Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

User's Manual for GRIZZLY

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

This work was supported by the US Department of Energy, Office of Basic Energy Sciences.

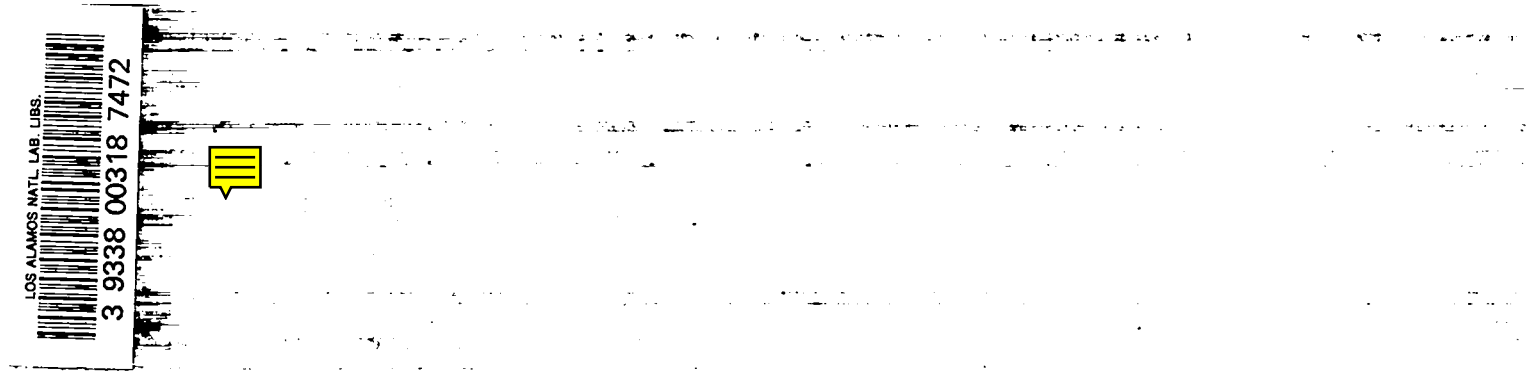
Prepared by Vickie Montoya, Group T-4

LA-10244-M

UC-32 and 34
Issued: September 1984

User's Manual for GRIZZLY

Joseph Abdallah, Jr.



Los Alamos National Laboratory
Los Alamos, New Mexico 87545

USER'S MANUAL FOR GRIZZLY

by

Joseph Abdallah, Jr.

ABSTRACT

This manual describes the first release of GRIZZLY, a computer program to construct tables of atomic data for use in applications programs. The first release of GRIZZLY has the capability to generate baseline equation-of-state tables for elements and mixtures using various physical models. GRIZZLY runs on the Los Alamos CRAY-1 computers.

I. INTRODUCTION

In the past it was usually necessary to run more than one code to calculate a total equation-of-state (EOS) table. Hence, such a calculation was often cumbersome and time consuming because of decentralization and data interfacing. It has become apparent that development of an automated and centralized computer program would improve the thoughput for producing EOS tables. The purpose of GRIZZLY is to provide such a capability. EOS tables are collected and incorporated into the SESAME data library[1-3] which can be accessed by several code packages[4-6] which are used in various hydrodynamics programs (for example, Ref. 7). The physical models used in the first release of GRIZZLY are not intended to be the latest in EOS theory, but they do represent computationally dependable models that may be used to generate a baseline EOS. Future releases of GRIZZLY will provide more sophisticated models capable of producing a higher quality EOS. In the meantime, tables calculated by newer models may be read into GRIZZLY for use if desired. Future plans for GRIZZLY also include the development of a data base of material properties. Also planned is the computation of transport properties such as opacity and conductivity.

GRIZZLY allows the users to

1. calculate contributions to the EOS based on physical models and to produce tables;
2. perform table operations, i.e., combining tables, energy shifting, density scaling, etc.;
3. mix tables using various schemes;
4. specify data to be used in calculating tables;
5. display input data and calculated tables in various formats;
6. read (write) tables from (to) files; and
7. execute procedures which are combinations of 1-6.

Items 1 through 7 are initiated via user supplied comands. These commands may be read in from a input command file or entered directly from the users terminal. Hence, GRIZZLY can be operated in both the production and interactive modes. GRIZZLY is a table oriented code from which many commands either generate tables or perform operations on tables. Table I-1 is an alphabetized list of GRIZZLY commands. Each entry provides a brief description of the command and a page number in this document where more detailed information may be found.

GRIZZLY consists of subpackages which evaluate the various models. These subpackages are called by a common driver program with a common input base. Most of the subroutines which evaluate models have been scavenged from existing programs. The cold curve and nuclear models used by GRIZZLY have been extracted from EOSCRAY[8] and PANDA.[9] The Thomas-Fermi-Dirac (TFD) model for electronic excitations has been extracted from CANDIDE.[10] The ideal mixture scheme has been taken from MIXB.[11] Models can be evaluated either individually or as part of multifunction procedures. Models are evaluated and tabulated on default or user supplied compression and temperature grids. Two temperature equation-of-state tables[12] are easily obtained because models are tabulated individually.

All the data used by GRIZZLY are assigned default values. These values are modified by issuing data specification commands. We plan to have default values based on material when the data base becomes available.

Every attempt has been made to keep GRIZZLY easy to use in order to appeal to various users. Even the occasional user should be able to generate a baseline EOS with relative ease.

Generated EOS tables may be written to SESAME files for use in programs using such data. Tables may also be read and written in GRIZZLY data base

formatted files. All displays of tables or thermodynamic functions are written to files which may be read by CURVES[13] to provide a graphics interface.

Not all of GRIZZLY has been adapted from other codes. In fact, the portions of GRIZZLY which are associated with items 2 through 7 represent new code development.

Table I-2 describes the units used by GRIZZLY. Note that the compression variable used in GRIZZLY is defined as

$$\eta = \frac{\rho}{\rho_o} \quad ,$$

where ρ_o is given by rhoref (Table I-1) and ρ is the mass density.

Section II discusses the general details of running GRIZZLY. Sections III and IV describe the procedures for calculating the EOS for elements and mixtures, respectively. Sections V, VI, and VII discuss the models used for cold curve, nuclear, and electronic table generation, respectively. Section VIII describes the data specification commands. Section IX describes the compression and temperature grids and the commands which control them. Section X describes the various grid suppression strings. Section XI describes mixing schemes, these include additive volume, partial pressure, and ideal mix algorithms. Section XII describes the various table operations which are available under GRIZZLY. Section XIII describes commands for displaying values of data used in EOS generation. Section XIV discusses commands to display EOS tables and commands to calculate and display thermodynamic properties along hugoniots, isobars, isentropes, isotherms, and isochores. Section XV describes commands for EOS table input and output. Section XVI presents several examples of running GRIZZLY.

II. GENERAL DETAILS

A. Running GRIZZLY

The executable binary file GRIZ and its associated data file GRZDB may be obtained from the common file system by using the command

```
MASS GET DIR=/LTE GRIZ GRZDB .
```

GRIZZLY may be executed using the CTSS execute line

```
GRIZ I = iname, P = pname, E = ename / t p.
```

The name of the input command file is specified by iname. The default for iname is I. If iname equals TTY (teletype), commands are entered interactively. If iname does not exist in the users local file space, control is transferred to the terminal for interactive input. If the command file does not have an END command, control is transferred to the TTY after all the commands from the command file have been processed. This allows the user to run interactively after performing a routine setup.

The name of the output print file is pname. The default for pname is P. All the printed output is routed to pname.

The name for the echo file is ename. The echo file contains all commands entered during a session. If ename is not specified or ename = E, then commands are echoed back to the TTY.

B. Command File Format

All GRIZZLY commands have the format

cname p_1 p_2 p_3 ... / .

The symbol cname is the alphanumeric command name, and the p_i are associated parameters delimited by blanks. The p_i may be numeric or alphanumeric depending on the command. A command parameter may be defaulted by entering an asterisk (*) for that parameter or by ending the command prematurely. A single command may extend over several lines. Each command must end with at least one blank and a slash (/).

A command file is a collection of such commands on a file. Each new command must start on a new line. For example,

$cname_1$ p_1 p_2 p_3

p_4 /

$cname_2$ p_1 /

Most of this manual will be concerned with describing the commands which are available under GRIZZLY.

C. Table Numbers

Grizzly currently has storage area allocated for seven 12,000 word tables. Each storage area is identified by a table number i ($1 \leq i \leq 7$). Table numbers are used as parameters on many commands.

D. EOS Evaluation

In general, the EOS of a material is calculated by combining three terms

$$P(\rho,T) = P_c(\rho) + P_n(\rho,T) + P_e(\rho,T)$$

$$E(\rho,T) = E_c(\rho) + E_n(\rho,T) + E_e(\rho,T)$$

$$A(\rho,T) = A_c(\rho) + A_n(\rho,T) + A_e(\rho,T) \quad ,$$

where P is the pressure, E is the energy density, A is the Helmholtz free energy density, ρ is the mass density, T is the temperature, the subscript c stands for cold curve, n for nuclear, and e for thermal electronic excitations.

III. EOS FOR ELEMENTS

Tables for elements may be generated using the EOS command. This command initiates a procedure which generates a separate cold curve table, nuclear table, and electronic table [see Eq. (1)] and combines them to form a total table. Default models are provided. The user may select different models by issuing commands prior to the EOS command. The MODC command is used to select a cold curve model, MODN to select a nuclear model, and MODE to select an electronic model. These commands are discussed in Sec. VIII. In addition, all data must be set to desired values before the execution of the EOS command. The data setting commands are discussed in Sec. VIII. The data requirements are included in Secs. V, VI, and VII with the description of each model. The energy zero is adjusted to correspond to zero pressure and to the reference temperature tref.

The EOS command format is

EOS i_c i_n i_e i_t / ,

where i_c is the cold curve table number, i_n is the nuclear table number, i_e the electronic table number, and i_t is the total EOS table number. After execution of the EOS command, the tables designated by i_c, i_n, i_e, and i_t should contain the calculated values. A table may be used as input to EOS by specifying TAB with the MODC, MODN, or MODE commands (see Sec. VIII). This is convenient because it avoids unnecessary recomputation of a table on successive executions of the EOS command. The calculation of a particular contribution may be avoided completely by specifying NONE with the MODC, MODN, or MODE commands.

Tables are generated on the compression and temperature grid existing when EOS is executed (see Sec. IX) subject to suppression strings (Sec. X).

EOS can be used in a somewhat crude way for generating EOS tables for mixtures. To use this method, the user enters atomic numbers and masses corresponding to average values for the mixture.

IV. EOS FOR MIXTURES

Tables for mixtures may be generated using the EOSMX command. The command initiates a procedure which generates a separate cold curve table, nuclear table, electronic table, and total EOS table. Default models are provided. The user may select different models by issuing MODC, MODN, and MODE commands prior to the EOSMX command. These commands are discussed in Sec. VIII. All data must be set to desired values before issuing the EOSMX command. In particular, the MXTURE command must be issued to define the mixture composition. The MXTURE command will set the atomic number, weight, reference density, and number of mixture components, (NMIX). MXTURE is discussed in Sec. VIII. The energy zero is adjusted to correspond to zero pressure and to the reference temperature tref.

The command format is

EOSMX i / .

On completion, table i contains the cold curve, table i + 1 contains the nuclear contribution, table i + 2 contains the electronic contribution, and table i + 3 contains the total EOS; at least NMIX + 2 table storage areas are required to execute EOSMX, hence $i + NMIX + 1 \leq 7$, or $NMIX \leq 6 - i$.

The cold curve calculated by EOSMX is that specified by MODC with a high density match to the mixed TFD cold curve. The mixed TFD cold curve is obtained by generating the TFD cold curve for each component and then applying the additive volume mixture rule. The nuclear table calculated is that specified by MODN for the average atom. The mixed electronic table is obtained by calculating the thermal electronic table for each component and then applying the additive volume mixing rule.

All tables are generated on the compression and temperature grids existing when EOSMX is executed (Sec. IX) subject to suppression strings (Sec. X).

V. COLD CURVE MODELS

The cold curve described here corresponds to the electronic contribution to the zero degree Kelvin isotherm. Contributions to the zero degree Kelvin isotherm due to zero point lattice vibrations are included in the nuclear model. In addition to the commands and options discussed in this section, there are specialized commands such as COLDMX, LJMATCH, MATCH, MATCH2, MXC, PCTAB, and TFDCMX which may aid the user in constructing a cold curve. These are discussed in Sec. XI.B and XII.B. All models may be calculated directly by using the commands discussed below or through the EOS and EOSMX commands. All models discussed in this section need specification of zbar, abar, and rhoref (see Table I-1) in addition to the specified data requirements.

A. TFD

A Thomas-Fermi-Dirac cold curve may be generated by using the command

TFDC i / ,

where i is the table number associated with the calculated cold curve. Upon completion of TFDC, table i will contain the TFD cold curve. The TFD cold curve may be used in the EOS and EOSMX procedure by setting modc (Table I-1) equal to TFD. The TFD cold curve is accurate at very high densities. The TFD calculations are described in Appendix A. The only data requirement is the exchange parameter xalpha (Table I-1).

B. CHUG

The CHUG cold curves consist of three models joined smoothly to each other. At compressions less than clj (see Table I-1) the Lennard-Jones match formula[9] is used. At intermediate compressions, the cold curve is chosen to reproduce experimental shock data.[9,14] The shock data is given in terms of a quadratic fit to the shock velocity-particle velocity (u_s-u_p) curve. At compressions greater than cmat (Table I-1), the high density match formula [see Appendix B] is used to connect the cold curve to TFD. The method used in the intermediate compression region is discussed in detail in Ref. 14. The coding for CHUG has been adapted from PANDA.[9]

The CHUG cold curve may be generated using

CHUG i mn_1 mn_2 / ,

where i is the output table number, and mn_1 and mn_2 specify the nuclear model. The parameters mn_1 and mn_2 may be given any of the values possible for $modn_1$ and $modn_2$ (see Table I-1 and Sec. VIII). In addition, if the user wishes to specify

a tabular nuclear model, then mn_1 may be set to TAB and mn_2 to the nuclear table number. The nuclear table must be loaded at the time of CHUG execution. If mn_1 and mn_2 are not specified the default nuclear model is used. The CHUG cold curve is obtained with the EOS and EOSMX commands with the setting modc = CHUG. The default value for modc is CHUG.

The parameters clj, faclj, ecoh, c_o, s_1, s_2, cmat, and xalpha are required. In addition, all parameters for the nuclear model must be set. The u_s-u_p shock fit parameters (c_o, s_1, s_2) are specified using the SHKFIT or SHKFITKS command.

C. CHUGT

The CHUGT cold curve is the same as CHUG except that a table of u_s, u_p (USUP command) points is provided instead of the quadratic fit. Linear interpolation is used to obtain the shock velocity at a given particle velocity. This option is convenient if the u_s-u_p curve for the material has a phase transition or some other complex structure which the user wishes to reproduce.

The command

CHUGT i mn_1 mn_2 /

generates the CHUGT cold curve. All parameters have the same meaning as in the CHUG command (Sec. V.B). The tabulated u_s-u_p points are specified using the USUP or USUPKS command.

D. MODMRS1

MODMRS1 is the first of four variations of the modified Morse[15] potential in GRIZZLY. The modified Morse parameters for MODMRS1 are determined such that (1) the cold pressure vanishes at a given density (rcold), (2) the cold isothermal bulk modulus equals a given value (bcold) at that density, and (3) the pressure goes to the free electron limit and high densities. MODMRS1 has been adapted from EOSCRAY.[8]

The MODMRS1 cold curve may be calculated using

MODMRS1 i / ,

where i is the associated output table number, or by using the EOS or EOSMX command with modc set equal to MODMRS1.

The parameters rcold and bcold are required for MODMRS1.

E. MODMRS2

The modified Morse parameters for MODMRS2 are determined such that (1) the pressure at reference density (rhoref) and reference temperature (tref) vanishes, (2) the isothermal bulk modulus at reference density and reference temperature

equals a given value (bref), and (3) the pressure goes to the free electron limit at high densities.

The MODMRS2 cold curve may be calculated using

MODMRS2 i mn_1 mn_2 /

or by using the EOS or EOSMX commands with modc set equal to MODMRS2. All parameters on the MODMRS2 command have same meaning as discussed in Sec. V.B.

The values tref, bref, and nuclear model parameters are required by MODMRS2.

F. MODMRS3

The modified Morse parameters for MODMRS3 are determined such that (1) the pressure at reference density (rhoref) and reference temperature (tref) vanishes, (2) the isothermal bulk modulus at reference density and temperature equals a given value (bref), and (3) that the cohesive energy (ecoh) is reproduced. In addition, the high density match formula is used to insure that the MODMRS3 cold curve connects with TFD.

The MODMRS3 cold curve may be calculated using

MODMRS3 i mn_1 mn_2 /

or by using the EOS or EOSMX commands with modc set equal to MODMRS3. All parameters have the same meanings as discussed in Sec. V.B.

The values tref, bref, cmat, xalpha, and nuclear model parameters are required by MODMRS3.

G. MODMRS4

The modified Morse parameters for MODMRS4 are determined using the same conditions as MODMRS2. In addition, the high density match formula is used to insure that the MODMRS4 cold curve connects with TFD.

The MODMRS4 cold curve may be calculated using

MODMRS4 i mn_1 mn_2 /

or by using the EOS or EOSMX commands with modc set equal to MODMRS4. All parameters have the same meaning as discussed in Sec. V.B.

The values tref, bref, cmat, xalpha, and nuclear model parameters are required by MODMRS4.

VI. NUCLEAR MODELS

The models presented in this section calculate the contribution to the equation of state from nuclear motion. Note that solid zero-point lattice vibra-

tions are included in the tables generated by these models. All models may be calculated directly via commands discussed below or through the EOS and EOSMX commands. Models discussed in this section usually require specification of zbar, abar, and rhoref (Table I-1) in addition to the specified data requirements. If the CHARTD, COWAN, DEBYE, DEBYEC, EINSTN, EINSTC, or GIKNUC models (see below) are involved, then a solid phase is present and a Grüneisen parameter is required. Hence, igrun, gamref, and debref are required. If igrun = 3, gamref and debref are not used. Also, in all commands discussed below, i refers to the table number associated with the calculated table. All models are calculated on the compression-temperature grid existing at the time of command execution. The default nuclear model is CHARTD with a virial match.

A. CHARTD

The coding for the CHARTD nuclear model[16] has been adapted from the EOSCRAY code.[8] This model may be calculated using

CHARTD i /

or by setting $modn_1$ equal to CHARTD for the EOS and EOSMX procedures. In GRIZZLY and EOSCRAY, the Debye integral is calculated and in Ref. 16 it is approximated.

B. COWAN

The COWAN nuclear model was developed at Los Alamos about 1957 by R. D. Cowan. The coding for this model has been adapted from the EOSCRAY code.[8] This model may be calculated using

COWAN i /

or by setting $modn_1$ equal to COWAN for the EOS and EOSMX procedures.

C. DEBYE, DEBYEC, EINSTN, EINSTC, and GIKNUC

These nuclear models have been extracted from the PANDA code.[9] DEBYE and EINSTN compute the Debye and Einstein solid models respectively. DEBYEC and EINSTC are modified versions of DEBYE and EINSTC in which only a finite number of terms are included in the sum over vibrational levels. GIKNUC is the solid-gas interpolation formula. These models are calculated using

DEBYE i /
DEBYEC i /
EINSTN i /
EINSTC i /
GIKNUC i /

or by setting $modn_1$ to the appropriate value for the EOS and EOSMX procedures.

D. IDGAS

The ideal gas formula is evaluated using

IDGAS i /

or by setting $modn_1$ equal to IDGAS for the EOS and EOSMX procedures.

E. VIRIAL

The virial match procedure has been extracted from PANDA.[9] This match procedure is used to provide a smooth interpolation between the solid and ideal gas regions. A nuclear table with a virial match included may be generated by using

VIRIAL i mn / ,

where mn may be CHARTD, COWAN, DEBYE, DEBYEC, EINSTN, EINSTC, or GIKNUC. If mn is not specified, the default nuclear model is used. The virial match may be used in conjunction with the EOS and EOSMX commands by setting $modn_1$ to VIRIAL and setting $modn_2$ to CHARTD, COWAN, DEBYE, DEBYEC, EINSTN, EINSTC, or GIKNUC. The virial match requires a match compression (cvir) and a step size (dvir) for taking a numerical derivative. See the comments in Ref. 9 concerning the restrictions for using the virial match.

VII. ELECTRONIC MODEL

The only model currently available in GRIZZLY for calculating the contribution to the equation of state from electronic excitations is the TFD method.

A. TFD

The coding for the TFD model has been adapted from a modified version of the CANDIDE program.[10] This model is discussed in Appendix A. The commands which evaluate the TFD model are

TFDC i /

TFDTOT i /

TFDTHM i / ,

where TFDC evaluates the cold curve (TFDC has already been discussed in Sec. V), TFDTOT evaluates the TFD model, and TFDTHM calculates the thermal contribution to the EOS. The thermal table generated by TFDTHM is the TFDTOT table with the cold curve subtracted. The thermal table is used for the electronic contributions in Eq. (1). The TFD model is computed using the EOS and EOSMX commands if mode is set equal to TFD. When the EOS command is used, the TFD model is evaluated for the average atom. When the EOSMX command is used, the TFD model is

evaluated for each constituent atom of the mixture. All tables are generated on the compression-temperature grids existing at the time of command execution subject to suppression strings. The only required data for the TFDC, TFDTOT, and TFDTHM commands are zbar, abar, rhoref, and xalpha. The parameter tstfd is used for TFDTOT and TFDTHM.

VIII. DATA SPECIFICATION COMMANDS

This section describes the commands which are used to specify the data required by the models discussed in Secs. III through VII. Initially, all data are assigned default values. Data specification commands are used to modify these values. These commands should be issued prior to the model computation commands. The LIST command (Sec. XIII) may be used to view data settings.

A. Commands

ABAR abar /

The ABAR command is used to specify the gram atomic weight of an element or the average gram atomic weight for a mixture. The default abar = 0.

ATOM zbar /

The ATOM command is used to initialize GRIZZLY for calculating an element. The current version just resets all data defaults and sets the atomic number (zbar) (see example 6 in Sec. XVI). In future versions of GRIZZLY, the ATOM command will be used to provide the "best" default values for the specified element by accessing the data base. The default zbar = 0.

