities associated with material layers can be edited by Chart D and plotted or printed by CSQHIST. For global quantities, the term "layer" in the Chart D manual is the same as "material" in the CSQHIST documentation [4]; i.e., layer one in Chart D is material one in CSQHIST.

The format of the edit file from Chart D (unit 55) is exactly the same as the edit file from CSQII. The file is written so that the Chart D coordinate (X) is the CSQHIST X coordinate. For cylindrical geometry calculations, Y is the axial coordinate. The Y-velocity and shear stress deviator σ^d_{xy} are zero. The position and velocity of a Lagrangian particle are interpolated from the cell boundary values. In particular, if the position of the particle was initially one-fourth the way between the boundaries then the position and velocity are

$$\hat{x} = .25 X_L + .75 X_R$$

$$\hat{V} = .25 V_L + .75 V_R$$

where X (V) is the position (velocity) of a particle, X_L (V_L), is the position (velocity) of the left-hand boundary, and X_R (V_R) is the position (velocity) of the right-hand boundary. All other edited variables are cell centered values. Cell variables

and velocities are written in CGS units but CSQHIST can display the data in a variety of units.

History edits may be requested from any Lagrangian point within a material. An edit cannot be generated for points in an internal void or beyond the external boundaries. Up to one hundred Lagrangian points may be included in a calculation. New points may be added or the location of an existing point may be redefined at the restart of a calculation. When inserting history points at a restart (cycle > 0), note that the location of the Lagrangian point is the position in the current mesh, not the initial mesh. The user is warned that the edit file (unit 55) can become very large if there are many Lagrangian points, several layers, or many cycles in a calculation.

4. GENERALIZED FAILURE SURFACE

A generalized failure surface of the following form is available in Chart D.

$$Y^{2} = \frac{3}{2} \sum_{i} (\sigma_{i}^{d})^{2} = \left\{ A - B \exp(CP) \right\}^{2} \left\{ F(E) \right\}^{2}, \quad P \ge 0$$

$$Y = Y_{O} F(E) , \quad P < 0$$
(4.1)

where $\sigma^{\bar{d}}$ is the deviatoric stress tensor, F(E) is described below, and P is the pressure (the negative of one third of the trace of the stress tensor). It resembles a Drucker-Prager failure surface at low pressures and a von Mises failure surface at high pressures. The failure surface of many geologic materials is better approximated by (4.1) than by a von Mises failure surface [5]. Once failure occurs, the stresses are relaxed back to the failure surface using the same algorithm described in the Chart D manual; i.e., the stress deviators are multiplied by an appropriate number so that (4.1) is satisfied. This flow rule is associated with the von Mises failure surface so this model uses a non-associated flow rule.

The input variables for this model are:

 Y_{∞} - the value of Y as P $\rightarrow \infty$, F(E) = 1,

 Y_{O} - the value of Y at P = 0, F(E) = 1,

 \mathscr{E}_{m} - (optional) the absolute melt energy,

 $\rho_{_{\rm O}}$ - (optional) the reference density,

ν - reference Poisson's ratio,

 α - the fraction of melt energy at which the material starts to lose strength (normally 0.8),

 $\frac{dY}{dP}$ - the derivative of Y with respect to P at P = 0.

The relationship between the input data and the constants in (4.1) is easily shown to be

$$Y_{\infty} = A$$
 , $Y_{O} = A - B$, $\frac{dY}{dP} = -BC$.

The values of ν and ρ_{0} are used to calculate the stress deviators as described in the Chart D manual [1]. \mathscr{E}_{m} and α are used to define the degradation of the material strength with increasing temperature,

$$F(E) = \begin{cases} 1 & \text{if } E \leq \alpha \mathscr{E}_{m} \\ \frac{(1 - E/\mathscr{E}_{m})}{1 - \alpha} & \text{if } \alpha \mathscr{E}_{m} < E < \mathscr{E}_{m} \\ 0 & \text{if } E \geq \mathscr{E}_{m} \end{cases}$$

where E is the specific internal energy of the material. The influence of Y_O , Y_∞ , and $\frac{dy}{dP}$ is displayed in Figure 1. Note that $Y = Y_O$ if P < 0.

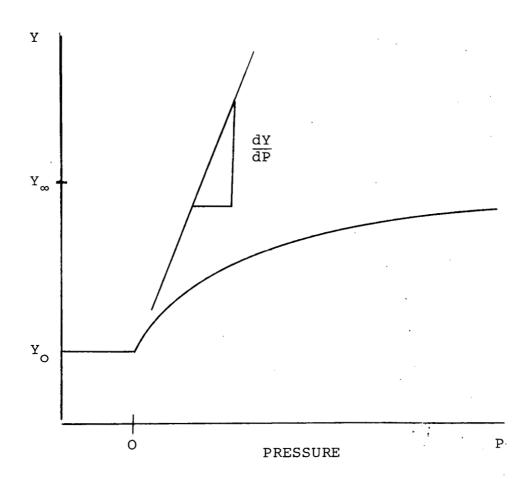


Figure 1. Generalized Failure Surface

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TRANSMITTING BOUNDARY CONDITION

Transmitting boundaries simulate semi-infinite homogeneous media in the sense that they absorb incident stress waves with little or no reflection. The only practical alternative to a transmitting boundary is to include enough material in the calculation so that the reflected stress wave from the boundary does not influence the region of interest. This alternative can be very expensive in both CPU time and storage. With transmitting boundaries, only the region of interest need be included in the calculation.

Several types of transmitting boundaries have been developed. The one we use is a generalization of the boundary condition developed by Lysmer and Kuhlemeyer [6].