BCOLD bcold /

The BCOLD command is used to specify the isothermal bulk modulus (Mbar) at density rcold (see RCOLD command) along the cold curve. The default bcold = 0.

BREF bref /

The BREF command is used to specify the isothermal bulk modulus (Mbar) at rhoref and tref (see RHOREF and TREF commands). The default bref = 0.

CLJ clj /

The CLJ command is used to specify the compression where the Lennard-Jones match procedure is to be applied to the cold curve. The default clj = 1.

CMAT cmat /

The CMAT command is used to specify the compression where the high density match formula is applied to the cold curve. The default cmat = 1.5

CVIR cvir /

The CVIR command is used to specify the compression where the virial match procedure is applied to nuclear models. The default cvir = 1.0.

DEBREF debref /

This command is used to specify the reference Debye temperature (eV) used in nuclear models. The default debref = 0.

DEBKEL debref /

This command is equivalent to DEBREF except that debref is specified in degrees Kelvin.

DEBSHK c_0 σ /

This command is used to calculate the Debye reference temperature (debref) from the sound speed c_0 (cm/μsec) and Poissons ratio σ. If c_0 is not specified it is taken from an existing value (see SHKFIT command), and σ is set to 1/3 if it is not specified. For example, DEBSHK / will compute debref from the current c_0 and σ = 1/3; DEBSHK 0.5 / will compute debref using c_0 = 0.5, σ = 1/3; DEBSHK 0.5 0.4 / will compute debref with c_0 = 0.5, and σ = 0.4; and DEBSHK * 0.4 / will compute debref with c_0 equal to the current value and σ = 0.4. The entered values of c_0 and σ are not saved. The calculated value of debref is stored for later use. The value of debref may be viewed by using the LIST / command.

DEBSHKKS c_0 σ /

This command is equivalent to DEBSHK except that c_0 is specified in km/sec.

DVIR dvir /

This command is used to specify the spacing used to calculate numerical derivatives for the virial match. The spacing is expressed as a fraction of the virial match density. The default value for dvir is .001.

ECOH ecoh /

This command is used to specify the cohesive energy (Mbar·cm^3/g). The default value for ecoh is 0.

ECOHKC ecoh /

This command is equivalent to ECOH except that ecoh is specified in kcal/mole.

EPSMIX epsmix /

This command is used to specify the accuracy criteria for additive volume mixing. The default value for epsmix is 10^{-6}.

FACLJ faclj /

This command is used to specify the exponent used in the Lennard-Jones match formula. The default value for faclj is 1.

GAMREF gamref /

This command is used to specify the reference Grüneisen parameter. The default value for gamref is 0.

GAMSHK s_1 ft /

This command uses the formulas of Ref. 9 to calculate the reference Grüneisen parameter from the slope of the u_s-u_p curve s_1 and parameter ft. If s_1 is not specified, the current value is used (see SHKFIT command). If ft is not specified, 0 is used. This command is similar to DEBSHK.

IGRUN igrun /

This command is used to specify the method for calculating the Grüneisen parameter as a function of density. The following table describes the possible values of igrun.

igrun	type
1	Chart-D[8,16]
2	SESAME[9]
3	Cowan[8]
4	$\rho\Gamma$ = constant
5	$\rho^{1/3}\Gamma$ = constant
6	Γ = constant

Note that the igrun = 3 option does not require specification of gamref and debref. The default value for igrun is 3.

MODC modc /

This command is used to specify the cold curve model. Possible values for modc are CHUG, CHUGT, MODMRS1, MODMRS2, MODMRS3, MODMRS4, and TFD (see Sec. V). In addition, for the EOS command only, modc may be set to TAB if the user wishes to supply a cold curve table, or modc may be set to NONE to neglect the cold curve contribution. The default value for modc is CHUG.

MODN $modn_1$ $modn_2$ /

This command is used to specify the nuclear model. Possible values for the $modn_1$ and $modn_2$ combination are given in the following table.

$modn_1$	$modn_2$
COWAN	
CHARTD	
DEBYE	
DEBYEC	
GIKNUC	
EINSTN	
EINSTC	
IDGAS	
VIRIAL	COWAN
VIRIAL	CHARTD
VIRIAL	DEBYE
VIRIAL	DEBYEC
VIRIAL	GIKNUC
VIRIAL	EINSTN
VIRIAL	EINSTC

In addition, for the EOS commands only, $modn_1$ may be set to TAB if the user wishes to supply a nuclear table, or $modn_1$ may be set to NONE to omit the nuclear model. The default values for $modn_1$ and $modn_2$ are VIRIAL and CHARTD, respectively.

MODE mode /

This command is used to specify the electronic model. The possible value for mode is TFD. In addition, for the EOS command only, mode may be set to TAB if the user wishes to supply a thermal electronic table or mode may be set to NONE to neglect the electronic contribution. The default value for mode is TFD.

MXTURE nw x_1 z_1 a_1 r_1 x_2 z_2 a_2 r_2 ... /

This command is used to specify a mixture. The parameter nw may be set to N if input is in number fractions or to W if input is in weight fractions. The parameters x_i, z_i, a_i, and r_i are the fraction, atomic number, atomic weight, and solid density for mixture component i. The parameters zbar, abar, rhoref, and a set of tables describing the mixture are saved for further use upon completion of MXTURE. These tables may be viewed using the LIST command.

RCOLD rcold /

The RCOLD command is used to specify the zero pressure density for the cold curve. The default rcold equals 0.

RHOREF rhoref /

The RHOREF command is used to specify the reference density at temperature tref (see TREF command). The default value for rhoref is 0.

SHKFIT c_0 s_1 s_2 /

This command is used to specify the fit to the u_s-u_p curve for a material. The fit formula is given by

$$u_s = c_0 + s_1 u_p + s_2 u_p^2 \quad .$$

Since u_s and u_p are required in units of cm/μsec, c_0 has the units of cm/μsec, s_1 is dimensionless, and s_2 has units of μsec/cm. The default values for these parameters are $c_0 = s_1 = s_2 = 0$.

SHKFITKS c_0 s_1 s_2 /

This command is equivalent to SHKFIT except that fit parameters are specified in km/sec units.

TREF tref /

This command is used to specify the reference temperature (eV). The default value for tref is room temperature or 0.025692 eV.

TREFKEL tref /

This command is equivalent to TREF except that tref is specified in degrees Kelvin.

TSTFD tstfd /

This command is used to specify the temperature (eV) below which the TFD energies are substituted by 1/2 TS, where T is the temperature, S is the entropy, and $T \leq$ tstfd. The substitution is used to eliminate noisy energy results at low temperatures. The substitution is exact at high densities and approximate at low densities. If tstfd is 0, a default is chosen based on atomic number. The default value for tstfd is 0.

USEALL i /

This command is a combination of USEZ, USEC, and USET (see Sec. IX).

USEZ i /

This command is used to load the values of zbar, abar, and rhoref from the values stored in table i.

USUP u_{p_1} u_{s_1} u_{p_2} u_{s_2} ... /

This command is used to specify a tabulated u_s-u_p curve. Linear interpolation is used to calculate shock velocities between table points. The maximum number of u_s-u_p points allowed is twenty. All pairs must be specified in order of increasing u_p. No shock table exists until a USUP command is executed. All velocities are given in units of cm/μsec.

USUPKS u_{p_1} u_{s_1} u_{p_2} u_{s_2} ... /

This command is equivalent to USUP except that velocities are entered in km/sec.

XALPHA xalpha /

This command is used to specify the exchange parameter for the TFD model. The default value for xalpha is 2/3.

ZBAR zbar /

This command is used to specify the average atomic number. The default value for zbar is 0.

IX. COMPRESSION AND TEMPERATURE GRIDS

A. General

The models in GRIZZLY are calculated at the mass density and temperature points specified by the compression and temperature grids existing at the time of command execution. The mesh at which a given model is calculated is also subject to the appropriate suppression string (see Sec. X). The density points are obtained by multiplying the compressions by the parameter rhoref. Initially default compression and temperature grids are read from the GRZDB file. These are general purpose grids which should be suitable for most applications. Hence, the cumbersome task of specifying a grid is eliminated. The default compression grid is presented in Table IX-1, and the default temperature grid is presented in Table IX-2. Commands are also provided so the user may construct alternative meshes. These commands are described in Sec. IX.B. The LIST command may be used to view the existing compression and temperature grids.

B. Grid Manipulation Commands

In this section all commands starting with the letter C are associated with the compression grid, and all commands starting with the letter T are associated with the temperature grid.

CSUP k η_1 η_1' η_2 η_2' ... /

TSUP k t_1 t_1' t_2 t_2' ... /

These commands construct grids based on suppressing portions of the default grid (see Tables IX-1 and IX-2). The parameter k is a sparsing factor, for example, if k equals 1 all default grid points are used, if k equals 2 every other grid point is used, etc. The parameters η_i, η_i', t_i, t_i' specify ranges of values in compression and temperature space, respectively, to be suppressed.

CGRD η_1 η_2 ... /

TGRD t_1 t_2 ... /

These commands allow the user to specify the grid points directly. The η_i are compression points and the t_i are temperature points. The points must be specified in ascending order.

CLIN n η_1 η_n /

TLIN n t_1 t_n /

These commands allow the user to construct grids based on a linear spacing of points. The parameter n is the number of points, η_1 and η_n are the compression limits, and t_1 and t_n are the temperature limits.

CLOG n n_1 n_n /

TLOG n t_1 t_n /

These commands allow the user to construct grids based on a logarithmic spacing of points. The parameters n, η_1 η_n, t_1, and t_n have the same meaning as in the CLIN and TLIN commands.

CGRDA η_1 η_2 ... /

TGRDA t_1 t_2 ... /

These commands allow the user to add the specified points to the current grid. The η_i are the compression values and the t_i are the temperature values to be added to the grid.

CLINA n η_1 η_n /

TLINA n t_1 t_n /

These commands allow the user to add a linearly spaced set of points to the current grid. The parameter n is the number of points to be added and η_1, η_n, t_1, and t_n specify the compression and temperature limits, respectively.

CLOGA n η_1 η_n /

TLOGA n t_1 t_n /

These commands have the same meaning as CLINA and TLINA except that the points have logarithmic spacing.

USEC i /

USET i /

These commands are used to specify the grids from existing tables. USEC sets the compression grid from table i, and USET sets the temperature grid from table i.

X. SUPPRESSION

A. General

Some of the physical models used by GRIZZLY do not work over the wide range of compressions and temperatures which need to be considered. Grid suppression is used to eliminate trouble regions for a particular model prior to calculation. Allowance is also made for sparsing the grids for a particular model. For each model or group of models there exists a suppression string which is initially read from the GRZDB file. Each string controls the suppression of compressions and temperatures. Each string contains sparsing factors and ranges of grid values to be suppressed. These values may be altered by issuing the appropriate commands (see below). The grid for a particular model is determined by applying the sparsing factor and suppression ranges to the current grid (see Sec. IX). Suppression strings may be viewed by using the LIST command (see Sec. XIII). The commands which control suppression strings are discussed in Sec. X.B.; suppression of data in existing tables is discussed in Sec. X.C.

B. Suppression Control Commands

This section describes the commands which allow the user to alter the suppression strings. There are four groups of models for which suppression strings exist. All the cold curve models are subject to a single compression suppression string (COLD). All the nuclear models are subject to a single suppression string (NUC). All mixing models are subject to a single suppression string (MIX). The TFD model is subject to its own suppression string (TFD). The sparsing factors k are defined such that k = 1 indicates no sparsing, k = 2 means every second point is used, k = j means every jth point is used.

KCOLD k /

KCMIX k /

KCNUC k /

KCTFD k /

These commands control the sparsing of compressions. KCCOLD controls sparsing for cold curve models, KCMIX controls the sparsing for mixture models, KCNUC

controls the sparsing for nuclear models, and KCTFD controls sparsing for the TFD model. The parameter k is the sparsing factor. The default value is 1 for all compression sparsing factors.

KTMIX k /

KTNUC k /

KTTFD k /

These commands control the sparsing of temperatures. KTMIX, KTNUC, KTTFD control sparsing for mixture, nuclear, and TFD models, respectively. The parameter k is the sparsing factor. The default value is 1 for all temperature sparsing factors.

SCCOLD η_1 η_1' η_2 η_2' /

SCMIX η_1 η_1' η_2 η_2' /

SCNUC η_1 η_1' η_2 η_2' /

SCTFD η_1 η_1' η_2 η_2' /

These commands control the parameters associated with compression suppression. SCCOLD, SCMIX, SCNUC, and SCTFD control suppression for cold curve, mixture, nuclear, and TFD models, respectively. The parameters η_i and η_i' (i = 1,2) define lower and upper limits, respectively, for suppression region i. The default values for all models are $\eta_1 = -1$, $\eta_1' = 10^{-10}$, $\eta_2 = -1$, and $\eta_2' = -1$. An asterisk (*) should be entered in any field for which the user wishes the associated value to remain unchanged.

STMIX t_1 t_1' t_2 t_2' /

STNUC t_1 t_1' t_2 t_2' /

STTFD t_1 t_1' t_2 t_2' /

These commands control the parameters associated with temperature suppression. STMIX, STNUC, and STTFD control suppression for mixture, nuclear, and TFD models, respectively. The parameters t_i and t_i' (i =1,2) define lower and upper limits, respectively, for suppresion region i. The default value for all t_i and t_i' is -1, except for the TFD model where $t_1 = 10^{-4}$ and $t_1' = 0.2499$. An asterisk (*) should be entered in any field for which the user wishes the associated value to remain unchanged.

C. Table Suppression

The user may sparse and suppress points of an existing EOS to remove bad data or for other reasons. This operation is performed by the SUP command. This command has the format

SUP i_1 i_2 / .

The SUP command suppresses data on table i_1 and creates the resultant (suppressed) table i_2. Suppression conditions are imposed by issuing the following commands prior to SUP execution. Note that this type of suppression is based on mass density and not compression.

KRTAB k /

KTTAB k /

These commands are used to specify the density and temperature sparsing factors respectively, for table suppression. The default value for k is 1.

SRTAB r_1 r_1' r_2 r_2' /

STTAB t_1 t_1' t_2 t_2' /

These commands are used to specify the density and temperature suppression regions, respectively, for table suppression. The r_i and r_i' define lower and upper bounds, respectively, for density suppression in region i. The t_i and t_i' define lower and upper temperature bounds, respectively, for region i. The default value for all r_i, r_i', t_i, and t_i' is -1 (no suppression). An asterisk (*) should be entered in any field for which the user wishes the associated value to remain unchanged.

XI. MIXTURES

A. General

The additive volume, ideal, and partial pressure mixing schemes are available in GRIZZLY. These schemes are discussed in Appendix C. All three schemes may be used in commands where the user specifies the constituent tables. The additive volume procedure is used when mixing involves specified mixtures (see MXTURE command). Sec. XI.B. discusses the commands associated with table mixing, and Sec. XI.C discusses utility commands available for specified mixtures.

B. Table Mixing Commands

AVMIX nw i_1 x_1 i_2 x_2 ... i /

IDMIX nw i_1 x_1 i_2 x_2 ... i /

PPMIX nw i_1 x_1 i_2 x_2 ... i /

These commands apply the corresponding mixing schemes to the specified tables and create a mixed EOS table. The commands AVMIX, IDMIX, and PPMIX apply the additive volume, ideal, and partial pressure mixing schemes, respectively. The parameter nw can be set to N if number fractions are input or to W if weight

fractions are input. The i_j's are table numbers for mixture component j, and the x_j's are number or weight fractions depending on the value of nw. The parameter i specifies the output "mixed" table number. All tables i_j must be loaded prior to command execution. Note that table numbers and fractions are not saved for further use.

C. Specified Mixtures

A specified mixture is defined using the MXTURE command (see Sec. VIII). In addition to the EOSMX command (see Sec. IV), several other miscellaneous commands which operate on specified mixtures are available. These commands are presented in this section. The definition of the current specified mixture may be viewed using the LIST command. In all the command discussed below, NMIX is the number of mixture components.

COLDMX i mc mn_1 mn_2 /

This command generates a mixed cold curve using the method described in Sec. IV. The parameter i specifies the "mixed" cold curve table number. This command uses NMIX + 1 table areas starting at table i; hence, table i through i + NMIX are used and any data in these tables will be overstored upon completion of COLDMX. The parameters mc, mn_1, and mn_2 may optionally be used to specify the cold curve and nuclear models. If these parameters are not specified, the default models are used.

ELECMX i m_e /

This command calculates a mixed thermal electronic table using the method described in Sec. IV. The parameter i specifies the "mixed" table number. The command requires NMIX + 1 table areas starting at table i; hence, table i through i + NMIX are used and any data in these tables will be overstored upon completion of ELECMX. The parameter m_e may optionally be used to specify the electronic model; if it is not specified, the default model is used.

MX i /

MXC i /

These commands perform additive volume mixing of EOS tables and cold curve tables, respectively. Tables i through i + NMIX - 1 are mixed, and the results are stored into table i + NMIX. Table i is assumed to be loaded with data for component 1, table i + 1 is assumed to be loaded with data for component 2, etc.

TFDCMX i /

TFDMX i /

These commands calculate TFD cold curves and TFD thermal electronic tables, respectively, for each component of the specified mixture. The calculated table for component 1 is stored on table i, the table for component 2 is stored in table i + 1, etc.

XII. TABLE OPERATIONS

A. General

This section describes commands which perform useful operations on EOS tables.

CHANGE i r t p e a /

This command changes the pressure, internal energy, and free energy to the specified value (p, e, and a, respectively) for the grid point closest to specified density r and temperature t of table i. An asterisk (*) may be entered for p, e, or a if the user does not want the associated values to be changed.

COPTAB i_1 i_2 /

Copies table i_1 to table i_2.

RAT i_1 i_2 /

This command creates table i_2 by interpolating table i_1 to the current compression and temperature grids using the rational function method.[17]

RSCALE i r /

This command scales table i to the specified reference density r. The low density and high temperature regions of the EOS are preserved. The scaling prescription is presented in Appendix D.

SCALE i a / .

This command scales table i to the specified atomic weight a. SCALE is useful for generating equations-of-state for various isotopic compositions of a material. This type of scaling is discussed in Ref. 4.

SHFT i es /

This command subtracts the specified energy shift (es) from internal energies and free energies of table i.

STAN i_1 i_2 /

This command computes the energy where the pressure vanishes at tref on table i_1 and subtracts this energy from both tables i_1 and i_2.

SUBCLD i /

This command subtracts the isotherm of lowest temperature of table i from all isotherms of table i.

TOTAL i_c i_n i_e i_t /

This command combines a cold curve table i_c, a nuclear table i_n, and an electronic table i_e to form a composite (total) EOS table i_t. The tables i_c, i_n, and i_e must be loaded prior to execution of TOTAL. Any contribution may be neglected by entering zero for i_c, i_n, or i_e.

B. Cold Curves

This section describes commands which perform table operations which are useful for constructing cold curves.

LJMATCH i_1 i_2 mn_1 mn_2 /

This command applies the LJMATCH formula[9] to cold curve table i_1 and generates table i_2 at the current compression grid. The parameters mn_1 and mn_2 specify the nuclear model (see Sec. V.B.). The default model is used if mn_1 and mn_2 are not specified. LJMATCH uses the parameters clj, faclj, ecoh, and nuclear model parameters.

MATCH i_1 i_2 i_3 /

This command applies the high density match (Appendix B) to low density table i_1 and high density table i_2 to form the composite table i_3 at the current compression grid. The high density match is applied at compression cmat.

MATCH2 i_1 i_2 i_3 mn_1 mn_2 /

This command applies the Lennard-Jones match formula[9] to cold curve table i_1 and the high density match (Appendix B) formula to i_1 and i_2 to form a composite table i_3. The parameters mn_1 and mn_2 have the same meaning as in Sec. V.B. In addition to nuclear parameters, clj, faclj, ecoh, and cmat are used.

PCTAB i r_1 p_1 r_2 p_2 .... /

This command constructs a cold curve table i from density (r_j) and pressure (p_j) data. Energies are calculated by numerically integrating the pressure.

XIII. DATA DISPLAY

LIST item itp /

This command generates displays of the raw data used in constructing an equation-of-state table. All values listed correspond to those existing at the time the LIST command is executed. The parameter item specifies the type of data to be listed. Possible values for item are DATA (default), TEMP, COMP, GRIDS,

MIX, SUP, and ALL. DATA will provide a list of raw data used by the models (see Sec. VIII), TEMP will display the temperature grid, COMP will display the compression grid, GRIDS will display both the temperature and compression grids, MIX will display information stored for specified mixtures, SUP will display suppression strings, and ALL will display all of the above. The parameter itp controls where the display is printed. If TTY is entered (default), the display is written to the user's terminal. Any other setting of itp will route the display to the print file. Note that the commands

```
LIST /
LIST DATA /
LIST DATA TTY /
LIST * TTY /
LIST * /
LIST * * /
```

are all equivalent. Example 6 in Sec. XVI uses the LIST command to display default data settings.

XIV. EOS DISPLAY

Commands are available in GRIZZLY for displaying EOS data from tables. There are commands which display actual table points and commands which use interpolation to display the EOS along hugoniots, isentropes (constant entropy), isobars (constant pressure), isochores (constant density), and isotherms (constant temperature). All displays can be sent to the user's terminal, the print file, or both. CURVES[13] may be used to generate graphical displays from print files. Sections XIV.A., B., C., D., E., and F. discuss the commands associated with displaying table points, hugoniots, isentropes, isobars, isochores, and isotherms, respectively.

Displays produced by commands in this section can be presented in other units provided that the conversion involves only simple multiplication. User units are defined through the DUNITS command. Note that if alternative units are defined then all commands in this section requiring data must be entered in user units.

DUNITS run tun pun eun vun /

This command allows the user to modify display units. The parameters run, tun, pun, eun, and vun are density, temperature, pressure, energy, and velocity

multipliers, respectively. All parameters correspond to conversion factors for converting GRIZZLY units (Table I-2) to user units. All factors have a default value of 1.

A. Table Points

DISPLAY i r_1 r_2 t_1 t_2 lab /
D i r_1 r_2 t_1 t_2 lab /
PRINT i r_1 r_2 t_1 t_2 lab /
P i r_1 r_2 t_1 t_2 lab /

These commands display the tabulated EOS values for table i. DISPLAY presents the table at the users terminal, and PRINT routes the table to the print file. D is shorthand for DISPLAY and P is shorthand for PRINT. The parameters r_1 and r_2 define a density window. The parameters t_1 and t_2 define a temperature window. Any points falling within both windows are displayed. The default values for r_1, r_2, t_1, and t_2 are -1.0, 1.0E300, -1.0, and 1.0E300, respectively. The parameter label is an optional eight character alphanumeric the user may define to label the display.

RHO i itp /

This command displays the density grid for table i. If the parameter itp is set to P then the display is sent to the print file; otherwise, the display is presented at the user's terminal.

TEMP i itp /

This command displays the temperature grid for table i. If the parameter itp is set to P then the display is sent ot the print file; otherwise, the display is presented at the user's terminal.

B. Hugoniots

The HUG command is used to display EOS information for a material undergoing shock compression from some initial state. Solutions to the Rankine-Hugoniot relation are displayed along a prescribed temperature mesh. The default temperature mesh is 0.026, 0.05, 0.1, 0.15, 0.2, 0.25, 0.30, 0.35, 0.40, 0.45, and 0.5 eV. Alternative temperature meshes may be constructed using the THGRD, THLIN, and THLOG commands. The initial state of the material is taken to be a compression of 1 and temperature of 0.025692 eV. The initial state may be altered by issuing a HUGI command.

HUG i idev /

This command displays a hugoniot from table i. If the parameter idev is omitted

or set to TTY, the display is sent to the user's terminal. If idev is set to P, the display is sent to the print file. If idev is set to B, the display is sent to both the terminal and print file.

CHGM chgm /

This command is used to specify the maximum hugoniot compression. The density corresponding to this compression (chgm) is used as a upper limit when searching for solutions of shock relationships. The default value for chgm is 3.

HUGI chgi thgi /

This command is used to alter the initial state used for computing the hugoniot. The parameter chgi specifies the initial compression and thgi the initial temperature.

THGRD t_1 t_2 ... /

THLIN n t_1 t_n /

THLOG n t_1 t_n /

These commands are used to alter the hugoniot temperature mesh. THGRD, THLIN, and THLOG are analogous to TGRD, TLIN, and TLOG (see Sec. IX), respectively. A maximum of 50 temperatures is allowed.

C. Isentropes

The ISENT command is used to display EOS information along paths of constant entropy. Isentropes are generated on a prescribed density mesh. The default density mesh consists of 13 logarithmically spaced points between 10^{-3} and 10^{3}. Alternative meshes may be constructed using the RENGRD, RENLIN, and RENLOG commands.

ISENT i r t idev /

This command displays an isentrope from table i. The density r and temperature t are used to determine the entropy for the isentrope. Table i must include the free energy. The parameter idev is defined in Sec. XIV.B. (HUG command).

RENGRD r_1 r_2 ... /

RENLIN n r_1 r_n /

RENLOG n r_1 r_n /

These commands are used to alter the density mesh. RENGRD is used to specify individual density points, RENLIN is used to specify a linear density mesh, and RENLOG is used to specify a logarithmic density mesh. The parameter n specifies the number of points, and r_1 and r_n specify the lower and upper density limits, respectively. The maximum number of densities allowed is 50.

TENT $tent_1$ $tent_2$ /

This command is used to alter the temperature search limits used in calculating isentropes. The parameters $tent_1$ and $tent_2$ specify the lower and upper limits, respectively. The default values for $tent_1$ and $tent_2$ are 0 and 100000 eV, respectively.

D. Isobars

The ISOBAR command is used to display EOS information along paths of constant pressure. Isobars are computed on a prescribed temperature mesh. The default mesh is 0, 0.025692, 0.1, 0.5, 1, 3, 10, 30, 100, 300, and 1000 eV. The commands TISBGRD, TISBLIN, AND TISBLOG may be used to construct alternative meshes.

ISOBAR i p idev /

This command displays an isobar from table i. The parameter p specifies the pressure, and idev has been discussed in Sec. XIV.B.

RISOB $risob_1$ $rosob_2$ /

This command is used to alter the density search limits. The parameters $risob_1$ and $risob_2$ are the lower and upper density search limits, respectively. The default values for $risob_1$ and $risob_2$ are the density limits of the table specified in the ISOBAR command. These parameters may be varied to avoid difficulties caused by nonuniqueness in the vapor dome region.

TISBGRD t_1 t_2 ... /

TISBLIN n t_1 t_n /

TISBLOG n t_1 t_n /

These commands are used to alter the isobar temperature mesh. TISBGRD, TISBLIN, and TISBLOG are analogous to TGRD, TLIN, and TLOG (see Sec. IX), respectively. The maximum number of temperatures allowed is 50.

E. Isochores

The command ISOCHR is used to generate the EOS at constant density along a mesh of temperatures. The default mesh is 0, 0.025692, 0.1, 0.5, 1, 3, 10, 30, 100, 300, and 1000 eV. The temperature mesh may be altered by using the TISCGRD, TISCLIN, or TISCLOG commands discussed below.

ISOCHR i r idev /

This command is used to display an isochore from table i. The parameter r specifies the isochore density. The parameter idev has been discussed in Sec. XIV.B. (HUG command).

TISCGRD t_1 t_2 ... /
TISCLIN n t_1 t_n /
TISCLOG n t_1 t_n /
These commands are used to prescribe a temperature mesh for displaying isochores. TISCGRD, TISCLIN, and TISCLOG are analogous to TGRD, TLIN, and TLOG. The maximum number of temperatures is 50.

F. Isotherms

The command ISOTHM is used to generate the EOS at constant temperature along a mesh of densities. The default mesh is 13 logarithmically spaced points between 10^{-3} and 10^{3}. The density mesh may be altered by using the RISTGRD, RISTLIN, and RISTLOG commands discussed below.

ISOTHM i t idev /
This command is used to display isotherms from table i. The parameter t is the isotherm temperature. The parameter idev has been discussed in Sec. XIV.B. (HUG commmand).

RISTGRD r_1 r_2 ... /
RISTLIN n r_1 r_n /
RISTLOG n r_1 r_n /
These commands are used to prescribe a density mesh for displaying isotherms. RISTGRD, RISTLIN, and RISTLOG are analogous to RENGRD, RENLIN, and RENLOG (see Sec. XIV.C.). The maximum number of densities allowed is 50.

XV. FILE INTERFACES

File interface commands allow the user to read and write EOS data to files of various formats. EOS tables can be written to SESAME files or GRIZZLY data base files. SESAME is currently the format supported by T-4 for storing EOS, opacity, and conductivity data. The GRIZZLY data base files are compatible with those being used for NLTE (Non-Local Thermodynamic Equilibrium) work in T-4.

SESAME files have the advantage that they interface with many computer codes existing at the laboratory.

GRIZZLY data base files have the advantage of a more flexible data identification scheme. Also, data records may be added to an existing file without running an intermediate data base management program.

The commands discussed below control the reading and writing of EOS tables.
RSES id fn i_1 t_1 i_2 t_2 ... /

WSES id fn i_1 t_1 i_2 t_2 ... ipe /

These commands read and write SESAME files, respectively. The parameter id is the SESAME material number, fn is the SESAME file name, i_k is the internal table number, and t_k is the SESAME table number. For RSES the SESAME file fn is read and tables t_k of material id are read into internal table numbers i_k. For WSES a SESAME file fn is created with one material of number id and SESAME table numbers t_k corresponding to internal table numbers i_k. These commands also perform the units conversions which are required. If the parameter ipe is set to PE only the pressure and internal energy tables are written; thus the Helmholtz free energy is not included in the SESAME table.

RTAB i fn ky_1 ky_2 ... /

WTAB i fn ky_1 ky_2 ... /

These commands are used to read and write data base files, respectively. The parameter i is the table number, fn is the file name, and the ky_k are a set of 1 to 3 numeric or hollerith identification keys. RTAB will read the data record with identification keys ky_k from file fn into GRIZZLY table i. WTAB will write internal table i to file fn with keys ky_k. If fn does not exist in the users local file space, fn will be created. If fn does exist in the user's space, then the data will be added to file fn. If the identification keys are identifical to ones existing on the file, the new data will replace the existing data.

XVI. EXAMPLES

1. Figure 16-1-1 shows a run of GRIZZLY to generate an aluminum EOS using the default models. The atomic number, atomic mass, normal density, and cohesive energy are specified by the first four commands. The SHKFIT command is used to supply the u_s-u_p fit[18] for the CHUG cold curve. The EOS command calculates the equation of state. The cold curve is stored in table 1, the nuclear contribution is stored in table 2, the electronic contribution is stored in table 3, and the total EOS is stored in table 4. The WSES command is used to write these tables to SESAME file S3716 with material number 3716. The code SES2D[19] was used to access this file and generate the plots shown in Figs. 16-1-2 to 16-1-10. Figures 16-1-2, 16-1-3, and 16-1-4 show the total pressure, total internal energy, and total Helmholtz free energy, respectively. Figures 16-1-5, 16-1-6, and 16-1-7 show the electronic contribution for the pressure, energy, and free energy, respectively. Figures 16-1-8, 16-1-9, and 16-1-10 show the nuclear

contribution for the pressure, energy, and free energy, respectively. The variables are plotted as a function of mass density for a given temperature.

2. Figure 16-2-1 shows a run of GRIZZLY which accesses the data generated in example 1 and calculates the hugoniot. The generated hugoniot is compared with experimental shock data in Fig. 16-2-2. Figure 16-2-2 was generated using CURVES[13] with the GRIZZLY output file, the experimental shock data were extracted from the HUGDATA[20] file.

3. Figure 16-3-1 shows a run of GRIZZLY to generate an EOS for silver. This example is more detailed than example 1 because more parameters are specified. The value for normal density, bulk modulus, Debye temperature, and cohesive energy were taken from Ref. 21. Note the user specified compression grid and the suppression of temperatures above 100 eV. The TSTFD command is used to eliminate some wiggles in the TFD energies at 10 eV and below. A mod-Morse cold curve is used with the solid-gas formula plus virial match nuclear model. Note the data and grids are listed before the EOS is computed. After the EOS is calculated the tables are written to a SESAME file and the principal hugoniot is sent to the print file with user defined units. Figures 16-3-2 through 16-3-10 display the calculated total, electronic, and nuclear EOS surfaces. Figures 16-3-11 and 16-3-12 compare the theoretical and experimental hugoniots.

4. Figure 16-4-1 presents the GRIZZLY run for beryllium oxide (BeO). The MXTURE command is used to define the mixture components. The actual normal density is supplied with the RHOREF command. The KCTFD command is used to sparse the TFD tables to make the run faster. The CHUGT cold curve option is used to replicate a complex hugoniot structure,[18] and hence a USUP command is issued. The EOSMX command is used to calculate the EOS. Note that suppression is used to get rid of data above a compression of 1000. Most of these data are not good because of applying the mixing scheme to densities beyond the validity of the constituent tables. The tables are then written to a SESAME file and a hugoniot is calculated. Figures 16-4-2 through 16-4-10 present the calculated EOS surfaces. The wiggles in the electronic tables (16-4-5 through 16-4-7) at low temperatures are caused by interpolation to temperatures not tabulated for each of the constituent materials. These wiggles do not appear on the total EOS surface because the electronic contribution is small in this region. Figures 16-4-11 shows a comparison of the calculated hugoniot with experiment. The theoretical hugoniot does not approach the sound speed (small particle velocities) because there are

not enough grid points around ambient conditions to resolve the structure of the EOS.

5. Figure 16-5-1 shows an example of mixing pre-existing tables. The tables are read from the SESAME library and mixed with the various schemes. The mixture corresponds to that of Appendix C. The print file generated by this example is shown in Fig. 16-5-2.

6. Figure 16-6-1 shows an interactive run of GRIZZLY to exercise the LIST command. Note the default values of the various parameters. Also note that a MXTURE command is invoked as a prerequisite to exercising a LIST MIX / command. The columns labeled WMIX, FMIX, ZMIX, AMIX, and RMIX correspond to weight fraction, number fraction, atomic number, atomic weight, and normal density of each component. Note that the MXTURE command also sets zbar, abar, and rhoref.

ACKNOWLEDGMENTS

The author is indebted to Bard Bennett, F. Dowell, Brad Holian, Kathy Holian, Walter Huebner, J. D. Johnson, Al Merts, and Galen Straub for their involvement with GRIZZLY. The author is also indebted to Jerry Kerley for PANDA, to David Liberman for providing Appendix A, and to Jean Trujillo and Vickie Montoya for typing the manuscript.

APPENDIX A

CANDIDE

CANDIDE is the computer program which uses a temperature dependent Thomas-Fermi-Dirac model to obtain equation of state data. Like other Thomas-Fermi models[22,23] it assumes an average atom. Unlike Ref. 23, it uses a zero temperature expression for exchange at all temperatures. This has the advantage of simplicity and also avoids the well known incorrect low temperature behavior characteristic of the Hartree-Fock expression for exchange. At high temperatures there is some error as a result of this approximation, but it is small in comparison with the thermal contributions to the kinetic and potential energies.

The model is based on an expression for the free energy, $F = E - TS$, where $E = K + U + V + W$ is the internal energy, and

$$K = \iint \frac{drdp}{h^3} \frac{p^2}{2m} 2f(p,r) \tag{A-1}$$

is the kinetic energy

$$U = - \int dr \frac{Ze^2}{r} \rho(r) \tag{A-2}$$

is the electron-nucleus potential energy,

$$V = \frac{e^2}{2} \iint dr\, dr' \frac{\rho(r)\rho(r')}{|r - r'|} \tag{A-3}$$

is the electron-electron potential energy,

$$W = - \frac{3e^2}{4\pi} \frac{3}{2} X_\alpha \int dr\, \rho(r) k_F(r) \tag{A-4}$$

is the zero temperature expression for the exchange energy, and

$$S = - k_B \iint \frac{drdp}{h^3} 2\{f(r,p)\log f(r,p) + [1 - f(r,p)]\log[1-f(r,p)]\} \quad \text{(A-5)}$$

is the entropy. In these equations

$$\rho(r) = \int \frac{dp}{h^3} 2f(r,p) \quad \text{(A-6)}$$

is the density of electrons,

$$k_F(r) = [3\pi^2\rho(r)]^{1/3} \quad \text{(A-7)}$$

is the Fermi wave number, f(r,p) is the Fermi-Dirac distribution function, and X_α is a parameter which normally is 2/3. All integrals on r are understood to run from 0 to R--the radius of the atomic sphere--while integrals on p run over all of momentum space.

The free energy, F, is to be minimized subject to the condition that the number of electrons in the atomic sphere,

$$N = \int dr\ \rho(r), \quad \text{(A-8)}$$

is fixed. For neutral atoms N = Z. The minimization of F, subject to the constraint that N is fixed, is accomplished by setting

$$\frac{\delta(F - \mu N)}{\delta F} = 0 = \frac{1}{h^3} \varepsilon(r,\rho) - \mu + k_B T \log \frac{f(r,p)}{1 - f(r,p)} \quad , \quad \text{(A-9)}$$

where

$$\varepsilon(r,p) = \frac{p^2}{2m} + v(r) \quad \text{(A-10)}$$

and

$$v(r) = - \frac{Ze^2}{r} + \int dr' \frac{e^2\rho(r')}{|r - r'|} - \frac{e^2}{\pi} (\tfrac{3}{2} X_\alpha)k_F(r) \quad . \quad \text{(A-11)}$$

The solution of this is the Fermi-Dirac distribution function

$$f(r,p) = 1/\{\exp[(\varepsilon(r,p) - \mu)/k_B T] + 1\} \quad . \tag{A-12}$$

The potential $v(r) + \frac{e^2}{\pi} \frac{3}{2} X_\alpha \, k_F(r)$ satisfies the Poisson equation

$$-\nabla^2[v(r) + \frac{e^2}{\pi} (\tfrac{3}{2} X_\alpha) k_F(r)] = 4\pi e^2[Z\delta(r) - \rho(r)] \quad , \tag{A-13}$$

and the electron density is

$$\rho(r) = \int \frac{dp}{h^3} \frac{2}{\exp\left[\frac{p^2}{2m} + v(r) - \mu\right]/k_B T + 1} \quad . \tag{A-14}$$

These last two equations are solved for $v(r)$ and $\rho(r)$ by CANDIDE. The chemical potential is adjusted to make the number of electrons, N, correct. When $\rho(r)$ and $v(r)$ are known, the thermodynamic functions, including the pressure, are calculated.

APPENDIX B

HIGH DENSITY MATCH

The high density match formula in GRIZZLY is a modified version of the TFD match formula of PANDA.[9] The major differences are (1) the GRIZZLY version has one less parameter and therefore one less condition to satisfy, and (2) the formula as implemented in GRIZZLY is not restricted to TFD.

The purpose of the high density match formula is to join smoothly a cold curve valid at densities below a match density (ρ_m) to a cold curve valid at higher densities. The match density used in GRIZZLY is the product of rhoref and cmat. For densities $\rho < \rho_m$, the low density cold curve energies E_L and pressure P_L are used. For densities $\rho \geq \rho_m$, the cold curve is expressed as

$$E_c(\rho) = [E_H(\rho) - E_H(\rho_M)]Y(\rho) + \Delta E_c \quad \text{and} \tag{B-1}$$

$$P_c(\rho) = P_H(\rho)Y(\rho) + \rho^2[E_H(\rho) - E_H(\rho_M)]\,\frac{dY}{d\rho} \quad , \tag{B-1}$$

where E_L and P_L are the cold energies and pressures, respectively, E_H and P_H are the high density cold energies and pressures, and Y is a interpolation function given by

$$Y(\rho) = 1 + \frac{b_1}{\rho} + \frac{b_2}{\rho^{4/3}} \quad . \tag{B-3}$$

The constants ΔE_c, b_1, and b_2 are determined by requiring that

$$E_c(\rho_M) = E_L(\rho_M) \quad , \tag{B-4}$$

$$P_c(\rho_M) = P_L(\rho_M) \quad , \tag{B-5}$$

and

$$\left.\frac{dP_c}{d\rho}\right|_{\rho_M} = \left.\frac{dP_L}{d\rho}\right|_{\rho_M} \quad . \tag{B-6}$$

The version of the TFD match in PANDA had an additional term in Eq. (B-3). In order to evaluate a coefficient for this term, an extra condition involving the second derivative of the pressure was imposed. This term is used in PANDA to insure the continuity of the second derivative of the pressure. This derivative is used in methods which compute the Grüneisen parameter from the cold curve. Since the current version of GRIZZLY has no such methods the term was dropped. Comparison runs show little qualitative difference between the two methods. The match formula in GRIZZLY is more often successful and less dependent on the value of the match density. Comparison runs indicate that removal of this condition in GRIZZLY has little qualitative effect on the generated cold curves. Substituting Eqs. (B-1)-(B-3) into Eqs. (B-4)-(B-6) we can obtain expressions for ΔE_c, b_1 and b_2.

APPENDIX C
MIXING SCHEMES

1. Additive Volume Mixing

In the additive volume scheme each component of the mixture is assumed to be in equilibrium at the same pressure, and the volume (density) of each component at this pressure is used to compute a resultant volume (density). The equations which describe this are

$$P(\rho,T) = P_i(\rho_i,T) \quad , \quad i = 1, \ldots, N \tag{C-1}$$

and

$$\frac{1}{\rho} = \sum_{i=1}^{N} \frac{W_i}{\rho_i} \quad , \tag{C-2}$$

where P and ρ are the pressure and density of the mixture, respectively, P_i and ρ_i are the pressure and density of component i, respectively, T is the temperature, N is the number of mixture components, and the W_i are the mass fractions for each component. In GRIZZLY, for a given mixture density ρ, P is varied until a set of ρ_i's are found that satisfy both Eqs. (C-1) and (C-2). The internal energy (E) and the Helmholtz free energy (A) for the mixture are then calculated using

$$E(\rho,T) = \sum_{i=1}^{N} W_i E_i(\rho_i,T) \tag{C-3}$$

and

$$A(\rho,T) = \sum_{i=1}^{N} W_i A_i(\rho_i,T) \quad , \tag{C-4}$$

where E_i and A_i are the internal energy and free energy for component i. The additive volume mixing scheme gets into trouble in regions where the pressure is not monotonic in density along an isotherm because then there exist multiple

solutions of Eq. (C-1). In particular, this scheme does not work in regions of Van der Waals loops. In other regions the results of additive volume mixing are probably more reliable than the other mixing schemes in GRIZZLY.

2. Ideal Mixing

The ideal mixing scheme used in GRIZZLY is an ideal gas adaption of the additive volume method. This scheme has been presented previously in Ref. 11. In this method the equation of state of the mixture is given by

$$P(\rho,T) = \sum_{i=1}^{N} f_i P_i(\rho_i,T) \quad , \tag{C-5}$$

$$E(\rho,T) = \sum_{i=1}^{N} W_i E_i(\rho_i,T) \quad , \tag{C-6}$$

and

$$A(\rho,T) = \sum_{i=1}^{N} W_i A_i(\rho_i,T) \tag{C-7}$$

where the component densities are now given by

$$\rho_i = \frac{A_i}{A} \rho \quad . \tag{C-8}$$

In Eqs. (C-5)-(C-8) the f_i are number fractions which may be calculated from the mass fractions by using

$$f_i = AW_i/A_i \quad , \tag{C-9}$$

where the A_i are atomic weights of the individual components, and the average atomic weight (A) of the mixture may be calculated using

$$\frac{1}{A} = \Sigma \frac{W_i}{A_i} \quad . \tag{C-10}$$

This method is fast because it is noniterative and does not encounter problems in regions of Van der Waals loops.

3. Partial Pressure Mixing

In the partial pressure mixing scheme thermodynamic quantities for the mixture are obtained by simply summing up the contribution for each component according to their individual mass densities. Therefore the mixture EOS is computed using

$$P(\rho,T) = \sum_{i=1}^{N} P_i(\rho_i,T) \quad , \tag{C-11}$$

$$E(\rho,T) = \sum_{i=1}^{N} W_i E_i(\rho_i,T) \quad , \tag{C-12}$$

and

$$A(\rho,T) = \sum_{i=1}^{N} W_i A_i(\rho_i,T) \quad , \tag{C-13}$$

where the individual mass densities are given by

$$\rho_i = W_i \rho \quad . \tag{C-14}$$

Partial pressure mixing is noniterative, fast, and does not encounter numerical difficulties.

4. Comparison

A comparison of the mixing scheme presented in this Appendix is shown in Fig. C-1. All methods give the same results in the ideal gas regions (low density or high temperature). Note that additive volume and partial pressure mixing differ significantly at high densities whereas ideal mixing agrees well with the partial pressure scheme at intermediate densities and with additive volume at high densities.