 $\delta \sigma = \rho c \delta u$

where $\delta\sigma$ is the increment of the boundary stress, ρ is the mass density, c is the sound speed, and δu is the increment of the boundary velocity. Using this boundary condition and the momentum balance equation, which is also a relationship between velocity and stress, the boundary velocity can be eliminated and a boundary stress calculated. This boundary condition was originally developed for linearly elastic materials so ρc was a constant. We have generalized it to nonlinear materials by letting ρc vary during the calculation. This boundary condition has worked very well on a variety of problems but the user should scrutinize the results.

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APPENDIX A

REVISED CHART: D INPUT INSTRUCTIONS

TAPE UNITS FOR Chart D

- Optional binary edit output tape for plots.*
- 3. Binary edit output tape for plots.
- 7. Standard DTF or BUCKL input tape.
- 10. Standard restart output tape and input tape.
- 11. Optional restart output tape.
- 12. Tabular EOS tape.
- 17. Optional DTF or BUCKL input tape.
- 55. Material history output tape.

Writing optional binary edit output requires modification of the PROGRAM card. Presently tape units 2 and 3 are equivalenced.

The Chart D input variables that have been changed are marked with a vertical line to the left of the description of the variable.

APPENDIX A

REVISED CHART D INPUT INSTRUCTIONS

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 (615, 3E10.3, 3I5)
Variable 1.	ITIMEL - Computer time limit in seconds.
(1-5)	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.	NG - A switch to signify whether the problem
(6-10)	is to be generated or restarted.
	NG = 0 generate new problem
·	< 0 restart without input data change
	> 0 restart with data change - input only the following variables.
•	Card Variable
•	3 4-NPRIN same format with
	16-MOVIE other variables zero.
	5 All
	8 All if MOVIE > 0
	If NG \neq 0, the code reads NG tape dumps
	from tape 10 before restarting.
Variable 3.	NDUMP - The time interval in seconds of com-
(11-15)	puter time between writing restart tape dump
	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 \leq 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 at the same frequency as the print edits. See note on tape units for Chart D.

Variable 6. (26-30)

NEDREJ - A switch to force edits whenever a
fracture or 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.</pre>

Variable 7. (31-40)

FRACDT Fraction of Courant stability limit used to calculate sound speed time step. (Normally 0.8, in no case greater than 1).

If FRACDT \(\leq 0.8 \), FRACDT = 0.8.

Variable 8. (41-50)

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

Variable 9. (51-60)

TEND - The end of problem time. If TEND ≤ 0 , TEND is set to a very large number and the run is terminated on ITIMEL variable.

Variable 10. (61-65)

NEXZON - Indicator for special edit of zone quantities.

If NEXZON = 0, no special edit.

If $1 \le \text{NEXZON} \le \text{number of zones, special}$ edit for the NEXZONth zone.

If $-100 \le \text{NEXZON} \le -1$, special edit for the first zone in the $(-\text{NEXZON})^{\text{th}}$ layer.

If NEXZON < -100, special edit for the last zone in the (-NEXZON -100)th layer.

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

Variable 12. IHIST - Switch for output on history data (71-75) tape (unit 55). This data file is for use with CSQHIST plot program.

If = 0, no output to tape 55.

If \neq 0, output data written on tape 55. The frequency of output is every |IHIST! the cycle.

For a new problem generation (CYCLE = 0) input card set 16.

For a restart (NG ≠ 0, variable 2),

IHIST > 0 indicates that no additional data is to be entered on card set 16; IHIST < 0 indicates that additional card set 16 data is to be entered.

If this calculation is <u>not</u> a restart, go to card 3. If this calculation is a restart (NG \neq 0 on card 2), enter only the information defined by variables 2 and 12 on card 2 (and on cards 3, 5, 8 and 16 if appropriate).

Card	3	Format (16I5)
Variable :	1.	IGM - A geometry switch.
(1-5)		<pre>If IGM = 1, plane geometry.</pre>
		<pre>If IGM = 2, cylindrical geometry.</pre>
		<pre>If IGM = 3, spherical geometry.</pre>
Variable 2	2.	NRZC - The number of different zoning regions
(6-10)		(see card set 11). There is no limit on the
		size of NRZC.
Variable :	3.	NMTRLS - The number of material layers in the
(11-15)		problem. A material layer is a group of cells

that all contain the same material, and has boundary cells that are either at the edge of the mesh or adjacent to cells containing a different material, (see card set 11). NMTRLS \leq NRZC. NMTRLS \leq 20.

- Variable 4. NPRIN The number of edit (print out) fre-(16-20) quency intervals (see card set 5). $1 \leq \text{NPRIN} \leq 24.$
- Variable 5. NDTMAX The number of maximum input Δt (21-25) intervals (see card set 6). $0 \le \text{NDTMAX} \le 24$. If NDTMAX ≤ 0 , the maximum Δt is set to a very large number.
- Variable 6. NDTMINN The number of minimum input Δt (26-30) intervals (see card set 7). $0 \le \text{NDTMINN} \le 24$. If NDTMINN ≤ 0 , the minimum Δt is zero.
- Variable 7. NBPRES The number of points in the boundary (31-35) pressure histories (see card set 9). NBPRES \leq 24. If NBPRES \leq 0, there are no boundary pressures.
- Variable 8. NOSOUR A switch for internal energy sources.

 (36-40) If NOSOUR ≤ 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. IBS A switch to determine if boundary NZP (41-45) (smallest X) is transmitting, free to move, or fixed in space.