APPENDIX D

DENSITY SCALING

The formulas presented in this appendix are used to scale an EOS table of a particular reference density to an EOS of a user specified reference density. These formulas are used by the RSCALE command. The high temperature and low density (ideal) regions of the EOS are preserved by the transformation. Other regions have no physical significance except that the scaled table has the specified reference point. This procedure is useful for adjusting the reference point for an approximate EOS such as one resulting from table mixing. The scaling formulas are

$$P(\rho,T) = s\ P'(\rho/s,T) \quad , \tag{D-1}$$

$$E(\rho,T) = E'(\rho/s,T) \quad , \tag{D-2}$$

$$A(\rho,T) = A'(\rho/s,T) \quad , \tag{D-3}$$

and

$$s = \rho_o/\rho'_o \quad , \tag{D-4}$$

where P', E', and A' are the pressure, internal energy, and free energy of the original EOS, P, E, and A are the pressure, internal energy, and free energy of the "scaled" EOS, s is the scale factor, ρ'_o is the reference density of the original EOS, ρ_o is the desired reference density, ρ is a given mass density, and T is the temperature.

TABLE I-1

COMMAND	DESCRIPTION	PAGE
ABAR abar /	specify atomic weight	12
ATOM zbar /	initialize element	12
AVMIX nw i_1 x_1 i_2 x_2 ... i /	compute additive volume mix	21
BCOLD bcold /	specify cold curve bulk modulus	12
BREF bref /	specify reference point bulk modulus	12
CGRD η_1 η_2 ... /	specify compressions	18
CGRDA η_1 η_2 ... /	add compressions	18
CHANGE i r t p e a /	change table point	23
CHARTD i /	compute CHART-D nuclear model	10
CHGM chgm /	specify maximum compression for hugoniot	27
CHUG i mn_1 mn_2 /	compute CHUG cold curve	7
CHUGT i mn_1 mn_2 /	compute CHUGT cold curve	8
CLIN n η_1 η_n /	specify linear compression grid	18
CLINA n η_1 η_n /	add linear compression grid	18
CLJ clj /	specify Lennard-Jones match compression	12
CLOG n η_1 η_n /	specify log compression grid	18
CLOGA n η_1 η_n /	add log compression grid	18
CMAT cmat /	specify high density match compression	12
COLDMX i mc mn_1 mn_2 /	compute mixture cold curve	22
COPTAB i_1 i_2 /	copy table	23
COWAN i /	compute COWAN nuclear model	10
CSUP k η_1 η_1' η_2 η_2' ... /	suppresses compression from default grid	17
CVIR cvir /	specify virial match compression	13
D i r_1 r_2 t_1 t_2 lab /	display table	26
DEBREF debref /	specify reference Debye temperature (eV)	13
DEBKEL debref /	specify reference Debye temperature (Kelvin)	13

DEBSHK c_0 σ /	compute Debye temperature	13
DEBSHKKS c_0 σ /	compute Debye temperature (c_0 in km/sec)	13
DEBYE i /	compute Debye nuclear model	10
DEBYEC i /	compute cutoff Debye nuclear model	10
DISPLAY i r_1 r_2 t_1 t_2 lab /	display table	26
DUNITS run tun pun tun vun /	define display units	25
DVIR dvir /	specify step for virial match derivative	13
ECOH ecoh /	specify cohesive energy ($Mb \cdot cm^3/g$)	13
ECOHKC ecoh /	specify cohesive energy (kcal/mole)	13
EINSTN i /	compute Einstein nuclear model	10
EINSTC i /	compute cutoff Einstein nuclear model	10
ELECMX i me /	compute mixture electronic model	22
END /	terminate	4
EOS i_c i_n i_c i_t /	compute EOS for elements	5
EOSMX i /	compute EOS for mixture	6
EPSMIX epsmix /	specify accuracy parameter for mixing	13
FACLJ faclj /	specify Lennard-Jones factor	13
GAMREF gamref /	specify reference gamma	14
GAMSHK s_1 ft /	compute reference gamma	14
GIKNUC i /	compute solid-gas nuclear model	10
HUG i idev /	compute hugoniot	26
HUGI chgi thgi /	specify hugoniot initial conditions	27
IDGAS i /	compute ideal gas nuclear model	11
IDMIX nw i_1 x_1 i_2 x_2 ... i	compute ideal mix	21
IGRUN igrun /	specify method for computing gamma	14
ISENT i r t idev /	compute isentrope	27
ISOBAR i p idev /	compute isobar	28
ISOCHR i r idev /	compute isochore	28
ISOTHM i t idev /	compute isotherm	29
KCCOLD k /	specify cold curve compression sparsing factor	19

KCMIX k /	specify mixture compression sparsing factor	19
KCNUC k /	specify nuclear compression sparsing factor	19
KCTFD k /	specify TFD compression sparsing factor	19
KRTAB k /	specify table suppression density sparsing factor	21
KTNUC k /	specify nuclear temperature sparsing factor	20
KTMIX k /	specify mixture temperature sparsing factor	20
KTTAB k /	specify table suppression temperature sparsing factor	21
KTTFD k /	specify TFD temperature sparsing factor	20
LIST item itp /	display raw data	24
LJMATCH i_1 i_2 mn_1 mn_2 /	compute Lennard-Jones match	24
MATCH i_1 i_2 i_3 /	compute high density match	24
MATCH2 i_1 i_2 i_3 mn_1 mn_2 /	compute high density and Lennard-Jones match	24
MODC modc /	specify cold curve model	14
MODN $modn_1$ $modn_2$ /	specify nuclear model	14
MODE mode /	specify electronic model	15
MODMRS1 i /	compute modified Morse cold curve	8
MODMRS2 i mn_1 mn_2 /	compute modified Morse cold curve	8
MODMRS3 i mn_1 mn_2 /	compute modified Morse cold curve	9
MODMRS4 i mn_1 mn_2 /	compute modified Morse cold curve	9
MX i /	mix tables for specified mixture	22
MXC i /	mix cold curves for specified mixture	22
MXTURE nw x_1 z_1 a_1 r_1 ... /	specify a mixture	15
P i r_1 r_2 t_1 t_2 lab /	print table	26
PCTAB i r_1 p_1 r_2 p_2 ... /	compute cold curve from pressure table	24

PPMIX nw i_1 x_1 i_2 x_2 ... i /	compute partial pressure mix	21
PRINT i r_1 r_2 t_1 t_2 lab /	print table	26
RAT i_1 i_2 /	interpolate table	23
RCOLD rcold /	specify cold curve density	16
RENGRD r_1 r_2 ... /	specify isentrope density grid	27
RENLIN n r_1 r_n /	specify linear isentrope density grid	27
RENLOG n r_1 r_n /	specify log isentrope density grid	27
RHO i itp /	display table density grid	26
RHOREF rhoref /	specify reference density	16
RISOB $risob_1$ $risob_2$ /	specify isobar search density limits	28
RISTGRD r_1 r_2 ... /	specify isotherm density grid	29
RISTLIN n r_1 r_n /	specify linear isotherm density grid	29
RISTLOG n r_1 r_n /	specify log isotherm density grid	29
RSCALE i r /	scale to new normal density	23
RSES id fn i_1 t_1 i_2 t_2 ... /	read tables from SESAME file	29
RTAB i fn ky_1 ky_2 ... /	read table from data base file	30
SCALE i a /	isotopically scale table	23
SCCOLD η_1 η_1' η_2 η_2' /	specify cold curve compression suppression string	20
SCMIX η_1 η_1' η_2 η_2' /	specify mixture compression suppression string	20
SCNUC η_1 η_1' η_2 η_2' /	specify nuclear compression suppression string	20
SCTFD η_1 η_1' η_2 η_2' /	specify TFD compression suppresion string	20
SHFT i es /	shift table energies	23
SHKFIT c_0 s_1 s_2 /	specify u_s-u_p fit	16
SHKFITKS c_0 s_1 s_2 /	specify u_s-u_p fit (km/sec)	16
SRTAB r_1 r_1' r_2 r_2' /	specify table density suppression string	21
STAN i_1 i_2 /	standardize table energies	23
STMIX t_1 t_1' t_2 t_2' /	specify mixture temperature suppression string	20
STNUC t_1 t_1' t_2 t_2' /	specify nuclear temperature suppression string	20

STTAB t_1 t_1' t_2 t_2' / .	specify table temperature supppresion string	21
STTFD t_1 t_1' t_2 t_2' /	specify TFD temperature suppression string	20
SUBCLD i /	subtract cold isotherm from table	23
SUP i_1 i_2 /	suppress table densities and temperatures	20
TEMP i itp /	list tables temperatures	26
TENT $tent_1$ $tent_2$ /	specify temperature limits for isentrope search	28
TFDC i /	compute TFD cold curve	7,11
TFDCMX i /	compute TFD cold curves for mixture components	22
TFDMX i /	compute TFD thermal tables for mixture components	22
TFDTHM i /	compute TFD thermal table	11
TFDTOT i /	compute TFD total table	11
TGRD t_1 t_2 ... /	specify temperature grid	18
TGRDA t_1 t_2 ... /	add temperatures	18
THGRD t_1 t_2 ... /	specify hugoniot temperature grid	27
THLIN n t_1 t_n /	specify linear hugoniot temperature grid	27
THLOG n t_1 t_n /	specify log hugoniot temperature grid	27
TISBGRD t_1 t_2 ... /	specify isobar temperature grid	28
TISBLIN n t_1 t_n /	specify linear isobar temperature grid	28
TISBLOG n t_1 t_n /	specify log isobar temperature grid	28
TISCGRD t_1 t_2 ... /	specify isochore temperature grid	28
TISCLIN n t_1 t_n /	specify linear isochore temperature grid	29
TISCLOG n t_1 t_n /	specify log isochore temperature grid	29
TLIN n t_1 t_n /	specify linear temperature grid	18
TLINA n t_1 t_n /	add linear temperature grid	18
TLOG n t_1 t_n /	specify log temperature grid	18
TLOGA n t_1 t_n /	add log temperature grid	18

TOTAL i_c i_n i_e i_t /	combine tables	24
TREF tref /	specify reference temperature	16
TREFKEL tref /	specify reference temperature (Kelvin)	16
TSTFD tstfd /	specify temperature for 1/2 TS substitution in TFD	16
TSUP k t_1 t_1' t_2 t_2' ... /	suppress temperatures from default grid	18
USEALL i /	combination of USEC, USET, and USEZ	16
USEC i /	use compressions from table	19
USET i /	use temperature from table	19
USEZ i /	use atomic number, weight and density from table	16
USUP u_{p_1} u_{s_1} u_{p_1} u_{s_1} ...	specify u_s-u_p table (cm/μsec)	17
USUPKS u_{p_1} u_{s_1} u_{p_1} u_{s_1} ...	specify u_s-u_p table (km/sec)	17
VIRIAL i mn /	compute virial match	11
WSES id fn i_1 t_1 i_2 t_2 ... ipe /	write tables to SESAME file	30
WTAB i fn ky_1 ky_2 ... /	write table to data base file	3
XALPHA xalpha /	specify exchange parameter	17
ZBAR zbar /	specify atomic number	17

TABLE I-2

QUANTITY	UNIT
mass density	grams per cubic centimeter (g/cm^3)
temperature	electron volts (eV)
pressure	Megabars (Mb)
energy density	$Mb \cdot cm^3/g$
velocity	cm/μsec

TABLE IX-1

DEFAULT COMPRESSION GRID (dimensionless)

0.0	10^{-6}	2×10^{-6}	5×10^{-6}
10^{-5}	2×10^{-5}	5×10^{-5}	10^{-4}
2×10^{-4}	5×10^{-4}	10^{-3}	1.5×10^{-3}
2×10^{-3}	4×10^{-3}	6×10^{-3}	10^{-2}
1.5×10^{-2}	2.5×10^{-2}	4×10^{-2}	6×10^{-2}
0.1	0.125	0.15	0.2
0.25	0.3	0.4	0.5
0.6	0.7	0.8	0.9
0.95	1.0	1.05	1.1
1.2	1.4	1.6	1.8
2.0	2.5	3.0	3.5
4.0	5.0	6.0	7.0
8.0	9.0	10.0	15.0
20.0	25.0	30.0	40.0
60.0	80.0	100.0	150.0
250.0	400.0	600.0	10^{3}
2×10^{3}	5×10^{3}	10^{4}	2×10^{4}

TABLE IX-2

DEFAULT TEMPERATURE GRID (eV)

0	0.0125	0.025692	0.05
0.1	0.25	0.5	0.75
1	1.5	2	2.5
3	4	5	8
10	15	20	25
20	40	50	80
100	150	250	400
600	1000	1500	2500
6000	10000	20000	50000
100000			

REFERENCES

1. Necia G. Cooper, "An Invitation to Participate in the LASL Equation of State Library," Los Alamos Scientific Laboratory brochure LA-79-62 (February 1980).
2. F. Dowell, "SESAME '83: Report on the Los Alamos Equation-of-State Library," Los Alamos National Laboratory report LALP-83-4 (February 1983).
3. B. I. Bennett, J. D. Johnson, G. I. Kerley, and G. T. Rood, "Recent Developments in the Sesame Equation-of-State Library," Los Alamos Scientific Laboratory report LA-7130 (February 1978).
4. J. Abdallah, Jr., G. I. Kerley, B. I. Bennett, J. D. Johnson, R. C. Albers, and W. F. Huebner, "HYDSES: A Subroutine Package for Using Sesame in Hydrodynamic Codes," Los Alamos Scientific Laboratory report LA-8209 (June 1980).
5. Charles W. Cranfill, "EOSPAC: A Subroutine Package for Accessing the Los Alamos Sesame EOS Data Library," Los Alamos National Laboratory report LA-9728-M (August 1983).
6. J. M. Hyman and M. M. Klein, "EOSMOD: A Subroutine Package for Calculating Equation of State and Opacities," Los Alamos National Laboratory report LA-8502-M (October 1981).
7. M. S. Shaw and G. K. Straub, "HYDROX: A One-Dimensional Lagrangian Hydrodynamics Code," Los Alamos National Laboratory report LA-8642-M (March 1981).
8. The T-4 code EOSCRAY was developed at Los Alamos by B. I. Bennett. No formal documentation exists for EOSCRAY.
9. G. I. Kerley, "User's Manual for PANDA: A Computer Code for Calculating Equations of State," Los Alamos National Laboratory report LA-8833-M (November 1981).
10. GRIZZLY uses a version of CANDIDE developed by D. A. Liberman and modified by J. D. Johnson. The basic physics is discussed in Appendix A.
11. Joseph Abdallah, Jr., "MIXB: A BCON Controller for Generating and Maintaining Sesame Library Files of Mixture Data," Los Alamos Scientific Laboratory report LA-8219-M (April 1980).

12. R. C. Albers, "An Introduction to Two-Temperature Equations of State," Los Alamos Scientific Laboratory report LA-7934-MS (July 1979).
13. Joseph Abdallah, Jr., "User's Manual for CURVES," Los Alamos National Laboratory report LA-8844-M (October 1981).
14. B. I. Bennett, "On Obtaining the Zero-Temperature Equation of State from Shock Data," Los Alamos National Laboratory report LA-9890-MS (January 1984).
15. B. I. Bennett, "A Computationally Efficient Expression for the Zero-Temperature Isotherm in Equations of State," Los Alamos Scientific Laboratory report LA-8616-MS (December 1980).
16. S. L. Thompson and H. S. Lawson, "Improvements the Chart-D Radiation-Hydrodynamic Code III: Revised Analytic Equations of State," Sandia National Laboratory report SC-RR-710714 (March 1972).
17. G. I. Kerley, "Rational Function Method of Interpolation," Los Alamos Scientific Laboratory report LA-6903-MS (August 1977).
18. S. P. Marsh, Ed., LASL Shock Hugoniot Data (University of California Press, Berkeley, 1980).
19. J. D. Johnson and S. P. Lyon, "SES2D User's Manual," Los Alamos National Laboratory report LA-9164-M (April 1982).
20. M. S. Hoyt, "User's Manual for LASL Shock Hugoniot Data File," Los Alamos Scientific Laboratory report LA-7887-M (July 1979).
21. K. A. Gschneider, Solid State Physics 16, 275 (1964).
22. R. P. Feynman, N. Metropolis, and E. Teller, Phys. Rev. 75, 1561 (1949).
23. R. D. Cowan and J. Ashkin, Phys. Rev. 105, 144 (1957).

```
GRIZ I=AL / 10 .1
ATOM 13 /
ABAR 26.98154 /
RHOREF 2.7 /
ECOH .12 /
SHKFIT .537 1.29 0 /
EOS 1 2 3 4 /
WSES 3716 s3716 4 301 3 304 2 305 1 306 /
END /
 STOP
GRIZ      CTSS TIME    379.648      SECONDS
CPU=  366.152    SYS=      .045    I/O+MEMORY=     13.452

 ALL DONE
```

Figure 16-1-1. Sample GRIZZLY run to generate default aluminum EOS in example 1.

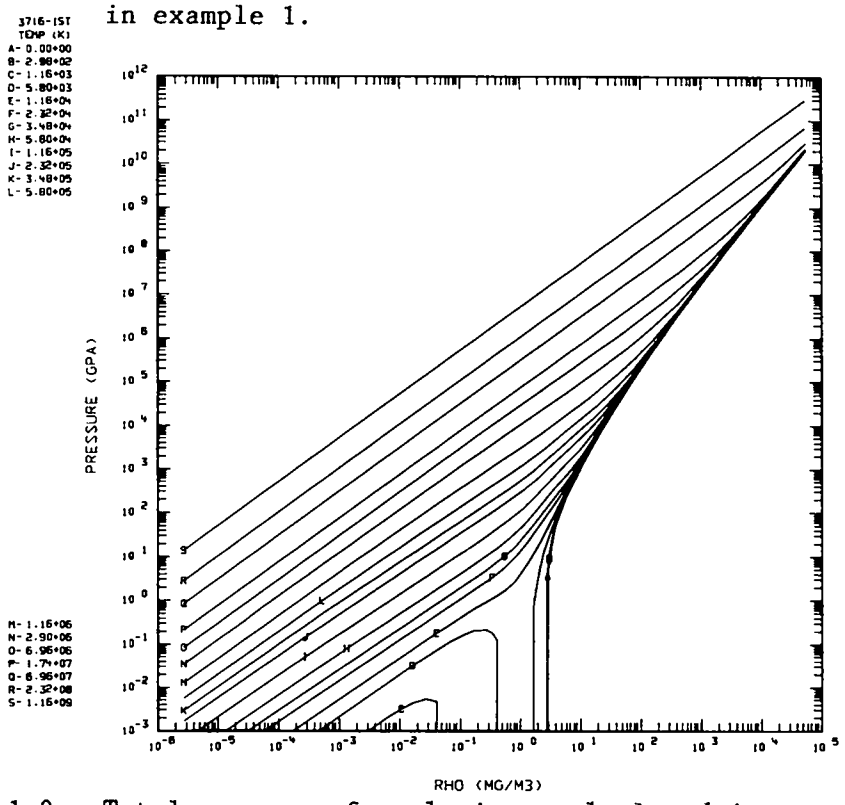


Figure 16-1-2. Total pressure for aluminum calculated in example 1. The pressure is plotted versus mass density for various temperatures.

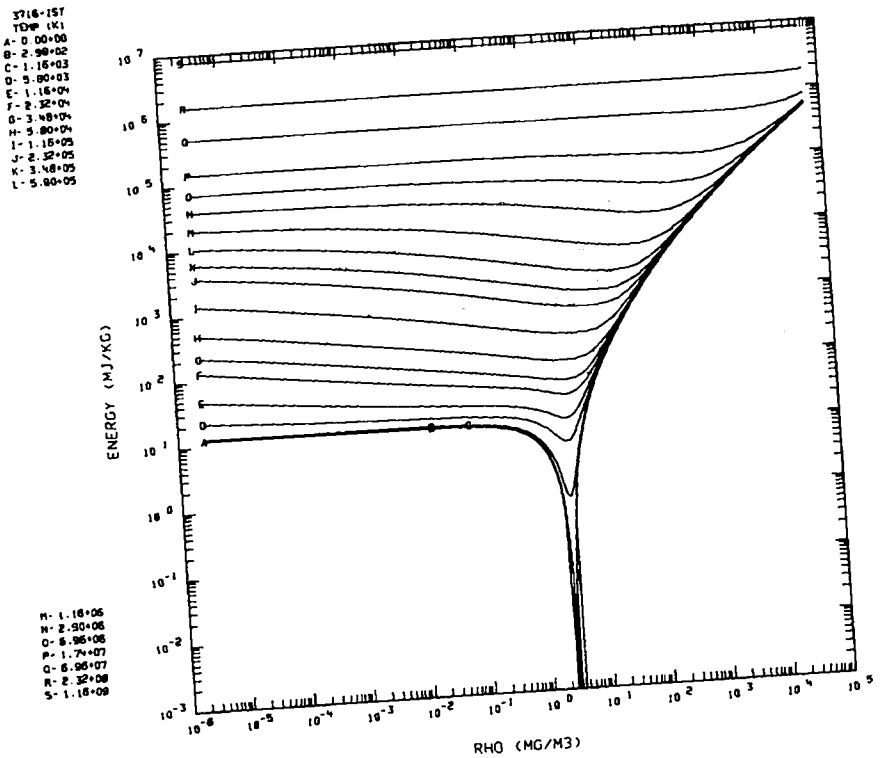


Figure 16-1-3. Total internal energy for aluminum calculated in example 1.