 If IBS = -1, boundary NZP is transmitting (available only if IGM = 1).

 If IBS = 0, boundary NZP is free.

 If IBS = 1, boundary NZP is fixed (V = 0).
- Variable 10. OBS A switch to determine if boundary 1 (46-50) (largest X) is transmitting, free to move, or fixed in space.

If OBS = -1, boundary 1 is transmitting. If OBS = 0, boundary 1 is free. If OBS = 1, boundary 1 is fixed $(V \equiv 0)$. NSPALL - A switch for fracture calculations. Variable 11. If NSPALL < 0, no material fracture is (51-55)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. NACTION - The number of regions with initially Variable 12. 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. If NORAD = 0, no radiation diffusion is cal-(61 - 65)culated. 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 the fastest of 1, 2, 3. The hydrodynamic calculation can be suppressed with options 1 through 4 by using the negative of the option number. NTHIST - The number of points in the boundary Variable 14. temperatures histories (see card set 10). (66-70)NTHIST \leq 24. (Ignored if NORAD = 0.) If NTHIST ≤ 0, there are no boundary tempera-

tures.

Variable 15.	NRADCK - A switch for the radiation flux
(71-75)	<pre>limiter. (Ignored if NORAD = 0.)</pre>
	If NRADCK = 0, the limiter is used (normal
	option).
	If NRADCK > 0, the limiter is not used.
	If NRADCK = -1 , the limitor is used but with
	<pre>1/4 maximum flux of NRADCK = 0. (See Section II.4 of [2].)</pre>
Variable 16.	MOVIE - The number of movie frame frequency
(76-80)	intervals. (See card set 8.) MOVIE ≤ 9.
•	If MOVIE = 0, no movie tape is produced.
	<pre>If MOVIE > 1, movie tape is produced on unit 3.</pre>
Card 4	Format (8E10.3)
Variable 1.	BL - The constant in the linear viscosity
(1-10)	term (normally 0.1).
Variable 2.	BQ - The constant in the quadratic viscosity
(11-20)	term (normally 2.0). Note: Both BL and BQ should not be zero.
	$\overline{I}f BL + BQ = 0$, code sets $BL = 0.1$ and
	BQ = 2.0.
Variable 3.	XM2(1) - Temporary storage for the fictitious
(21-30)	outer boundary mass (boundary 1) (normally 0).
	Must be zero if using transmitting boundary.
Variable 4.	XM2(2) - Temporary storage for the fictitious
(31-40)	inner boundary mass (boundary NZP) (normally
	0). Must be zero if using transmitting
· ·	boundary.
Variable 5.	SCRADF - A scale factor for the front surface
(41-50)	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.</pre>

Variable 6. SCRADB - A scale factor for the back surface (51-60) 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 ≥ 0, any radiation passing into the void will be lost. SCRADB < 0 is the physically realistic choice.

Variable 7. TRADOFF - The earliest time at which the code (61-70) will check to see if the radiation can be turned off (normally 0).

Variable 8. SWEP - Elastic-plastic switch.

(71-80) 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 NDTMINN > 0 (see card 3).

There are NDTMINN sets of these variables.

Variable Odd. TDTMINN (I) - The time at which the minimum time step switches from DTMINN (I-1) to DTMINN (I).

[TUTMINN (1) = 0, always.]

Variable Even. DTMINN (I) - The minimum time step allowed between TDTMINN (I) and TDTMINN (I+1). For times > TDTMINN (NDTMINN), the last value of DTMINN 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.

MOVIE 2 2 to function property.

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

 (1-10) pressure history point. [TBPRES(1) = 0, always.]
- Variable 2. PINNER (I) The boundary pressure at (11-20) boundary NZP (smallest X) at time TBPRES(I).
- Variable 3. POUTER (I) The boundary pressure at (21-30) boundary 1 (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
 (1-10) temperature history point.
 [TITH(1) = 0, always.]
- Variable 2. TEINTH(I) The boundary temperature at (11-20) boundary NZP (smallest X) at time TITH(I).

Variable 3. TEOUTH(I) - The boundary temperature at
(21-30) boundary 1 (largest X) at time TITH(I).
 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. There 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. In a material layer with multiple zoning regions, Chart D uses region information cards 2 and 3 from the last zoning region for all the zoning regions in the material layer. The region information cards for the other zoning regions are read but not used.

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 (1-5) used for this region.
- Variable 2. X_{up} The upper boundary (largest X) of the region (6-15) being zoned. Except 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 (16-25) the last region 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 (26-35) zone in this 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 (36-45) zone in this region. When Type 1 zoning is used, this temperature can be superseded for specified zones.

If $T_O \le 0$, code sets $T_O = 0.02567785$ (298°K).

- Variable 6. V_O The initial velocity to be used for the upper boundary 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 (56-60) material in this 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.

Region Information Card 2 Format (8E10.3)

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 or type 7 zoning (void).
 a blank card
 All eight variables read and stored but not used.
- TI. Elastic-Plastic von Mises Material (see Section IV-2 of [1] and variable 8, card 4).

Variable 1. Y_{O}

Variable 2. Y_]

- Variable 3. 0. Computed internally. The absolute melt

 (21 30) energy (%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. $\rho_{_{\mbox{O}}}$ Reference density. If zero, the density (31-40) is taken to be the same as $\rho_{_{\mbox{O}}}$ on region information card 1.
- Variable 5. v_0 Reference Poisson's ratio. (41-50)
- Variable 6. α Fraction of melt energy at which the (51-60) material starts to lose strength (normally 0.8). If $\alpha \le 0$, code sets $\alpha = 0.8$.

Variable 7. 0.

(61-70)

Variable 8. 0.

(71 - 80)

- III. Distended or Porous Material (see Section V-5 of [1] and Section II.2 of [2]).
 - Variable 1. ρ_{SO} Normal solid density at the temperature (1-10) given by T_{O} on region information card 1. This is used to calculate the initial distention ratio.
 - Variable 2. k_0' A constant used in computing the tempera(11-20) ture dependence of the crush strength. (See
 Section II.2 of [2]).

 If $k_0' = 0$, code sets $k_0' = -2$.

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

(21 - 30)

- Variable 4. \mathscr{P}_{e} The elastic limit pressure of the (31-40) material at full distention.
- Variable 5. \mathscr{P}_s The elastic limit pressure as all voids (41-50) vanish in the quadratic model, $\frac{\text{or}}{}$

(-a) - constant in the exponential model.

- Variable 6. C_{eo} Sound speed in the material at full (51-60) distention. If no value is given, the normal solid sound speed is used.
- Variable 7. $\Gamma_{\rm eff} {\rm Effective~Gr\"{u}neisen~coefficient~for}$ $(61-70) \qquad {\rm revised~P-\alpha~model~(see~Section~II.2~of~[2])}.$ ${\rm If~}\Gamma_{\rm eff} \leq 0, {\rm code~uses~older~P-\alpha~model}.$
- Variable 8. δ Constant (see Section II.2-2 of [2]). (71-80) If $\delta \leq 0$, code sets $\delta = 1/2$.

Variable 1. Y_{∞} (1-10)

Variable 2. Y_O (11-20)

Variable 3. 0. -Computed internally. The absolute melt (21-30) energy $(\mathscr{E}_{\mathfrak{m}})$ 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 (31-40) is taken to be the same as ρ_O on region information card 1.

Variable 5. ν_{o} - Reference Poisson's ratio. (41-50)

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

Variable 7. 0. - Not used. (61-70)

Variable 8. $\frac{dY}{dP}$ - Must be greater than 0. (71-80)

Region Information Card 3 Format (8E10.3)

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 of [1] for notation).

Variable 1. σ_u - Ultimate tensile strength (σ_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_0 - Static tensile strength ($\sigma_0 > 0$).

(51-60) If $\sigma_0 = 0$, code sets $\sigma_0 = \sigma_u$.

Variable 7. Switch to suppress tensions in partially

(61-70) melted material.

- = 0, can have tensions above incipient melt.
- = 1, cannot have tensions above incipient melt.

See Section (II.3 of [2]).

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 of [2]).

0 or 1 - normal materials

√ 4 or 5 - porous materials

- 1/2 - materials like fused silica

```
Cumulative Damage Model (see Section VII of [1] for
III.
      notation).
                               (normally 0).
      Variable 1.
                      K(O).
       (1-10)
                      T_s - Strength vanishing temperature.
      Variable 2.
                      If T_s \le 0, code sets T_s = 10.
       (11-20)
                      \sigma_{o} - Static tensile strength (\sigma_{o} > 0).
      Variable 3.
       (21 - 30)
      Variable 4.
                      λ.
       (31-40)
                      (-C) (must be negative).
      Variable 5.
       (41-50)
      Variable 6.
       (51-60)
      Variable 7.
                      Same as option II.
       Variable 8.
       (71 - 80)
      Tensile Strength Limit (see Section VII of [1] for notation).
 IV.
       Variable 1.
                      \sigma_{c} - Maximum tensile strength (\sigma_{c} > 0).
       (1-10)
                      T_s - Strength vanishing temperature.
       Variable 2.
       (11-20)
                      If T_s \le \text{code sets } T_s = 10.
                      Blank
       Variable 3.
       (21 - 30)
       Variable 4.
                      Blank
       (31-40)
       Variable 5.
                      C.
                       If C = 0, code sets C = 1.
       (41-50)
       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. NDXC - The number of ΔX zoning cards used (1-5) to zone this region.

Next NDXC Data Cards Format (I5, 4E10.3)

Variable 1. The number of zones desired with this ΔX . (1-5)

Variable 2. The ΔX to be used for these zones. (6-15)

Variable 4. 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. V_0^* - Used as the velocity of the upper (36-45) boundary for these zones if $V_0^* \neq 0$; it overrides the specified region velocity. If $V_0^* = 0$, 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 of [1])

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.

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.

Only Data Card Format (4E10.3)

Variable 1. W_1 - Width of first zone in region (1-10) (largest X). 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 (11-20) (smallest X).

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 and the other variable must be nonzero. RATIO then applies to moving away from the nonzero value.

Zoning Type 5 - Specifications of Mass Ratio and Number of Zones (See Appendix B of [1])

Only Data Card Format (I5, E10.3)

Variable 1. Number of zones desired in region (> 2). (1-5)

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

(6-15) from interior 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 $\ell \le 0$, 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 B 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 of [1] for notation.

Source Type 1 - Hand Input for Each Zone

Card l Format (I10)

Variable 1. NOSOUR - The last zone (largest zone

(1-10) number) in the problem to have a source.

All Other Cards Format (I5, 6El0.3)

Variable 1. I = Zonc 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_{Δ} - For Zone I.

(36-45)

Variable 6. \mathscr{S}_2 - For Zone I.

(46-55)

Variable 7. $\dot{\mathscr{S}}_3$ - 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.

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)

Source Type 2 - Input Total Energy Per Zone

 $\tau_1 = \tau_2$.

(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.

$$\dot{\mathscr{G}}_2 = \dot{\mathscr{G}}_3 = \frac{\text{zone energy}}{(\tau_4 - \tau_1)M_1}$$

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 L.

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

(1-10)

(largest X).

Variable 2.

Left-hand boundary of source region

(11-20)

(smallest X).

Variable 3.

Energy source strength, the total energy

(21 - 30)

to be introduced between right and left

boundaries.

Variable 4.

 $\tau_1 = \tau_2$.

(31-40)

Variable 5.

 $\tau_{\alpha} = \tau_{\alpha}$

(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.

<u>Caution note</u>: 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) $F_0 = \pm |total|$ incident flux. Variable 1. If $F_0 \ge 0$ flux in ergs/cm². (1-10)If $F_0 < 0$ flux in cal/cm². Variable 2. τ,. (11-20)Variable 3. τ,. (21 - 30)Variable 4. τ,. (31-40)Variable 5. τ4. (41-50) $\dot{\mathcal{G}}_2/\dot{\mathcal{G}}_3$ (see Type 1, same for all zones) Variable 6. (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. A switch for time retardation from front Variable 8. surface. (66-70)If \neq 1, there is no time retardation.

If = 1, time retardation is included.

See Section VII-5 of [1]. If card input is indicated, insert cards discussed in Appendix D of [1] at this point.