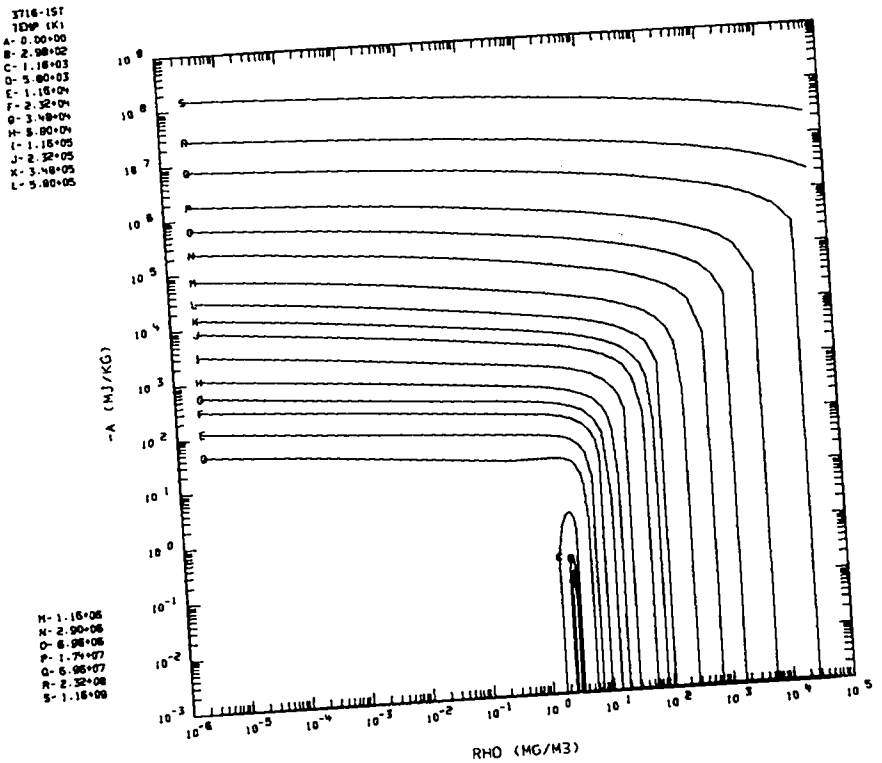


Figure 16-1-4. Total free energy for aluminum calculated in example 1.

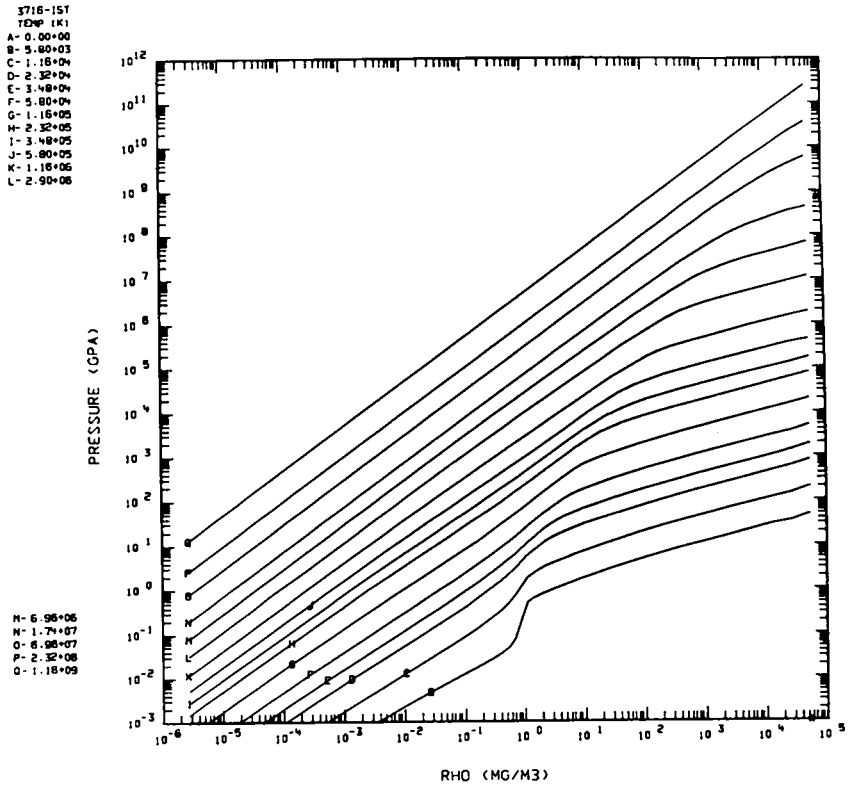


Figure 16-1-5. Thermal electronic contribution to the pressure for aluminum calculated in example 1.

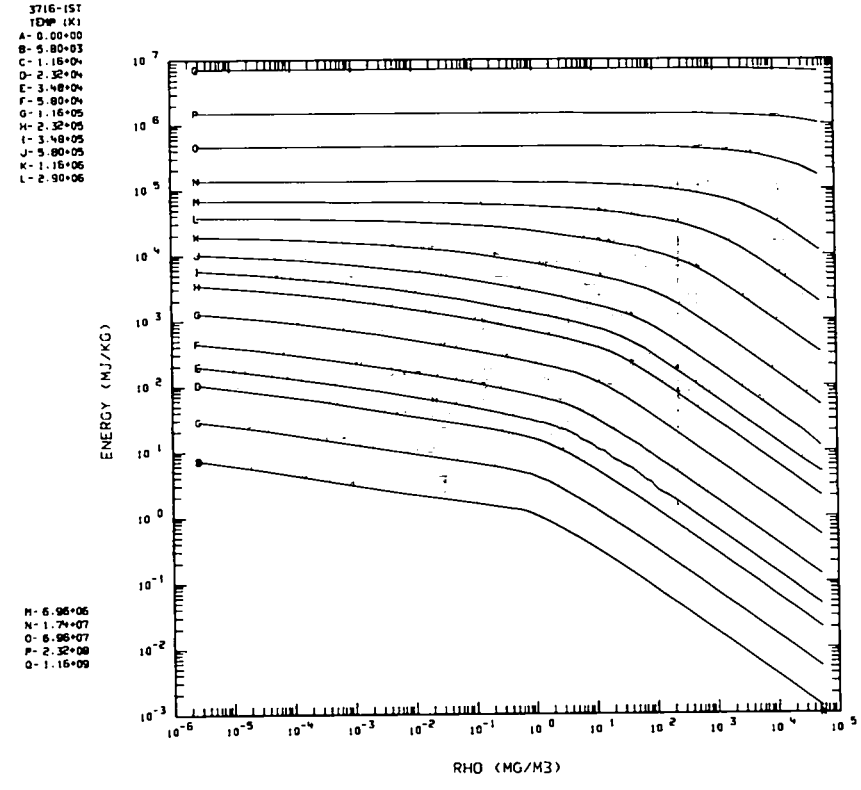


Figure 16-1-6. Thermal electronic contribution to the internal energy for aluminum calculated in example 1.

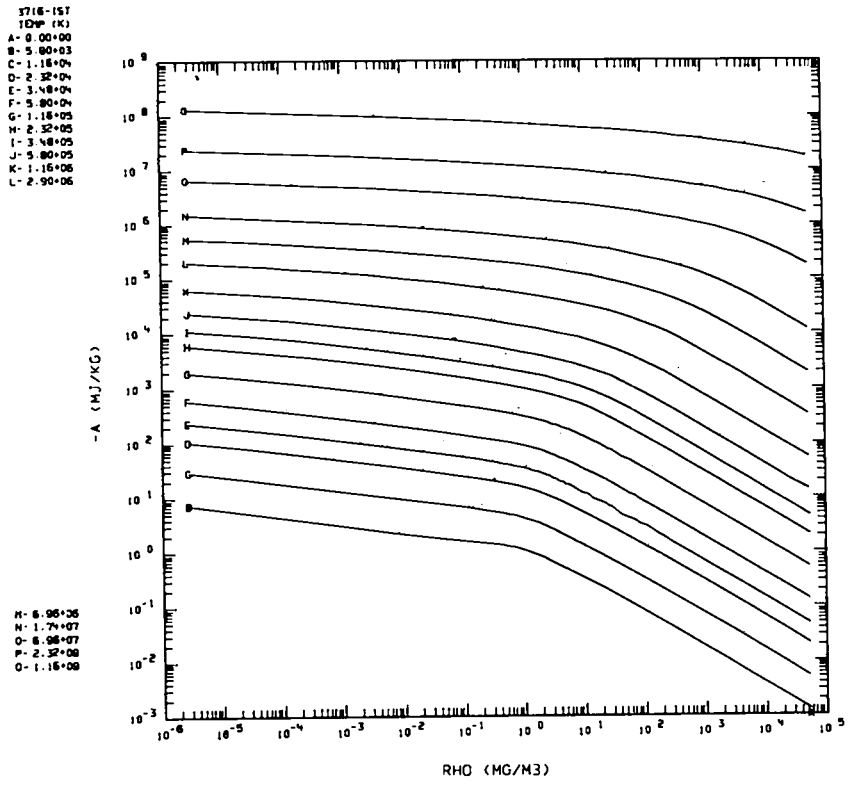


Figure 16-1-7. Thermal electronic contribution to the free energy for aluminum calculated in example 1.

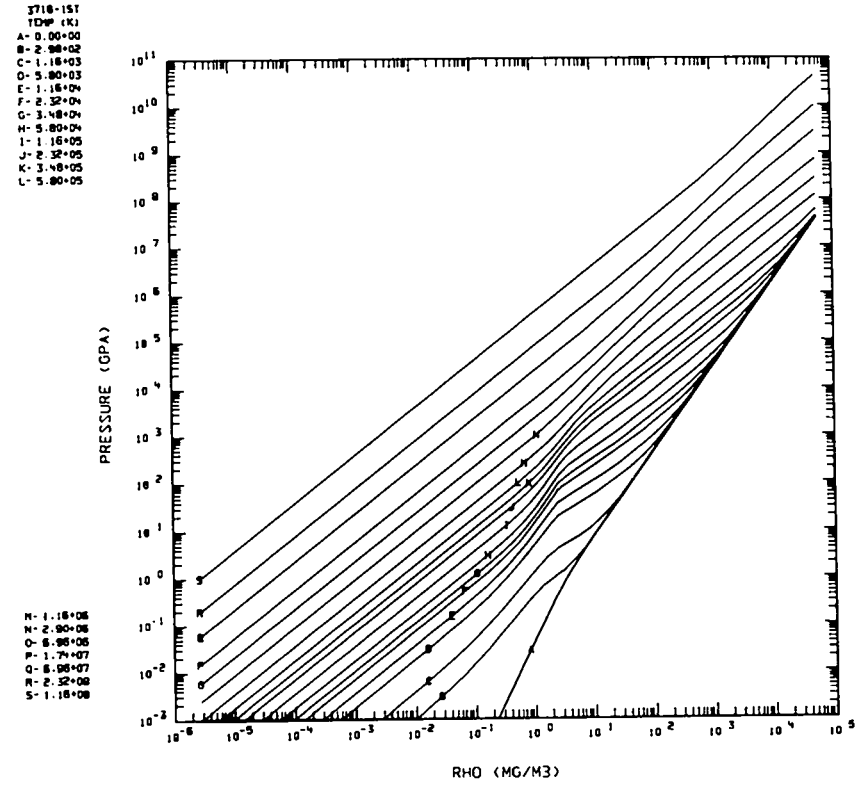


Figure 16-1-8. Nuclear contribution to the pressure for aluminum calculated in example 1.

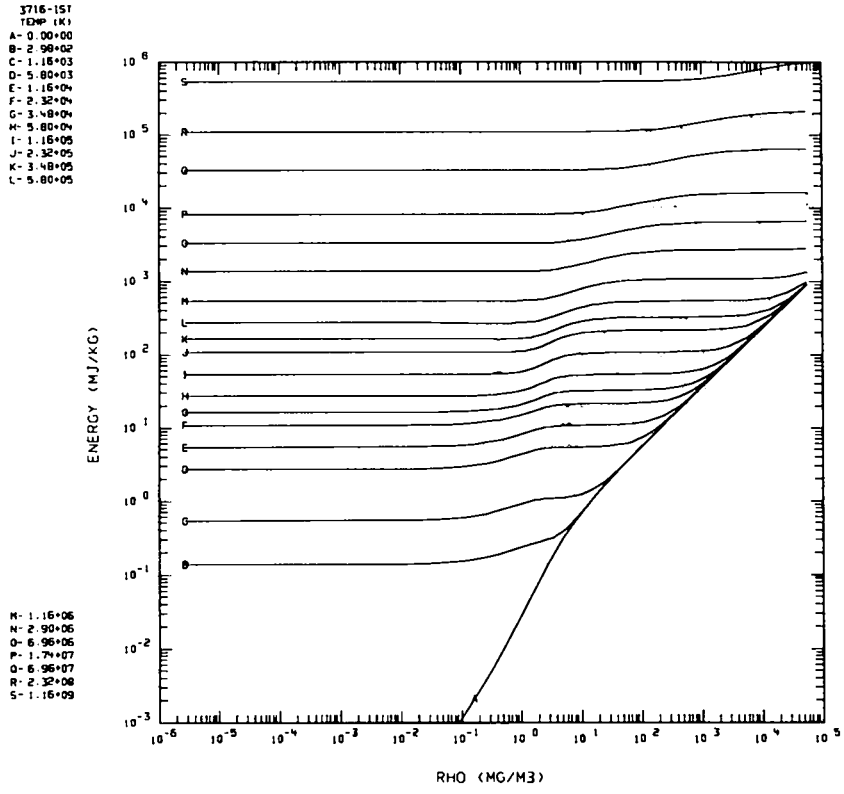
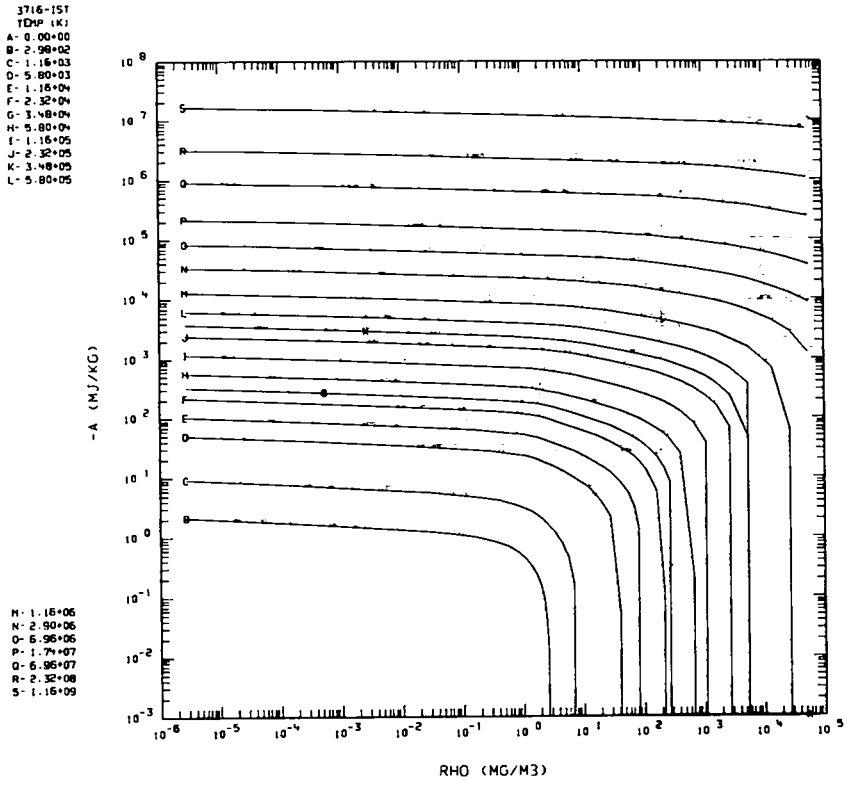


Figure 16-1-9. Nuclear contribution to the internal energy for aluminum calculated in example 1.



16-1-10. Nuclear contribution to the free energy for aluminum calculated in example 1.

```
GRIZ I=ALHUG
RSES 3716 s3716 1 301 /
HUG 1 E /
START      HUGONIOT
C     RH            TH            PH            EH            AH            UP            US
   2.721E+00   2.600E-02   6.188E-03   8.9c7E-06  -2.957E-03   4.234E-03   5.398E-01
   3.316E+00   5.000E-02   2.502E-01   8.608E-03   9.914E-04   1.312E-01   7.062E-01
   3.669E+00   1.000E-01   4.724E-01   2.310E-02   1.890E-03   2.149E-01   8.140E-01
   3.914E+00   1.500E-01   6.635E-01   3.811E-02   9.770E-04   2.761E-01   8.900E-01
   4.081E+00   2.000E-01   8.170E-01   5.121E-02  -3.873E-03   3.200E-01   9.455E-01
   4.200E+00   2.500E-01   9.411E-01   6.226E-02  -1.171E-02   3.529E-01   9.878E-01
   4.298E+00   3.000E-01   1.052E+00   7.241E-02  -2.153E-02   3.806E-01   1.024E+00
   4.382E+00   3.500E-01   1.155E+00   8.210E-02  -3.308E-02   4.052E-01   1.055E+00
   4.458E+00   4.000E-01   1.253E+00   9.148E-02  -4.579E-02   4.277E-01   1.085E+00
   4.527E+00   4.500E-01   1.347E+00   1.007E-01  -5.936E-02   4.487E-01   1.112E+00
   4.591E+00   5.000E-01   1.438E+00   1.097E-01  -7.356E-02   4.683E-01   1.137E+00
END /
 STOP
GRIZ      CTSS TIME        .378      SECONDS
CPU=      .061    SYS=      .035    I/O+MEMORY=       .282

 ALL DONE
```

Figure 16-2-1. Sample GRIZZLY run to access EOS tables written in example 1 and calculate the principal hugoniot.

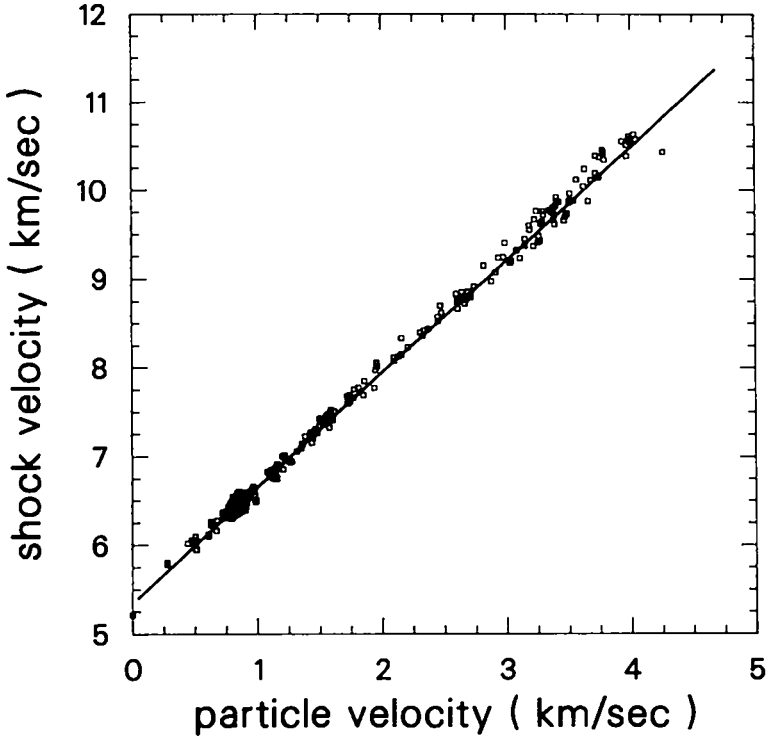


Figure 16-2-2. Comparison of the calculated aluminum hugoniot (solid line) of example 2 with experiment (Ref. 20) (squares).

```
GRIZ I=AG;F=PAG / 10 .1
ATOM 47 /
AMAS 107.868 /
RHOREF 10.49 /
PREF 1.0071 /
DEBYEL 221 /
GAMREF 2.46 /
IGRUN 1 /
ECOHPC 68.3 /
TSTFD 11 /
TSUP 1 101 1.0E9 /
CLIN 8 .1 1 /
CLINA 10 1 1.5 /
CLOGA 20 1.5 100 /
MODC MODMRE3 /
MODN VIRIAL GIRNUC /
LIST DATA /
```

---------- RAW DATA ----------

ZMAS	47.00000	AMAS	107.86800
ALPHA	6.6667E-01	IGRUN	1
RHOREF	1.0490E+01	GAMREF	2.4600E+00
DEBREF	1.9044E-02	CVIB	1.0000E+00
DVIB	1.0000E-03	TSTFD	1.1000E+01
CL36	2.0000E+00	CL3Y	1.0000E+02
TMELT	0.0000E+00		
RCOLD	0.0000E+00	ECOLD	0.0000E+00
TREF	2.5692E-02	C0	0.0000E+00
S1	0.0000E+00	S2	0.0000E+00
CMAT	1.5000E+00	CLJ	1.0000E+00
FACLJ	1.0000E+00	ECOH	2.6492E-02
PREF	1.0071E+00	MODC	MODMRE3
MODN(1)	VIRIAL	MODN(2)	GIRNUC
MODE	TFD	EPSMIX	1.0000E-06
NU	0		

```
LIST GRIDE /
```

TEV 25

0.0000E+00	1.2500E-02	2.5692E-02	5.0000E-02
1.0000E-01	2.5000E-01	5.0000E-01	7.5000E-01
1.0000E+00	1.5000E+00	2.0000E+00	2.5000E+00
3.0000E+00	4.0000E+00	5.0000E+00	8.0000E+00
1.0000E+01	1.5000E+01	2.0000E+01	2.5000E+01
3.0000E+01	4.0000E+01	5.0000E+01	8.0000E+01
1.0000E+02			

COMF 36

1.0000E-01	2.2857E-01	3.5714E-01	4.8571E-01
6.1429E-01	7.4286E-01	8.7143E-01	1.0000E+00
1.0556E+00	1.1111E+00	1.1667E+00	1.2222E+00
1.2778E+00	1.3333E+00	1.3889E+00	1.4444E+00
1.5000E+00	1.8711E+00	2.3339E+00	2.9112E+00
3.6314E+00	4.5297E+00	5.6502E+00	7.0479E+00
8.7913E+00	1.0966E+01	1.3679E+01	1.7062E+01
2.1283E+01	2.6548E+01	3.3115E+01	4.1307E+01
5.1525E+01	6.4270E+01	8.0169E+01	1.0000E+02

```
EOS 4 3 2 1 /
USES 4000 SILVER 1 301 2 304 3 305 4 306 /
DUNITS * 11604.85 100 100 10 /
THLIN 40 300 5000 /
HUG 1 P /
END /
 STOP
GRIZ      CTSS TIME     98.714      SECONDS
CPU=    94.509    SYS=      .052    I/O+MEMORY=      4.153

 ALL DONE
```

Figure 16-3-1. Sample GRIZZLY run to calculate the silver EOS of example 3.