```
Source Type 6 - HE Burn Format (8E10.3) (See Section X-2 of
                 [1] and Section IV.2 of [2])
                        X_{O} - Point of initiation of burn.
    Variable 1.
    (1-10)
                        t - Detonation time (start of burn).
    Variable 2.
    (11-20)
                        X_{p} - Right-hand boundary (largest X) of
    Variable 3.
                        burn region.
    (21 - 30)
                        X_{\tau} - Left-hand boundary (smallest X) of
    Variable 4.
    (31-40)
                        burn region.
                        D - Detonation velocity.
    Variable 5.
    (41-50)
                        Q - Chemical energy release per unit mass.
    Variable 6.
    (51-60)
                        (-P<sub>C,1</sub>) - Chapman-Jouguet pressure.
                        self-detonation calculation is active
                        only if P_{C,T} is defined.
                        N - Number of zones in the detonation
    Variable 7.
                        front (normally \sim 3).
     (61-70)
                        Switch = 1 if more HE burn region cards
    Variable 8.
                                    are to tollow.
                        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, El5.7)

Variable 1. JJ - The material zone boundary number (1-5) at the break.

Variable 2. The space between the parts of the (6-20) material.

Initial space can only be made at an interior boundary, i.e., $2 \le JJ \le NMTRLS$.

Card Set 16 - Lagrangian Particle History Edit for CSQHIST Program

Present only if

- 1. CYCLE = 0 (new problem) and IHIST \neq 0
- 2. CYCLE > 0 (restart) and IHIST < 0

There is one of the following cards for each point where it is desired to save the history. Maximum of 100 allowed.

Card	Format (I10, E10.3, A10)
Variable 1. (1-10)	NUMB = History particle number. If input blank or zero, will default to next available number (1 for 1st, 2 for 2nd, etc.) NUMB ≤ 100.
Variable 2. (11-20)	<pre>X = Position in current mesh. If CYCLE > 0 (restart) this is not the same as the initial mesh. X must lie</pre>

within a material. It cannot be in an internal void or beyond the external boundaries.

Variable 3. (21-30)

END FLAG = If this field is blank, the code will continue reading more of these cards. If anything is in the field, no more cards will be read.

APPENDIX E

ANEOS INPUT INSTRUCTIONS

APPENDIX B

ANEOS INPUT INSTRUCTIONS

The numbers in square brackets [] refer to sections or equations in reference 3 unless otherwise stated.

Inputs for ANEOS options 0 to +4

17 5		
	Card 1	Format (I3, I5, I2, 5Al0, 2El0.3)
	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 calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the

^{*}See Appendix C in [3] for contents.

reference temperature (variable 4, card 2 below).

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) See [3] 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 l., but with a detailed treatment of the liquid-vapor region.

Variable 3. ρ_{O} - Reference density. (21-30)

Variable 4. T_{O} - Reference temperature. (31-40) If $T_{O} \leq 0$, code sets $T_{O} = 0.02567785$ ev (298°K).

Variable 5. P_{Q} - Reference pressure (normally 0). (41-50)

B - Reference bulk modulus (positive Variable 6. number) [III-3], (51-60)(-S_o) - Constant in linear Hugoniot shockparticle velocity relation (negative number) [VIII-1]. To - Reference Grüneisen coefficient. Variable 7. (61 - 70) $\pm\theta_{O}$ - Reference Debye temperature. Variable 8. If $\theta_{o} = 0$, code sets $\theta_{o} = 0.025$. (71 - 80)If $\theta_0^2 > 0$, use high temperature approximation as in [3]. If θ_{O} < 0, calculate complete Debye functions. See Section III-1 of [2]. T_{P} - Parameter [3.10]. Variable 9. $T_{r} = -1$, Slater theory, (1-10) $T_r = 0$, Dugdale and MacDonald theory, $T_{\Gamma} = 1$, free-volume theory, S₁ - Constant in linear Hugoniot shockparticle velocity relation [VIII-1]. Input variable is defined in relation to variable 6. $3C_{24}$ - Three times the limiting value of Variable 10. the Grüneisen coefficient for large com-(11-20)pressions, usually either 2 or 0. When a value of 2 is used, $C_{24} = 2/3$ [4.11]. E - Zero temperature separation energy Variable 11. [3.23]. (21 - 30) T_m - Melting temperature [V-5], Variable 12. (31-40) $(-E_m)$ - Energy to the melting point at zero pressure from the reference point [V-5].

Variable 13. (41-50)	${ m C}_{53}$ - Parameter for low density P modification to move critical point (normally zero) [3.33].
Variable 14. (51-60)	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. (61-70)	H_O - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = H_O^C 41$ 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 ρ_{\min} = 0.8 ρ_{O} [V-3].
Variable 18. (11-20)	Parameter D ₁
Variable 19. (21-30)	Parameter D ₂
Variable 20. (31-40)	Parameter D ₃ Solid-solid phase transition parameters
Variable 21. (41-50)	Parameter D ₄ (normally 0) [V-7].
Variable 22. (51-60)	Parameter D ₅
Variable 23. (61-70)	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 $H_f = 1.117 \times 10^{12}$ $T_m/\Lambda (ergs/gm)$, where A is the average atomic weight.

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

Variable 24. (71-80)

 ρ_{ℓ}/ρ_{s} - Ratio of liquid to solid density at melt point,

or

 $(-\rho_{\ell})$ - Density of liquid at melt point,

 $1 + \Delta V = 1 + V_{\ell} - V_{s}$ - 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 $\rho_{\ell}/\rho_s = 0$, code sets $\rho_{\ell}/\rho_s = 0.95$ [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-1 (Low temperature solid)

Card 1 Format (I3, I5, I2, 5Al0, 2El0.3)

Variable 1. Equation-of-state number (negative (1-3) number). -1 to -20 always.

Variable 2. Library equation-of-state number if (4-8) desired; otherwise zero.

Variable 3. Used only with a library equation of (9-10) state. This variable determine the type of analytic calculation (see variable 2, card 2 below). Must be -l in this case.

Variable 4-8. Fifty-column identification label: any (11-60) BCD information.

Variable 9. RHUG = The initial density for the

(61-70) 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. THUG = The initial temperature for the (71-80) 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).

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

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

The number of elements in this material. Variable 1. (1-10)Variable 2. Switch for type of equation of state. (11-20)Must be -1 for this option. ρ_{0} - Reference density. Variable 3. (21 - 30) T_{O} - Reference temperature. Variable 4. If $T_O \leq 0$, code sets $T_O = 0.02567785$ eV (31-40)(298°K). Variable 5. Blank. (41-50)S - Reference point bulk sound speed. Variable 6. (51-60) $\Gamma_{\rm o}$ - Reference Grüneisen coefficient. Variable 7. (61-70)Blank. Variable 8. (71-80)S, - Constant in linear Hugoniot shock-Variable 9. (1-10)particle velocity relation for use of (III.4.22)(-100) - For power series representation of P_H (III.4.23 of [2]). Enter variables 18 to 21. (-S₁ -100) - For power series representation with S_1 for low density (see Section III.4-1 of [2]). Variable 10. Blank. (11-20)C_v - Heat capacity. Variable ll. If $C_v \leq 0$, code sets $C_v = 3 N_o k$. (21-30)

```
T_{\rm m} - Melting temperature
Variable 12.
(31-40)
                   (-E_m) - Energy to the melting point at
                   zero pressure from the reference point
                   (see eq. III.4.34 of [2]).
                   Blank.
Variable 13.
(41-50)
Variable 14.
                   Blank.
(51-60)
                   H - Thermal conductivity coefficient.
Variable 15.
                   If zero, thermal conduction is not in-
(61-70)
                   cluded. Note that the units of
                   H = H_0 T^C 41 are ergs/(cm sec eV) [7.6].
                   C_{A1} - Temperature dependence of thermal
Variable 16.
                   conduction coefficient (see variable 15)
(71 - 80)
                   [7.6].
                   \rho_{\text{min}} - Lowest allowed solid density,
Variable 17.
                   usually about 0.8 \rho_{\text{O}}. If zero or negative,
(1-10)
                   code sets \rho_{min} = 0.8 \rho_{o} [V-3].
Variable 18.
                   к<sub>1</sub>.
(11-20)
                                 Constants in equation (III.4.23
                   K<sub>2</sub>.
Variable 19.
                                 of [2]). Enter only if vari-
(21-30)
                                 able 9 \leq -100. Blank other-
Variable 20.
                   К3.
                                 wise.
(31-40)
Variable 21.
                   K_{\Delta}.
(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-2 (ideal gas)

Card 1 Format (I3, I5, I2, 5Al0, 2El0.3)

Variable 1. Equation-of-state number (negative ...

(1-3) number). -1 to -20 always.

Variable 2. Library equation-of-state number if (4-8) desired; otherwise zero.

Variable 3. Used only with a library equation of (9-10) state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -2 in this case.

Variable 4-8. Fifty-column identification label: any (11-60) BCD information.

Variable 9. RHUG = The initial density for the

(61-70) 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. THUG = The initial temperature for the (71-80) 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).

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

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