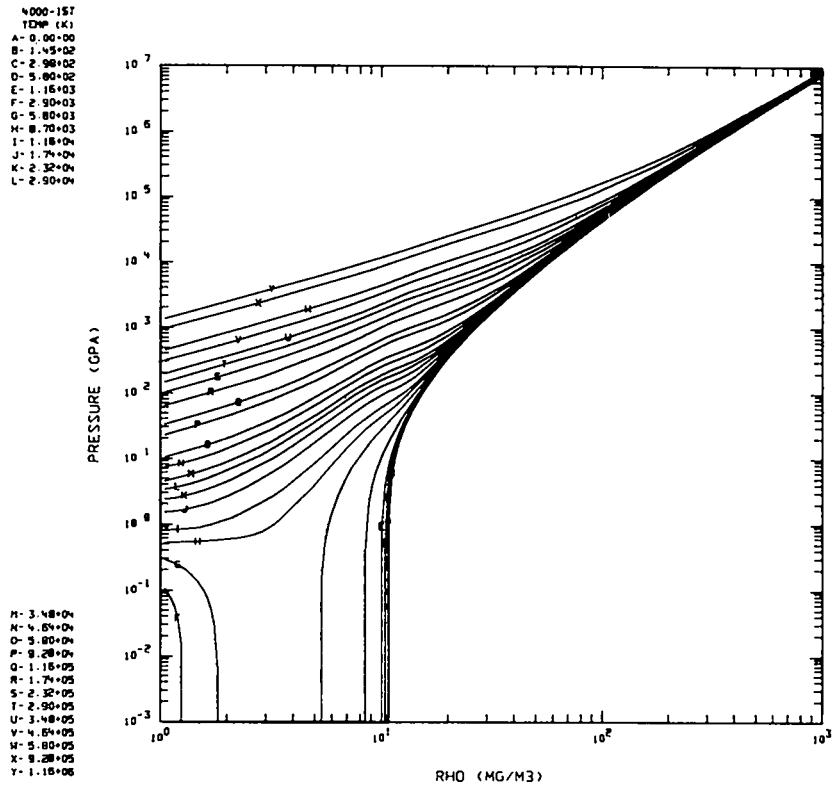


Figure 16-3-2. Total pressure for silver calculated in example 3.

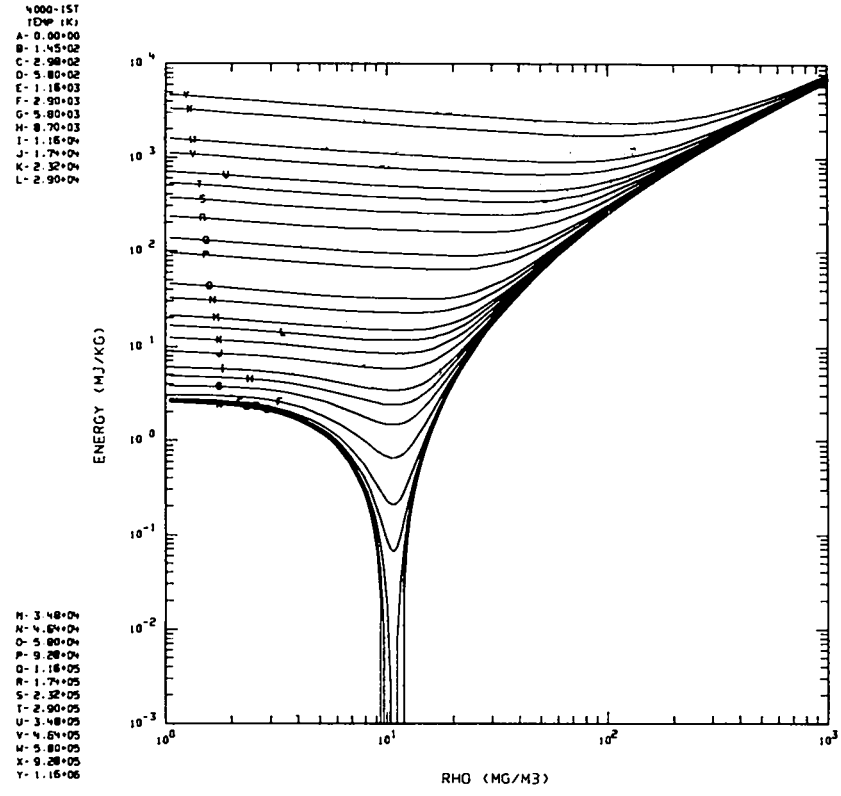


Figure 16-3-3. Total internal energy for silver calculated in example 3.

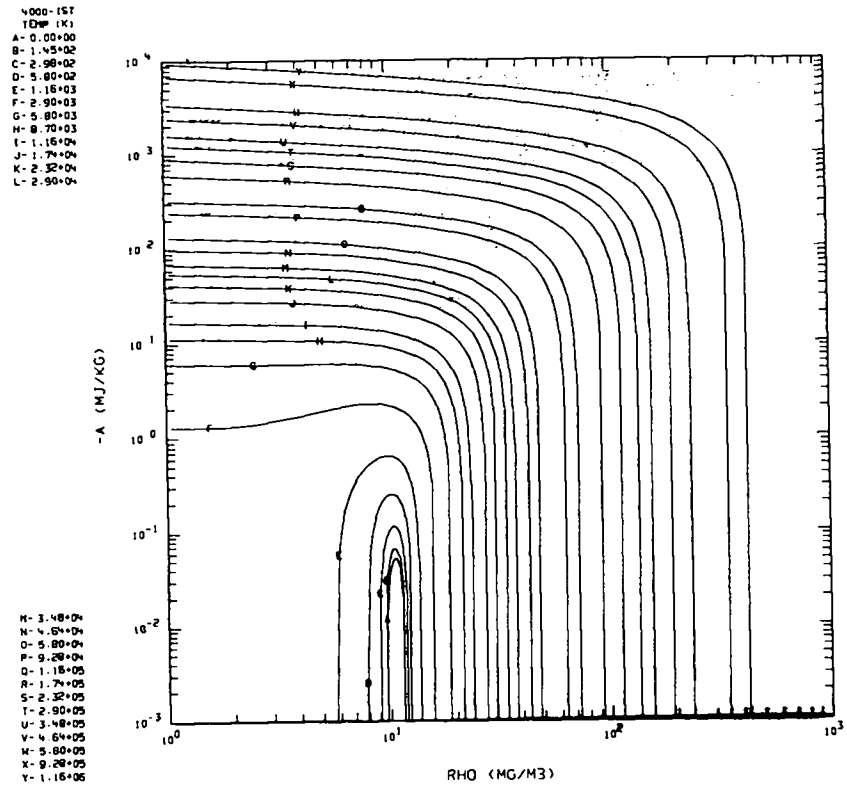


Figure 16-3-4. Total free energy for silver calculated in example 3.

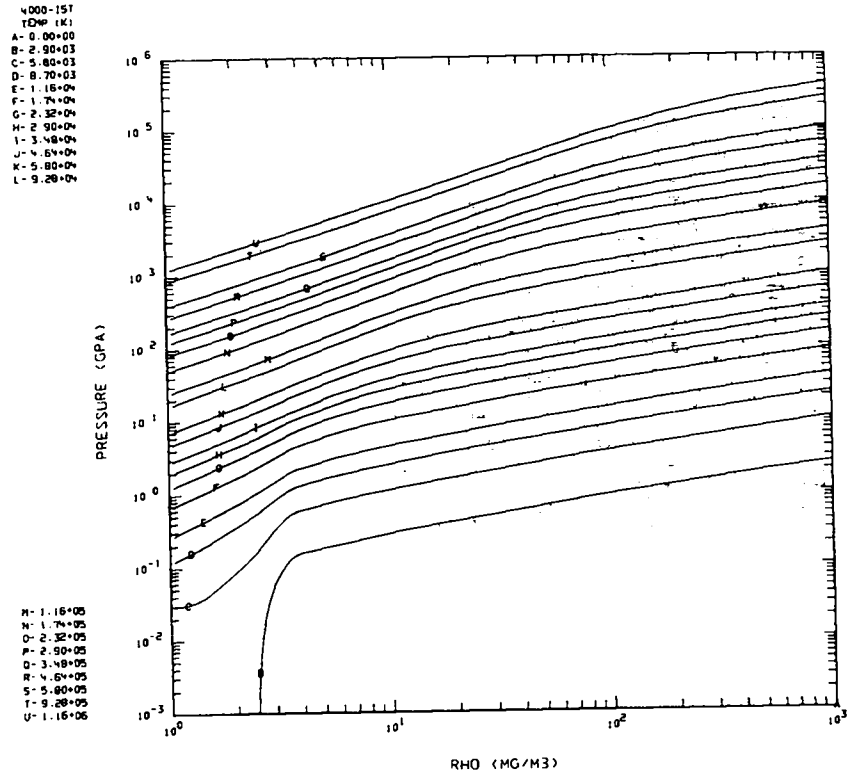


Figure 16-3-5. Thermal electronic contribution to the pressure for silver calculated in example 3.

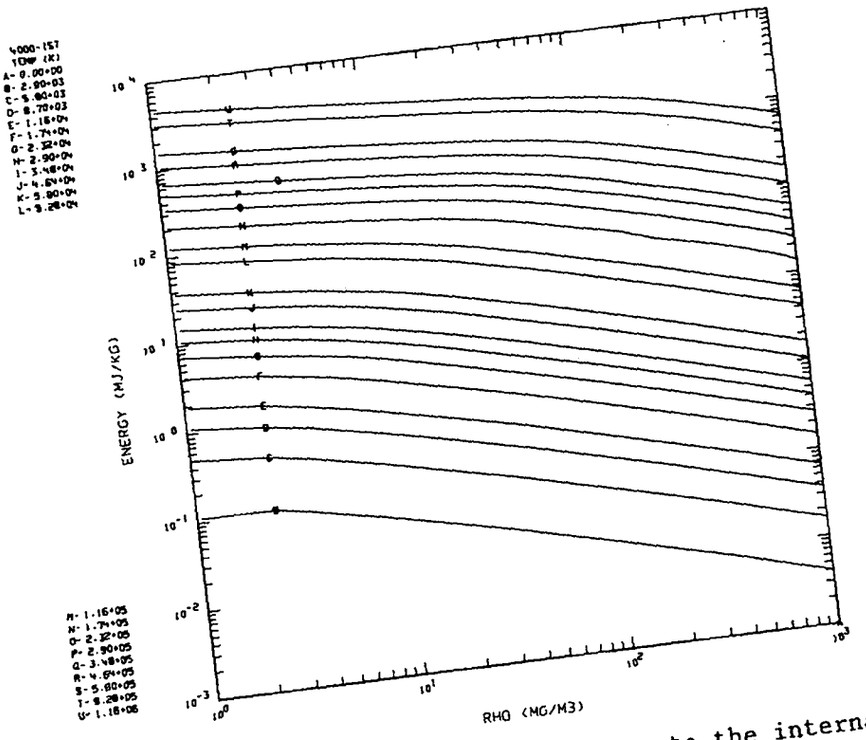


Figure 16-3-6. Thermal electronic contribution to the internal energy for silver calculated in example 3.

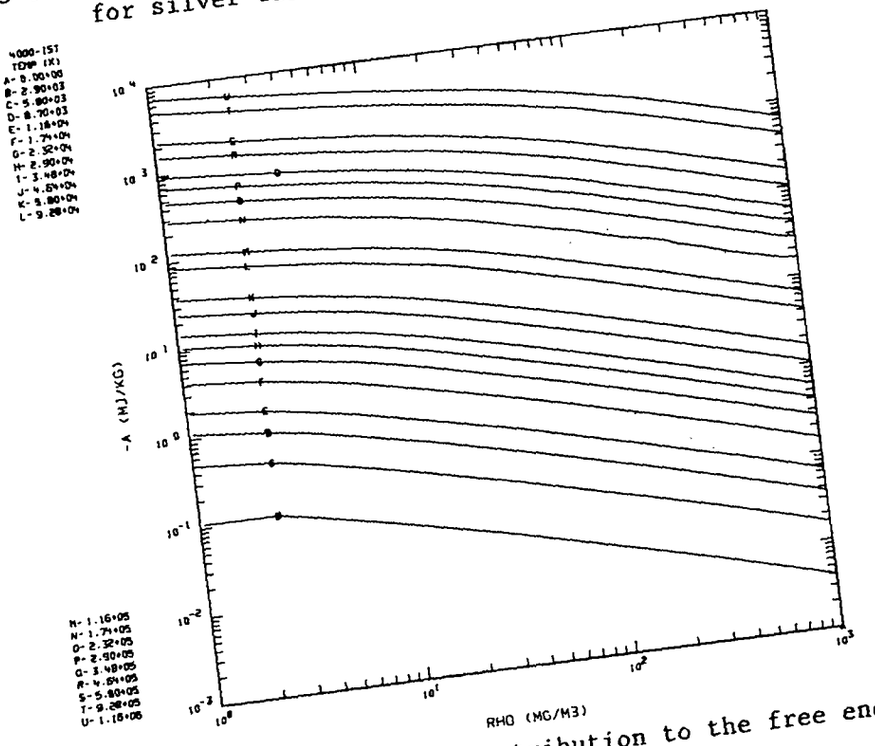


Figure 16-3-7. Thermal electronic contribution to the free energy for silver calculated in example 3.

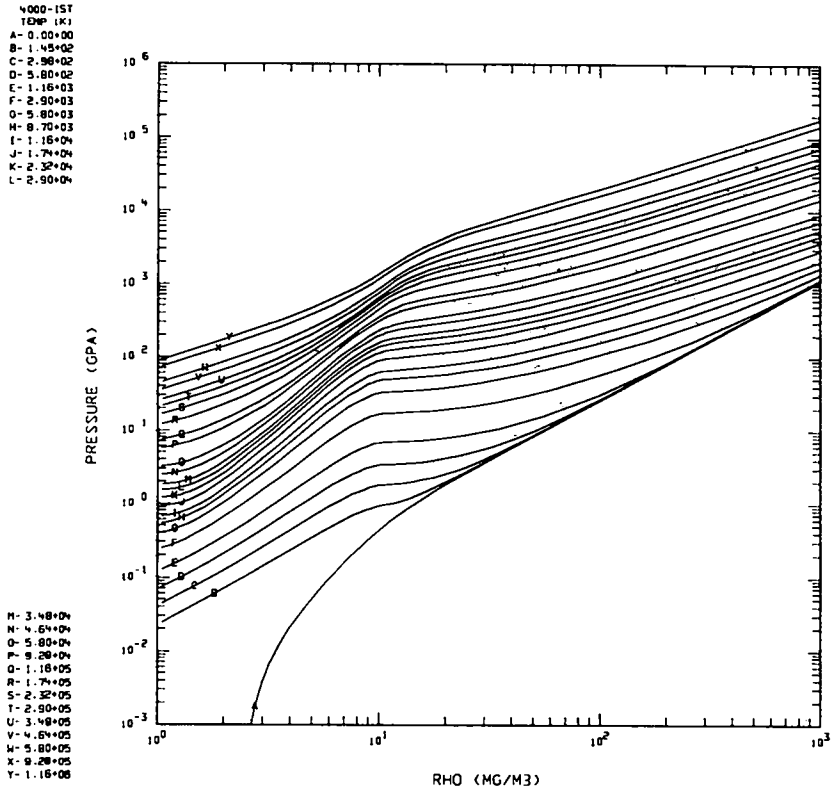


Figure 16-3-8. Nuclear contribution to the pressure for silver in example 3.

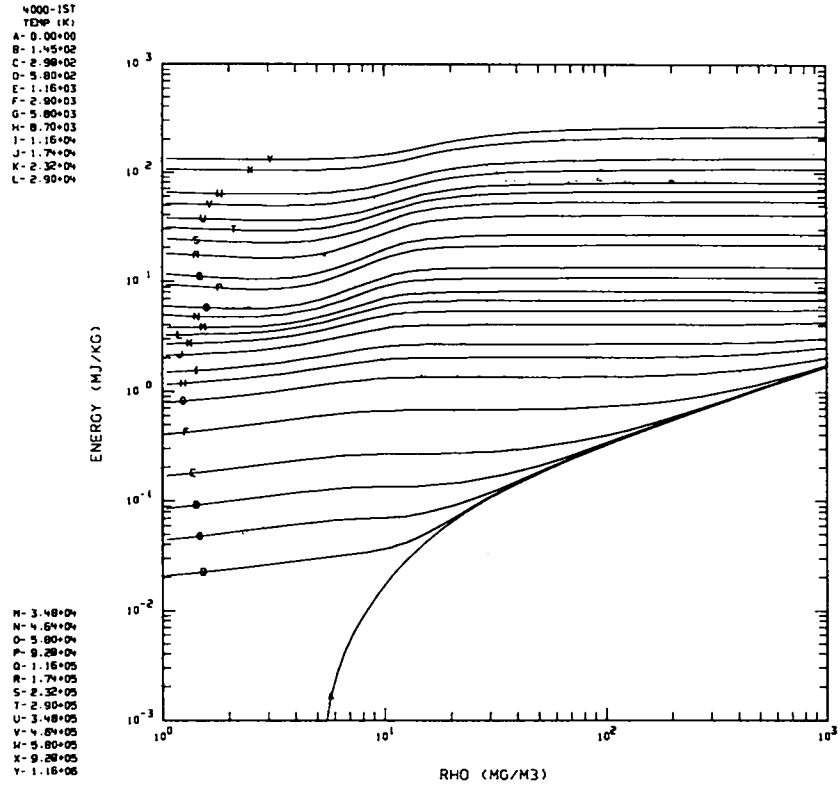


Figure 16-3-9. Nuclear contribution to the internal energy for silver in example 3.

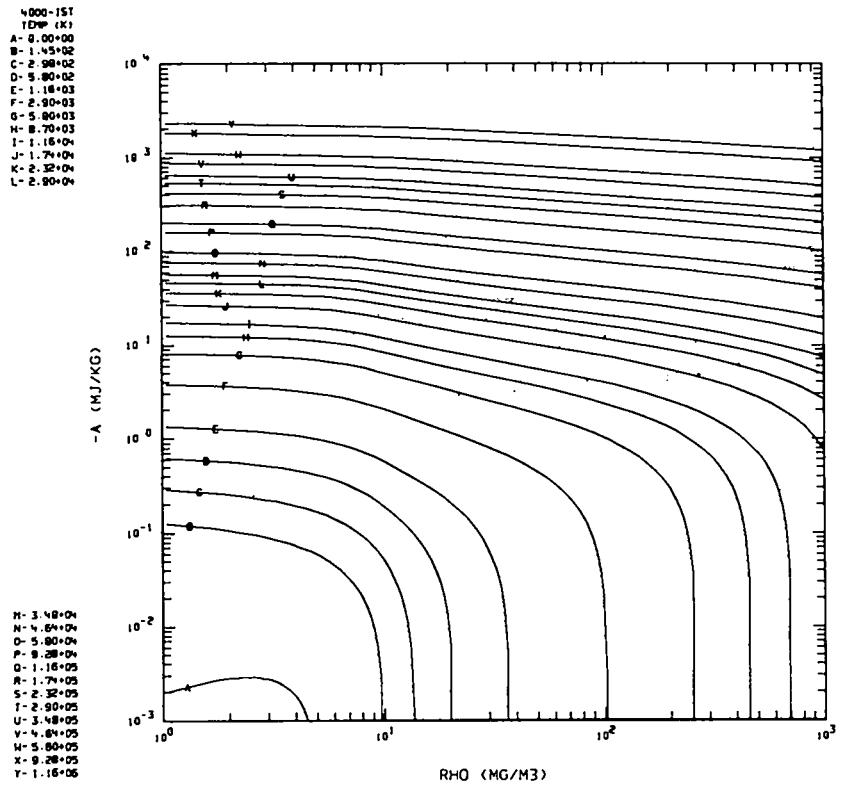


Figure 16-3-10. Nuclear contribution to the free energy for silver in example 3.

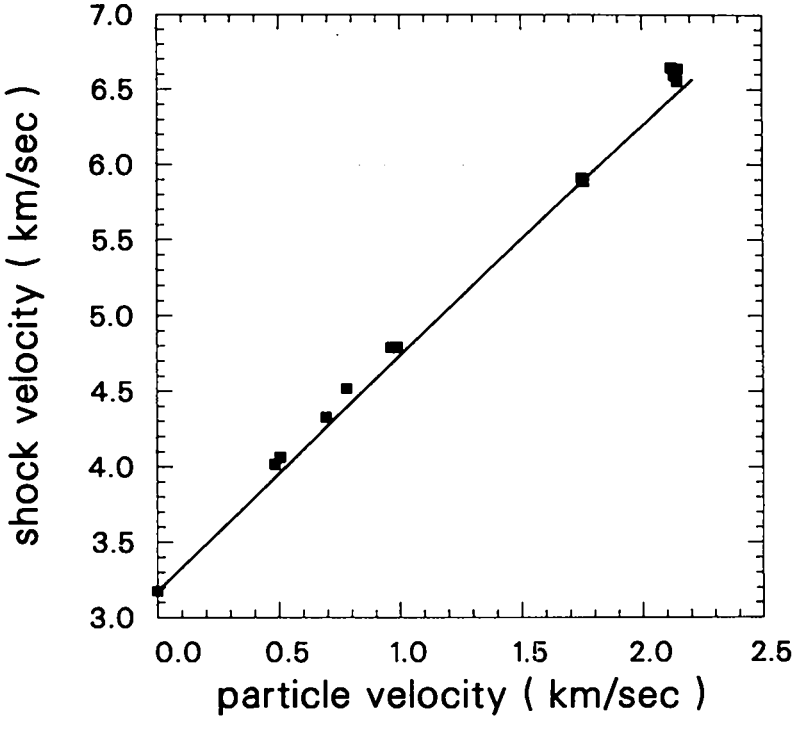


Figure 16-3-11. Comparison of the calculated silver hugioniot (solid line) of example 3 with experiment (Ref. 18) (squares).

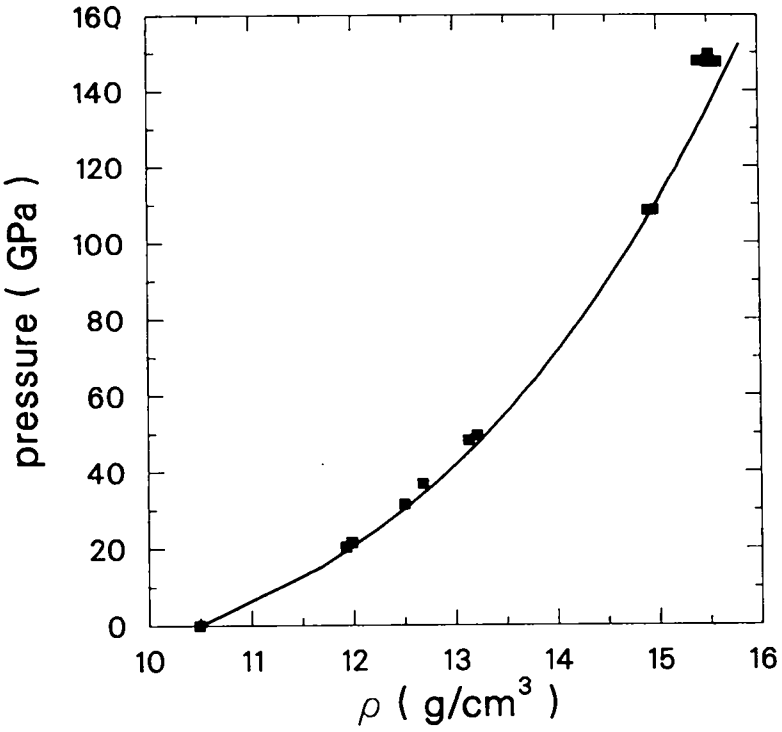


Figure 16-3-12. Comparison of the calculated silver hugoniot (solid line) of example 3 with experiment (Ref. 18) (squares). Pressure is plotted versus mass density.

```
GRIZ I=BEO,P=PBEO / 10 .1
MIXTURE N 1 4 9.01218 1.85 1 8 15.9994 1.426 /
RHOREF 2.989 /
MCTPD 2 /
ECOH .1 /
USUP 0 .8437 .03 1.05 .18 1.05 .2822 1.2054 /
MODC CHUGT /
EOSMX 1 /
SRTAB 3.0E3 3.0E10 /
SUP 1 5 /
COPTAB 5 1 /
SUP 2 5 /
COPTAB 5 2 /
SUP 3 5 /
COPTAB 5 3 /
SUP 4 5 /
COPTAB 5 4 /
WEES 6020 s6020 4 301 3 304 2 305 1 306 /
THLIN 30 .026 .1 /
HUG 4 P /
END /
 STOP
GRIZ      CTSS TIME    411.430      SECONDS
CPU=  396.428    SYS=      .051    I/O+MEMORY=     14.951

 ALL DONE
```

Figure 16-4-1. Sample run of GRIZZLY to calculate a beryllium oxide EOS.

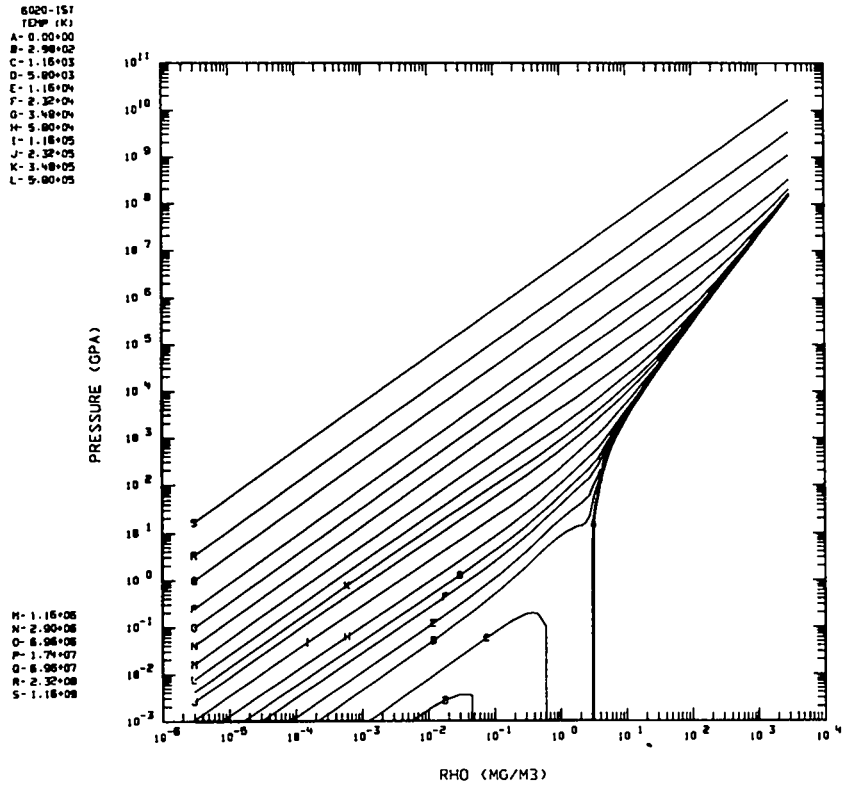


Figure 16-4-2. Total pressure for BeO calculated in example 4.

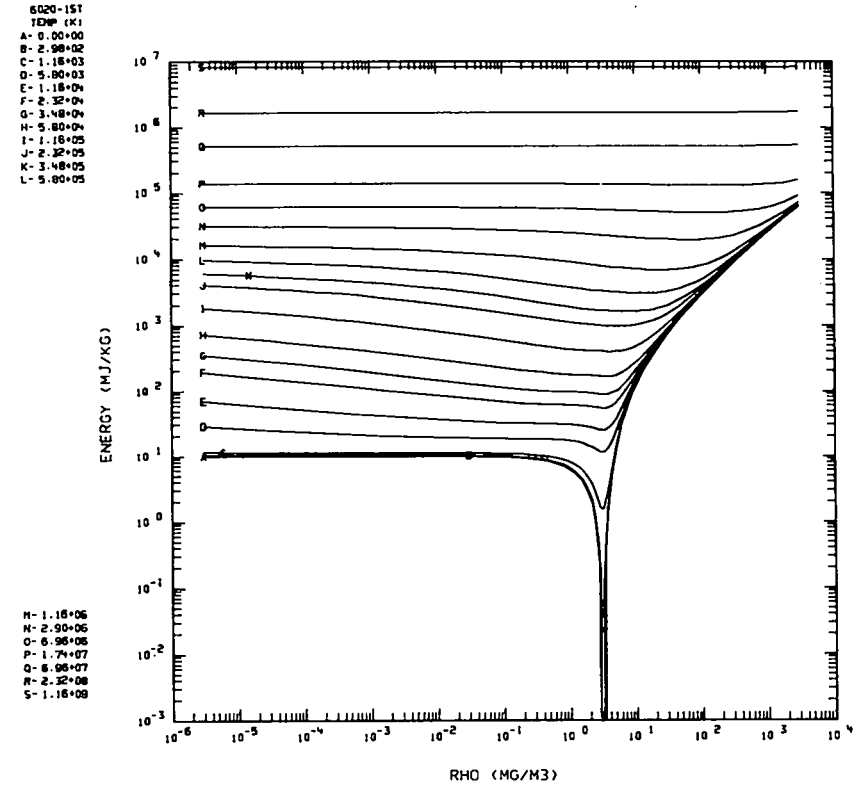


Figure 16-4-3. Total internal energy for BeO calculated in example 4.

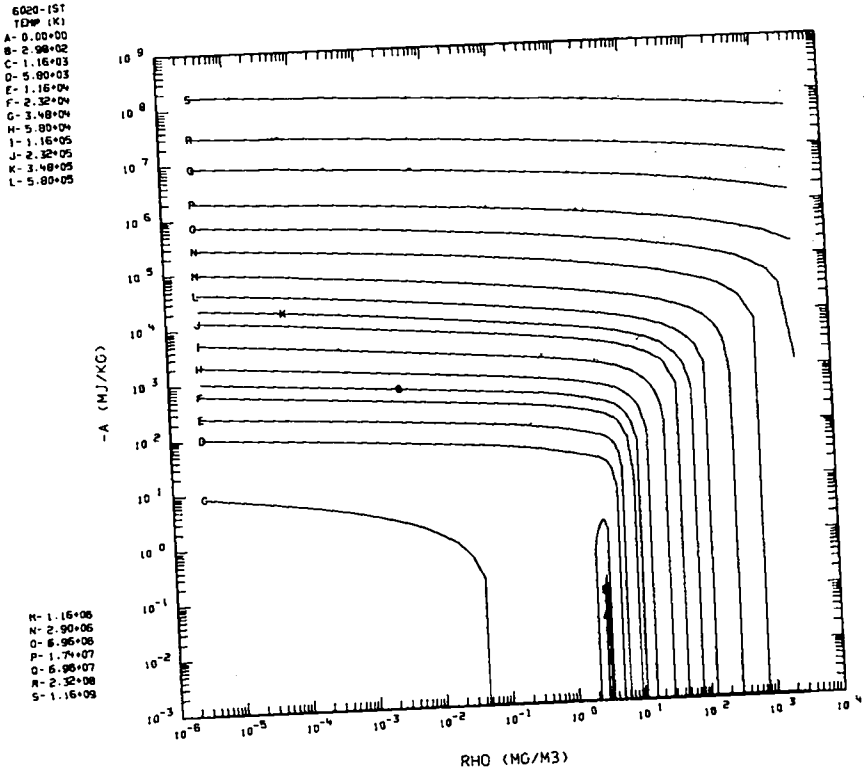


Figure 16-4-4. Total free energy for BeO calculated in example 4.

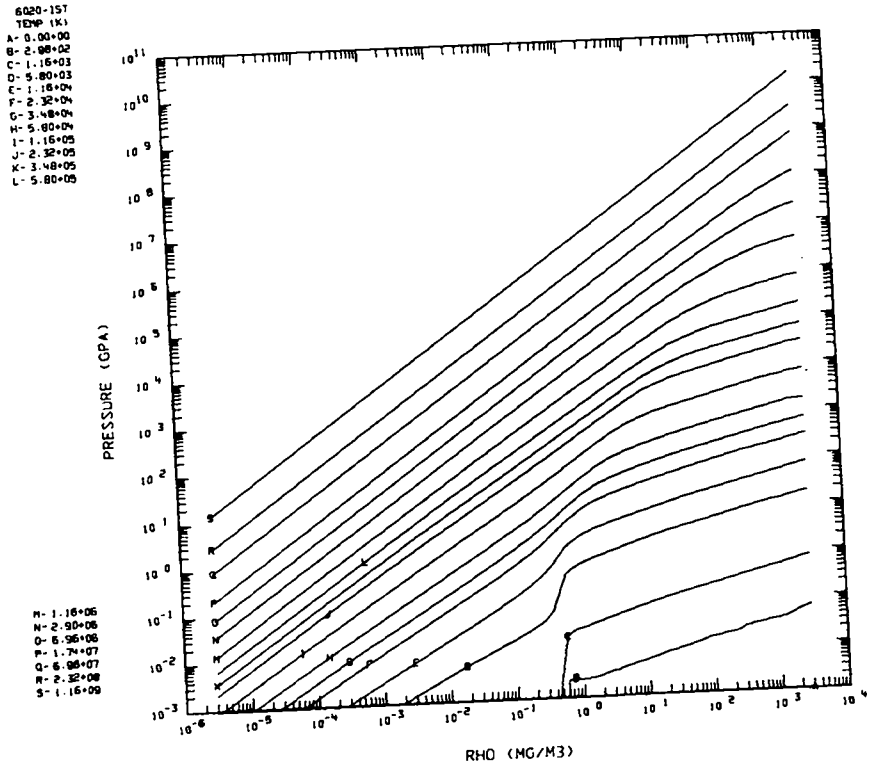


Figure 16-4-5. Thermal electronic contribution to pressure for BeO calculated in example 4.

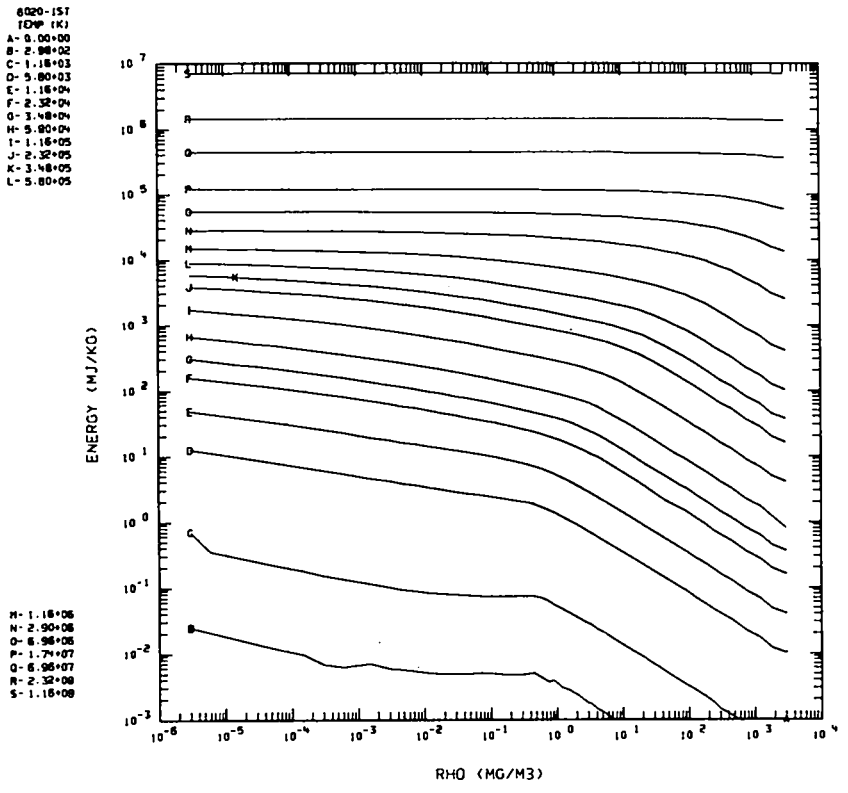


Figure 16-4-6. Thermal electronic contribution to internal energy for BeO calculated in example 4.

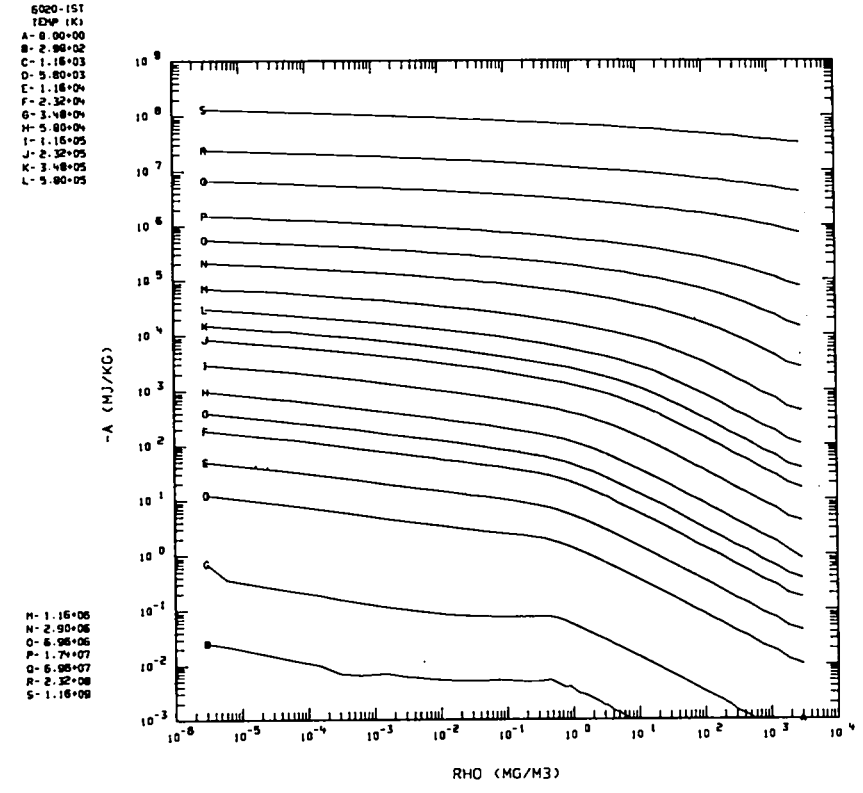


Figure 16-4-7. Thermal electronic contribution to free energy for BeO calculated in example 4.

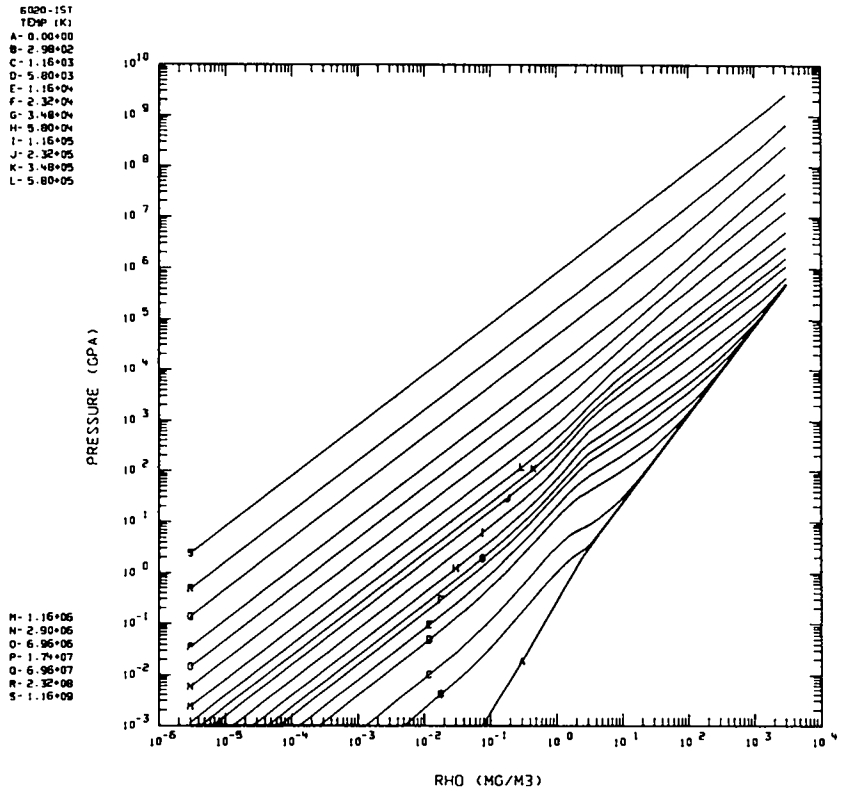


Figure 16-4-8. Nuclear contribution to pressure for BeO calculated in example 4.

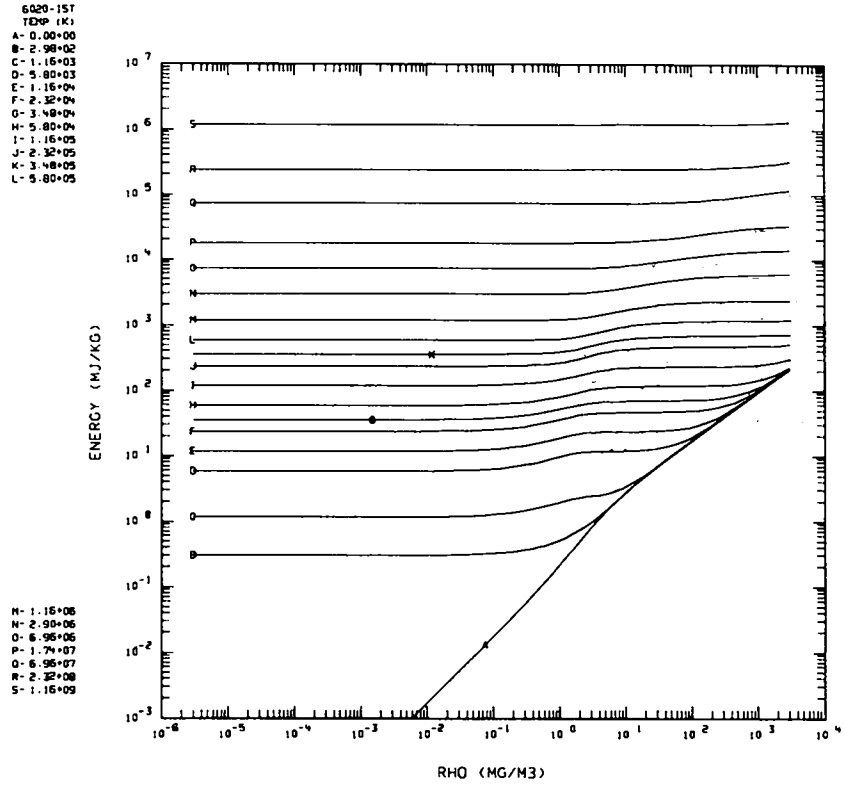


Figure 16-4-9. Nuclear contribution to internal energy for BeO calculated in example 4.

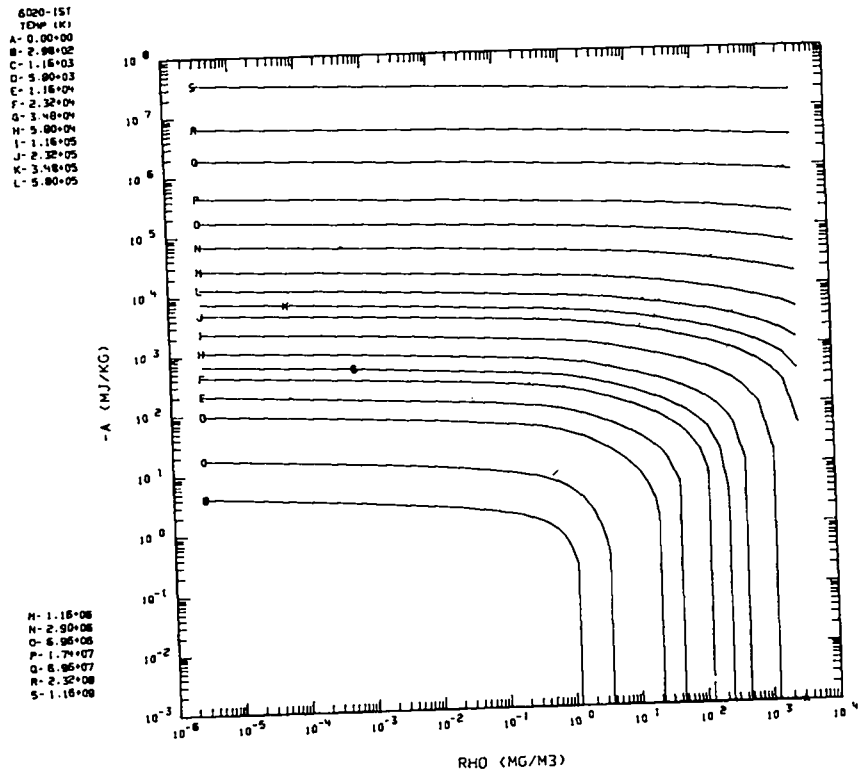


Figure 16-4-10. Nuclear contribution to free energy for BeO calculated in example 4.