```
Variable 1.
                   The number of elements in this material.
(1-10)
                   Switch for type of equation of state.
Variable 2.
                   Must be -2 for this option.
(11-20)
                   \rho_{O} - Reference density.
Variable 3.
(21 - 30)
                   T - Reference temperature.
Variable 4.
                   If T_{\Omega} \leq 0, code sets T_{\Omega} = 0.02567785 eV
(31-40)
                    (298°K).
                   K, - Constant in Rosseland opacity
Variable 5.
                   expression. Units are cm<sup>2</sup>/gm.
(41-50)
                   Blank.
Variable 6.
(51 - 60)
                    (\gamma-1) - Specific heat ratio minus one.
Variable 7.
(61-70)
                   K<sub>2</sub> - Constant in Rosseland opacity
Variable 8.
                   expression. Units arc cV.
(71 - 80)
                   If K_2 \le 0, code sets K_2 = .025 eV.
                    Blank.
Variable 9.
(1-10)
Variable 10.
                    Blank.
(11-20)
                   C, - Heat capacity.
Variable ll.
                    If C_{V} \leq 0, code sets C_{V} = 3/2 N_{O} k.
(21-30)
                    Blank.
Variable 12.
(31-40)
Variable 13.
                  Blank.
(41-50)
Variable 14.
                    Blank.
(51-60)
Variable 15.
                  Blank.
(61 - 70)
```

			/F /DF 0	m10	211		
Variable (71-80)	24.	Blank.					
Variable (61-70)	23.	Blank.					
Variable (51 - 60)	22.	Blank.					
Variable (41 - 50)	21.	Blank.					
Variable (31-40)	20.	Blank.					
Variable (21-30)	19.	Blank.					
Variable (11-20)	18.	Blank.					
Variable (1-10)	17.	Blank.		·			
Variable (71 - 80)	16.	Blank.				•	

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 (JWL high explosive)

Card 1 Format (I3, I5, I2, 5A10, 2E10.3)

Variable 1. Equation-of-state number (negative

(1-3) number). -1 to -20 always.

Variable 2. Library equation-of-state number if

(4-8) desired; otherwise zero.

Variable 3. Used only with a library equation of (9-10) state. This variable determines the type of analytic calculation (see variable 2, card 2 below).

Must be -3 in this case.

Variable 4-8. Fifty-column identification label: any (11-60) BCD information.

Variable 9. RHUG = The initial density for the

(61-70) Hugoniot calculation. If zero, the calculation is skipped. If negative, the

initial density is taken to be the

reference density (variable 3, card 2

Variable 10. THUG - The initial temperature for the (71-80) Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card

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

below).

2 below).

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

```
The number of elements in this material.
Variable 1.
(1-10)
Variable 2.
                   Switch for type of equation of state.
                  Must be -3 for this option.
(11-20)
                   \rho_{o} - Reference density.
Variable 3.
(21 - 30)
                  T - Reference temperature.
Variable 4.
                   If T_0 \leq 0, code sets T_0 = 0.02567785 eV
(31-40)
                   (298°K).
                  K, - Constant in Rosseland opacity
Variable 5.
                  expression. Units are cm<sup>2</sup>/gm.
(41-50)
Variable 6.
                   1. - Number which must be entered but
(51-60)
                  not used.
                   \omega - LLL constant. (See variable 18
Variable 7.
(61-70)
                  below.)
                  K<sub>2</sub> - Constant in Rosseland opacity
Variable 8.
                   expression. Units are eV.
(71 - 80)
                   If K_2 \le 0, code sets K_2 = 0.025 eV.
Variable 9.
                   Blank.
(1-10)
Variable 10.
                   Blank.
(11-20)
Variable 11.
                   C, - Heat capacity.
                   If C_v \le 0, code sets C_v = 3 N_0 k.
(21 - 30)
                   T_{\rm m} - Melting temperature.
Variable 12.
(31-40)
                   (-E_m) - Energy to the melting point at
                   zero pressure from the reference point
                   (see eq. III.4.34 of [2]).
Variable 13.
                   Blank.
(41-50)
```

Variable (51-60)	14.	Blank.
Variable (61-70)	15.	$_{\rm O}$ - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $_{\rm O}$ + $_{\rm O}$
Variable (71-80)	16.	C ₄₁ - Temperature dependence of thermal conduction coefficient (see variable 15 [7.6].
Variable (1-10)	17.	ρ_{min} - Lowest allowed solid density, usually about 0.8 ρ_{o} . If zero or negative, code sets ρ_{min} = 0.8 ρ_{o} [V-3].
Variable (11-20)	18.	A.
Variable (21-30)	19.	B. LLL Constants. See reference 7.
Variable (31-40)	20.	R ₁
Variable (41-50)	21.	R ₂
Variable (51-60)	22.	Blank.
Variable (61-70)	23.	Blank.
Variable (71-80)	24.	Blank.

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 7 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 [3]. The following is the corresponding information for the new options. An * next to an equation number means the equation is in reference 3.

	ANEOS -1	ANEOS -2	ANEOS -3
C.			
1.	not used	not used	not used
2.			-
3.	Eo	Υ	E
4.	c _v	C _v	$^{\rm c}{}_{ m v}$
5.	$\rho_{o}\Gamma_{o}C_{v}$	(γ - 1)C _v	R ₁
6.	error message counter	$\ln \left\{ T_{O} \rho_{O} (1-\gamma) \right\}$	R ₂
7.			
8.			=
9.			
10.			
11.	ρ _o	ρ _o .	Po
12.	T _O	T _O	ТО

	ANEOS -1	ANEOS -2	ANEOS -3
13.			
14.			
15.	Γ ₀ .	γ - 1	ω
16.			
17.			
18.	$\mathtt{T}_{\mathtt{m}}$		T _m
19.			ρ _{oo}
20.			
21.	poso ²	K ₁ K ₂ ³	K ₁ K ₂ ³
22.	constant in (7.8)*		constant in (7.8)*
23.	$^{ ho}$ min	not used	$^{ ho}_{ exttt{min}}$
21.			
25.		^K 2	к ₂
26.	$n_{\tilde{m}}[Eq. (6.5)]*$	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.	Ā[Eq. (6.2)]*	Ā	Ā
30.	EOS type switch,	-2	-3
31.	Internal storage location	Internal storage location	Internal storage location
32.	So		A
33.	s ₁		В
34.			

ANEOS	-1	ANEOS -2	ANEOS -3
35. T _m for er	ror test.		$\left\{ Ae^{-R_1/\rho_{OO}} + Be^{-R_2/\rho_{OO}} \right\}$
			$\left(\omega\rho_{OO}^{\omega+1}\right)$
36. 1/2 ρ _ο			
37			
38			
39			
40			
41. Constant	in (7.8)*		
42			
43			
44. K ₁			
45. K ₂			
46			
47			
48		<u></u>	
49			
50			
51			
52			
53. K ₃			
54. K ₄			
-			

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APPENDIX C

MASPLT INPUT INSTRUCTIONS

TAPE UNITS FOR MASPLT

- 1. Input Tape
- 2. Input Tape
- 3. Input Tape
- 4. Input Tape
- 39. Output Tape
- 40. Output Tape

APPENDIX C

MASPLT INPUT INSTRUCTIONS

MASPLT Input Instructions

MASPLT is a graphical post-processor for Chart D. It can plot a variety of cell variables and uses the SCORS plotting package.

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

N(1),N(2)	Variable	Standard Unit
1	<pre>I = zone or boundary number</pre>	
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	<u> </u>
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) N(1) = X (abscissa) variable code (see Table). (1-5)Not used if N(16) = 1. N(2) = Y (ordinate) variable code (see Table). (6-10)or -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.N(3) = 0 for output on tape unit 40. (11-15)= 1 for output on tape unit 39. N(4) = 0 plot frequency determined by record (16-20)number. = 1 plot frequency determined by time inpuls. See card set 8. Not used if N(16) = 1.N(5) = 0 for linear X scale. (21-25)= 1 for log X scale. N(6) = 0 for linear Y scale. (26 - 30)= 1 for log Y scale. N(7) = 0 no plot grid is shown on graph. (31-35)= 1 plot grid is shown on graph. determines number of title and The End (36-40)N(8) trames. If N(8) > 0, N(8) is the number of frames of each. If N(8) = 0, no title or The End frames.

If $-1000 \le N(8) < 0$, 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 $N(8) \le 0$ 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.
- (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 $0 < N(13) \le 10$. If N(16) = 1, then N(13) = 0.
 - (66-70) N(14) = number of plot symbols in card 6. $1 \le N(14) \le 50.$
 - (71-75) N(15) = input tape number (1, 2, 3, or 4).

TIMEVA.

Card 2	I	Format (3A10)
(1-30)]	Input label l (for first title frame,
	S	should be centered).
Card 3	I	Format (3AlO)
(1-30)	:	Input label 2 (for first title frame,
	\$	should be centered).
Card 4]	Format (3Al0)
(1-30)	• •	Input label 3 (for second title frame,
	:	should be centered).
Card 5]	Format (3Al0)
(1-30)		Input label 4 (for second title frame,
	:	should be centered).
Card 6	. 1	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	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 Y variable.
- (31-40) DLABY = same as DLABX except for Y label.
- (41-50) EXTR = the number of data point pairs to be read in card set 10. $0 \le \text{EXTR} \le 90$. 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.
- (21-30) TM(I) = time to start plotting at time intervals of <math>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.

- (61-70) YMIN(I) = same as XMIN(I) except for Y.
- (71-80) YMAX(I) = same as XMAX(I) except for Y.

		Notes:	Points outside of minimum-maximum range are dropped. If N(13) > 1, plotting
•	•		will start at first record ≥ 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)
	•		Present only if DLABX = 1 (card 7).
-	(1-50)		X label for this interval. Should be
		•	centered.
	Card 8.3		Format (5Al0)
	Caru 6.5	· 	
			Present only if DLABY = 1 (card 7).
	(1-50)		Y label for this interval. Should be
		,	centered.
	Card Set	9	Present only if N(16) - 1.
	Card 9.1		Format (2110, 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 (2El0.3)
	Present only if EXTR > 0 (card 7).
	There are EXTR sets of the following variables.
	I = 1,EXTR
(1-10)	EXTRX(I)
(11-20)	<pre>EXTRY(I) This set of variables is plotted on</pre>
·	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 (415)
	Present only if $N(2) = -1, -2$.
(1-5)	MULT(1) Y variable code for
(6-10)	lst curve. MULT(2) Y variable code for
(1 -1)	2nd curve. See
(11-15)	MULT(3) Y variable code for Table
(16-20)	3rd curve. MULT(4) Y variable code for
· /	4th curve.
	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.

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R. C. Bass
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     L. R. Hill
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     L. J. Vortman
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     G. E. Clark
2152
     D. E. Anderson
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     J. E. Kennedy
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     J. G. Harlan
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     P. L. Stanton
      J. G. Taylor
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     D. E. Mitchell
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     M. Cowan
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      J. R. Freeman
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      M. M. Widner
      L. Baker
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      M. A. Sweeney
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     T. J. Tucker
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      M. Berman
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      R. K. Cole
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     G. A. Samara
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      B. Morosin
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      M. P. Sears
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      B. J. Thorne
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      J. R. Asay
5534
5534
      T. J. Burns
8121
      L. E. Voelker
      M. A. Pound
8214
      J. F. Lathrop
8332
                        (5)
      L. J. Erickson
3141
                        (3)
      W. L. Garner
         for DOE/TIC
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       3154-4 J. Hernandez
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