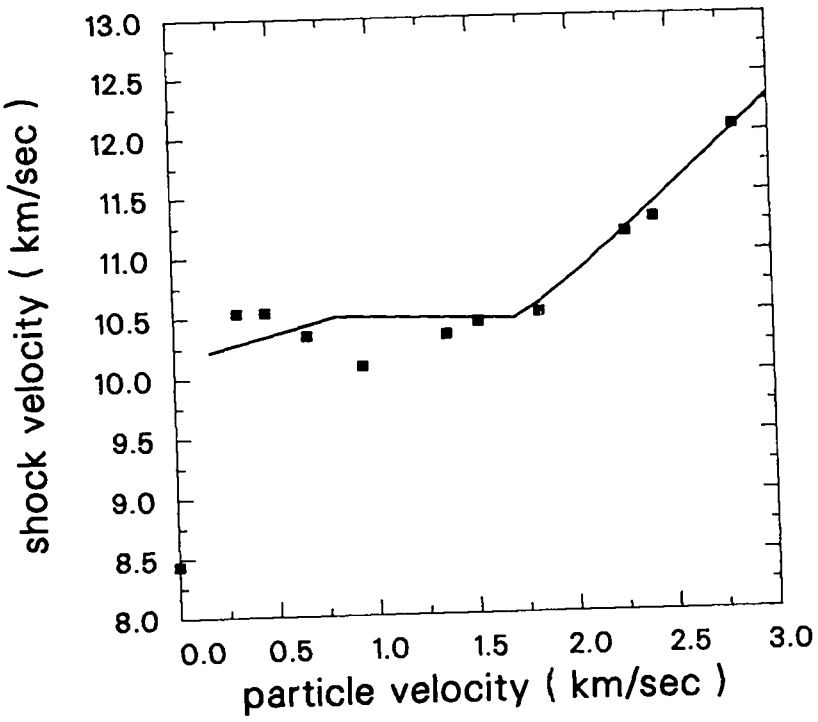


Figure 16-4-11. Comparison of the calculated BeO hugoniot (solid line) of example 4 with experiment (Ref. 18) (squares).

```
GRIZ I=MOFE / 1 1
RSES 2980 SESAME 1 301 /
RSES 2140 SESAME 2 301 /
TGRD 1 /
AVMIX N 1 .5 2 .5 3 /
PPMIX N 1 .5 2 .5 4 /
IDMIX N 1 .5 2 .5 5 /
P 3 .1 100 ◆ ◆ AV /
P 4 .1 100 ◆ ◆ PP /
P 5 .1 100 ◆ ◆ ID /
END /
 STOP
GRIZ      CTSS TIME      1.344      SECONDS
CPU=      .964    SYS=      .040    I/O+MEMORY=      .339

 ALL DONE
```

Figure 16-5-1. Sample run of GRIZZLY to calculate mixture of iron and molybdenum using various schemes at a temperature of 1 eV.

```
C EOS TABLE FOR   Z,A,R0=    34.00000  75.89500   9.18796
START     T(EV) =      1.000           AV
C      R              T              P              E              A
   1.37819E-01   1.00000E+00   1.96752E-03   1.13081E-01   0.00000E+00
   2.29699E-01   1.00000E+00   3.29324E-03   1.13034E-01   0.00000E+00
   3.67518E-01   1.00000E+00   3.83052E-03   1.12940E-01   0.00000E+00
   5.51278E-01   1.00000E+00   4.65330E-03   7.51858E-02   0.00000E+00
   9.18796E-01   1.00000E+00   8.96399E-03   7.45399E-02   0.00000E+00
   1.14850E+00   1.00000E+00   1.20354E-02   7.41505E-02   0.00000E+00
   1.37819E+00   1.00000E+00   1.52690E-02   7.37423E-02   0.00000E+00
   1.83759E+00   1.00000E+00   2.22345E-02   7.28101E-02   0.00000E+00
   2.29699E+00   1.00000E+00   2.93036E-02   7.16876E-02   0.00000E+00
   2.75639E+00   1.00000E+00   3.62768E-02   7.03432E-02   0.00000E+00
   3.67518E+00   1.00000E+00   4.98639E-02   6.69285E-02   0.00000E+00
   4.59398E+00   1.00000E+00   6.66580E-02   6.25712E-02   0.00000E+00
   5.51278E+00   1.00000E+00   9.59077E-02   5.74423E-02   0.00000E+00
   6.43157E+00   1.00000E+00   1.54447E-01   5.21182E-02   0.00000E+00
   7.35037E+00   1.00000E+00   2.59208E-01   4.75288E-02   0.00000E+00
   8.26916E+00   1.00000E+00   4.23434E-01   4.44333E-02   0.00000E+00
   8.72856E+00   1.00000E+00   5.28069E-01   4.36160E-02   0.00000E+00
   9.18796E+00   1.00000E+00   6.48361E-01   4.33231E-02   0.00000E+00
   9.64736E+00   1.00000E+00   7.85910E-01   4.35619E-02   0.00000E+00
   1.01068E+01   1.00000E+00   9.15300E-01   4.42450E-02   0.00000E+00
   1.10256E+01   1.00000E+00   1.20301E+00   4.67073E-02   0.00000E+00
   1.28631E+01   1.00000E+00   2.09800E+00   5.78799E-02   0.00000E+00
   1.47007E+01   1.00000E+00   3.38160E+00   7.64919E-02   0.00000E+00
   1.65383E+01   1.00000E+00   5.05644E+00   1.01701E-01   0.00000E+00
   1.83759E+01   1.00000E+00   7.14876E+00   1.32877E-01   0.00000E+00
   2.29699E+01   1.00000E+00   1.43685E+01   2.33765E-01   0.00000E+00
   2.75639E+01   1.00000E+00   2.46644E+01   3.62910E-01   0.00000E+00
   3.21579E+01   1.00000E+00   3.82831E+01   5.16009E-01   0.00000E+00
   3.67518E+01   1.00000E+00   5.54220E+01   6.89804E-01   0.00000E+00
   4.59398E+01   1.00000E+00   1.00874E+02   1.08983E+00   0.00000E+00
   5.51278E+01   1.00000E+00   1.62006E+02   1.54784E+00   0.00000E+00
   6.43157E+01   1.00000E+00   2.39519E+02   2.05338E+00   0.00000E+00
   7.35037E+01   1.00000E+00   3.33936E+02   2.59869E+00   0.00000E+00
   8.26916E+01   1.00000E+00   4.45730E+02   3.17800E+00   0.00000E+00
   9.18796E+01   1.00000E+00   5.75391E+02   3.78704E+00   0.00000E+00
```

Figure 16-5-2. Printed output generated in example 5.

```
C EOS TABLE FOR   Z,A,R0=   34.00000  75.89500  17.23489
START     T(EV) =      1.000          PP
C      R              T              P              E              A
   1.03409E-01   1.00000E+00   1.37657E-03   1.13089E-01   0.00000E+00
   1.72349E-01   1.00000E+00   2.36111E-03   1.13088E-01   0.00000E+00
   2.58523E-01   1.00000E+00   3.66526E-03   1.13083E-01   0.00000E+00
   4.30872E-01   1.00000E+00   6.31307E-03   1.13052E-01   0.00000E+00
   6.89395E-01   1.00000E+00   9.58188E-03   1.12916E-01   0.00000E+00
   1.03409E+00   1.00000E+00   1.32375E-02   1.12511E-01   0.00000E+00
   1.72349E+00   1.00000E+00   2.10889E-02   1.10902E-01   0.00000E+00
   2.15436E+00   1.00000E+00   2.60698E-02   1.09415E-01   0.00000E+00
   2.58523E+00   1.00000E+00   3.07911E-02   1.07635E-01   0.00000E+00
   3.44698E+00   1.00000E+00   3.94931E-02   1.03380E-01   0.00000E+00
   4.30872E+00   1.00000E+00   4.71865E-02   9.85149E-02   0.00000E+00
   5.17047E+00   1.00000E+00   5.40938E-02   9.32646E-02   0.00000E+00
   6.89395E+00   1.00000E+00   6.91613E-02   8.25270E-02   0.00000E+00
   8.61744E+00   1.00000E+00   8.91911E-02   7.22048E-02   0.00000E+00
   1.03409E+01   1.00000E+00   1.20088E-01   6.29940E-02   0.00000E+00
   1.20644E+01   1.00000E+00   1.71142E-01   5.53635E-02   0.00000E+00
   1.37879E+01   1.00000E+00   3.46503E-01   4.96283E-02   0.00000E+00
   1.55114E+01   1.00000E+00   6.58223E-01   4.60150E-02   0.00000E+00
   1.63731E+01   1.00000E+00   8.64037E-01   4.50578E-02   0.00000E+00
   1.72349E+01   1.00000E+00   1.09288E+00   4.46779E-02   0.00000E+00
   1.80966E+01   1.00000E+00   1.35216E+00   4.48546E-02   0.00000E+00
   1.89584E+01   1.00000E+00   1.64293E+00   4.55679E-02   0.00000E+00
   2.06819E+01   1.00000E+00   2.32241E+00   4.85310E-02   0.00000E+00
   2.41288E+01   1.00000E+00   3.93662E+00   6.00517E-02   0.00000E+00
   2.75758E+01   1.00000E+00   6.20281E+00   7.78833E-02   0.00000E+00
   3.10228E+01   1.00000E+00   9.13147E+00   1.01767E-01   0.00000E+00
   3.44698E+01   1.00000E+00   1.27973E+01   1.31123E-01   0.00000E+00
   4.30872E+01   1.00000E+00   2.54259E+01   2.25664E-01   0.00000E+00
   5.17047E+01   1.00000E+00   4.34646E+01   3.46381E-01   0.00000E+00
   6.03221E+01   1.00000E+00   6.73663E+01   4.89436E-01   0.00000E+00
   6.89395E+01   1.00000E+00   9.74969E+01   6.51918E-01   0.00000E+00
   8.61744E+01   1.00000E+00   1.77590E+02   1.02637E+00   0.00000E+00
```

Figure 16-5-2.(continued).

```
C EOS TABLE FOR   Z,A,R0=   34.00000  75.89500   8.61744
START     T(EV) =      1.000          ID
C     R              T              P              E              A
  1.29262E-01   1.00000E+00   1.83263E-03   1.13083E-01   0.00000E+00
  2.15436E-01   1.00000E+00   3.15654E-03   1.13052E-01   0.00000E+00
  3.44698E-01   1.00000E+00   4.79094E-03   1.12916E-01   0.00000E+00
  5.17047E-01   1.00000E+00   6.61874E-03   1.12511E-01   0.00000E+00
  8.61744E-01   1.00000E+00   1.05445E-02   1.10902E-01   0.00000E+00
  1.07718E+00   1.00000E+00   1.30349E-02   1.09415E-01   0.00000E+00
  1.29262E+00   1.00000E+00   1.53956E-02   1.07635E-01   0.00000E+00
  1.72349E+00   1.00000E+00   1.97466E-02   1.03380E-01   0.00000E+00
  2.15436E+00   1.00000E+00   2.35933E-02   9.85149E-02   0.00000E+00
  2.58523E+00   1.00000E+00   2.70469E-02   9.32646E-02   0.00000E+00
  3.44698E+00   1.00000E+00   3.45806E-02   8.25270E-02   0.00000E+00
  4.30872E+00   1.00000E+00   4.45956E-02   7.22048E-02   0.00000E+00
  5.17047E+00   1.00000E+00   6.00440E-02   6.29940E-02   0.00000E+00
  6.03221E+00   1.00000E+00   8.55708E-02   5.53635E-02   0.00000E+00
  6.89395E+00   1.00000E+00   1.73251E-01   4.96283E-02   0.00000E+00
  7.75570E+00   1.00000E+00   3.29111E-01   4.60150E-02   0.00000E+00
  8.18657E+00   1.00000E+00   4.32019E-01   4.50578E-02   0.00000E+00
  8.61744E+00   1.00000E+00   5.46439E-01   4.46779E-02   0.00000E+00
  9.04832E+00   1.00000E+00   6.76082E-01   4.48546E-02   0.00000E+00
  9.47919E+00   1.00000E+00   8.21464E-01   4.55679E-02   0.00000E+00
  1.03409E+01   1.00000E+00   1.16120E+00   4.85310E-02   0.00000E+00
  1.20644E+01   1.00000E+00   1.96831E+00   6.00517E-02   0.00000E+00
  1.37879E+01   1.00000E+00   3.10141E+00   7.78833E-02   0.00000E+00
  1.55114E+01   1.00000E+00   4.56574E+00   1.01767E-01   0.00000E+00
  1.72349E+01   1.00000E+00   6.39866E+00   1.31123E-01   0.00000E+00
  2.15436E+01   1.00000E+00   1.27129E+01   2.25664E-01   0.00000E+00
  2.58523E+01   1.00000E+00   2.17323E+01   3.46381E-01   0.00000E+00
  3.01611E+01   1.00000E+00   3.36832E+01   4.89436E-01   0.00000E+00
  3.44698E+01   1.00000E+00   4.87485E+01   6.51918E-01   0.00000E+00
  4.30872E+01   1.00000E+00   8.87949E+01   1.02637E+00   0.00000E+00
  5.17047E+01   1.00000E+00   1.42798E+02   1.45592E+00   0.00000E+00
  6.03221E+01   1.00000E+00   2.11426E+02   1.93087E+00   0.00000E+00
  6.89395E+01   1.00000E+00   2.95177E+02   2.44411E+00   0.00000E+00
  7.75570E+01   1.00000E+00   3.94438E+02   2.99011E+00   0.00000E+00
  8.61744E+01   1.00000E+00   5.09502E+02   3.56461E+00   0.00000E+00
```

Figure 16-5-2.(continued).

```
? LIST DATA /
LIST DATA /
-------------------- RAW DATA --------------------
 ZBAR            0.00000          ABAR            0.00000
 XALPHA      6.6667E-01           IGRUN                 3
 RHOREF      0.0000E+00           GAMREF      0.0000E+00
 DEBREF      0.0000E+00           CVIR        1.0000E+00
 DVIR        1.0000E-03           TSTFD       0.0000E+00
 CL3G        2.0000E+00           CL3K        1.0000E+02
 TMELT       0.0000E+00
 RCOLD       0.0000E+00           BCOLD       0.0000E+00
 TREF        2.5692E-02           C0          0.0000E+00
 S1          0.0000E+00           S2          0.0000E+00
 CMAT        1.5000E+00           CLJ         1.0000E+00
 FACLJ       1.0000E+00           ECOH        0.0000E+00
 BREF        0.0000E+00           MODC          CHUG
 MODN(1)       VIRIAL             MODN(2)       CHARTD
 MODE          TFD                EPSMIX      1.0000E-06
 NU                    0
-------------------------------------------------------
? LIST COMP /
LIST COMP /
-------------------------------------------------------
 COMP                        68
   0.0000E+00  1.0000E-06  2.0000E-06  5.0000E-06
   1.0000E-05  2.0000E-05  5.0000E-05  1.0000E-04
   2.0000E-04  5.0000E-04  1.0000E-03  1.5000E-03
   2.5000E-03  4.0000E-03  6.0000E-03  1.0000E-02
   1.5000E-02  2.5000E-02  4.0000E-02  6.0000E-02
   1.0000E-01  1.2500E-01  1.5000E-01  2.0000E-01
   2.5000E-01  3.0000E-01  4.0000E-01  5.0000E-01
   6.0000E-01  7.0000E-01  8.0000E-01  9.0000E-01
   9.5000E-01  1.0000E+00  1.0500E+00  1.1000E+00
   1.2000E+00  1.4000E+00  1.6000E+00  1.8000E+00
   2.0000E+00  2.5000E+00  3.0000E+00  3.5000E+00
   4.0000E+00  5.0000E+00  6.0000E+00  7.0000E+00
   8.0000E+00  9.0000E+00  1.0000E+01  1.5000E+01
   2.0000E+01  2.5000E+01  3.0000E+01  4.0000E+01
   6.0000E+01  8.0000E+01  1.0000E+02  1.5000E+02
   2.5000E+02  4.0000E+02  6.0000E+02  1.0000E+03
   2.0000E+03  5.0000E+03  1.0000E+04  2.0000E+04

-------------------------------------------------------
? LIST TEV /
LIST TEV /
-------------------------------------------------------
 TEV                         37
   0.0000E+00  1.2500E-02  2.5692E-02  5.0000E-02
   1.0000E-01  2.5000E-01  5.0000E-01  7.5000E-01
   1.0000E+00  1.5000E+00  2.0000E+00  2.5000E+00
   3.0000E+00  4.0000E+00  5.0000E+00  8.0000E+00
   1.0000E+01  1.5000E+01  2.0000E+01  2.5000E+01
   3.0000E+01  4.0000E+01  5.0000E+01  8.0000E+01
   1.0000E+02  1.5000E+02  2.5000E+02  4.0000E+02
   6.0000E+02  1.0000E+03  1.5000E+03  2.5000E+03
   6.0000E+03  1.0000E+04  2.0000E+04  5.0000E+04
   1.0000E+05
-------------------------------------------------------
```

Figure 16-6-1. Sample interactive run of GRIZZLY to print default data settings.

```
? MXTURE N 1 4 9.01218 1.85 1 8 15.9994 1.426 /
MXTURE N 1 4 9.01218 1.85 1 8 15.9994 1.426 /
? LIST MIX /
LIST MIX /
 ------------------------------MIXTURE--------------------------
       WMIX          FMIX          ZMIX          AMIX          RMIX
  1  3.6032E-01   5.0000E-01      4.00000       9.01218   1.8500E+00
  2  6.3968E-01   5.0000E-01      8.00000      15.99940   1.4260E+00
-----------------------------------------------------------------
? LIST /
LIST /
-------------------- RAW DATA --------------------
 ZBAR          6.00000          ABAR         12.50579
 XALPHA    6.6667E-01           IGRUN               3
 RHOREF    1.5544E+00           GAMREF    0.0000E+00
 DEBREF    0.0000E+00           CVIR      1.0000E+00
 DVIR      1.0000E-03           TSTFD     0.0000E+00
 CL3G      2.0000E+00           CL3K      1.0000E+02
 TMELT     0.0000E+00
 RCOLD     0.0000E+00           BCOLD     0.0000E+00
 TREF      2.5692E-02           C0        0.0000E+00
 S1        0.0000E+00           S2        0.0000E+00
 CMAT      1.5000E+00           CLJ       1.0000E+00
 FACLJ     1.0000E+00           ECOH      0.0000E+00
 BREF      0.0000E+00           MODC        CHUG
 MODN(1)     VIRIAL             MODN(2)     CHARTD
 MODE        TFD                EPSMIX    1.0000E-06
 NU                  0
--------------------------------------------------
```

Figure 16-6-1.(continued).

```
? LIST SUP /
LIST SUP /
-----------------------------------------------
 KCTFD                1
 SCTFD                2     -1.0000E+00   1.0000E-10
                            -1.0000E+00  -1.0000E+00

 KTTFD                1
 STTFD                2      1.0000E-04   2.4990E-01
                            -1.0000E+00  -1.0000E+00

 KCNUC                1
 SCNUC                2     -1.0000E+00   1.0000E-10
                            -1.0000E+00  -1.0000E+00

 KTNUC                1
 STNUC                2     -1.0000E+00  -1.0000E+00
                            -1.0000E+00  -1.0000E+00

 KCCOLD               1
 SCCOLD               2     -1.0000E+00   1.0000E-10
                            -1.0000E+00  -1.0000E+00

 KCMIX                1
 SCMIX                2     -1.0000E+00   1.0000E-10
                            -1.0000E+00  -1.0000E+00

 KTMIX                1
 STMIX                2     -1.0000E+00  -1.0000E+00
                            -1.0000E+00  -1.0000E+00

 KRTAB                1
 SRTAB                2     -1.0000E+00  -1.0000E+00
                            -1.0000E+00  -1.0000E+00

 KTTAB                1
 STTAB                2     -1.0000E+00  -1.0000E+00
                            -1.0000E+00  -1.0000E+00

-----------------------------------------------
? END /
END /
 STOP
GRIZ      CTSS TIME      1.713      SECONDS
CPU=      .035    SYS=      .035    I/O+MEMORY=      1.643

 ALL DONE
```

Figure 16-6-1.(continued).

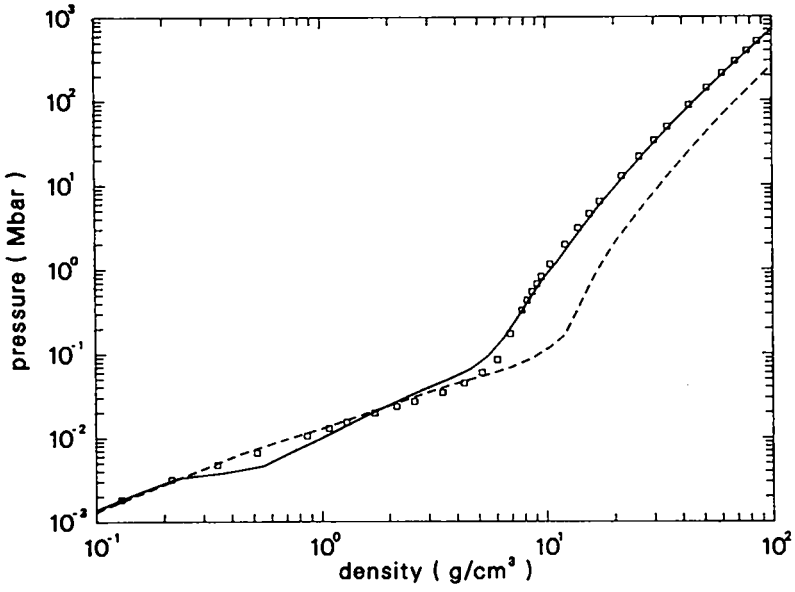


Figure C-1. Pressure as a function of density at a temperature of 1 eV for a one to one mixture of iron and molybdenum using the various mixing schemes. The iron table used was SESAME 2140 and molybdenum table was SESAME 2980. The solid line is additive volume mix, the dashed line is partial pressure mix, and the boxes are ideal mix.

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

Microfiche (A01)

Page Range	NTIS Price Code
001-025	A02
026-050	A03
051-075	A04
076-100	A05
101-125	A06
126-150	A07
151-175	A08
176-200	A09
201-225	A10
226-250	A11
251-275	A12
276-300	A13
301-325	A14
326-350	A15
351-375	A16
376-400	A17
401-425	A18
426-450	A19
451-475	A20
476-500	A21
501-525	A22
526-550	A23
551-575	A24
576-600	A25
601-up*	A99

*Contact NTIS for a price quote.