

EOSPRO CODE: AN INTERIM REPORT

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G. I. Kerley
Kerley Technical Services
Appomattox, VA

INTRODUCTION

EOSPro is a new, revised, expanded, more user-friendly version of the PANDA II code [1]. In addition to many other changes, the code has recently been rewritten in Fortran 2003. It is still undergoing changes, and there has not yet been time to write a new set of manuals and tutorials. This interim report gives a preliminary discussion of the current version. It should be used in conjunction with the 1991 PANDA manual [1], the EOSPro command summary [2], the KTS website tutorials [3], and other references listed at the end of this document.

CODE OVERVIEW

EOSPro is an interactive, command-line code for computing equations of state (EOS) for materials over a wide range of densities and temperatures. It offers options for constructing EOS for one-component solids and fluids, for inert or reactive mixtures of many chemical components, and for materials having several phases. The user enters commands that define EOS models, make calculations and compare the models to experimental data, and generate tabular EOS libraries for use in hydrocodes and other applications.

EOSPro can be run from commands entered at the keyboard, from input command files, or by switching back and forth between the keyboard and input files. It does not generate plots. Instead, it generates files of data that are suitable for plotting with other programs, such as the Gnuplot code [4].

CODE PACKAGE & INSTALLATION

When the code package (zip or gz file) is extracted, it creates an eospro directory, with five subdirectories:

- exe: code executables for three platforms—MacOSX (Intel), Linux, and Windows (XP).
- docs: three documents—EOSProIR.pdf (interim report, this file), EOSProCS.pdf (command summary), and SAND88-2291.pdf (PANDA II manual).
- data: a library of tables for the mixture model, Hugoniot data files, and orbital data files.
- input: several directories containing input files illustrating use of various code options.
- util: source code for some simple Fortran and C programs:

To set up the code for use:

- move directories and files and rename executables as desired; set up paths and aliases.
- run eospro and use ASC2BIN command to generate binary file from asplib file in data directory.
- compile programs in util directory, if desired.

PRELIMINARY COMMENTS

EOS modeling is not merely the task of fitting experimental data; in most practical applications, the modeler will not have enough data to warrant use of “least-squares” algorithms. *The goal of EOS modeling should be to describe the material behavior.* In order to achieve that goal, one must understand the chemical and physical phenomena that govern the behavior. Armed with that understanding, the modeler has a reasonable chance of constructing a good model, even in cases where experimental data are very limited.

When constructing an EOS model, it is essential to learn as much as possible about the material and the class of materials to which it belongs. Different types of materials require different models; there is no truly “universal” EOS model that can be applied to all cases. Experimental data are valuable, of course, but they

are not sufficient. The following questions comprise a partial list of what should be considered:

- What is the chemical composition and molecular structure of the material?
- What forces are present in the material—metallic, covalent, ionic, van der Waals?
- How will the structure and forces depend on density and temperature?
- Is the material likely to have phase transitions? (Yes!) What transitions?
- How important are strength effects, and how should they be treated?
- How important are porosity effects, and how should they be treated?
- If chemical reactions occur with changes in state, will they be reversible or irreversible?

EOSPro can assist in the modeling process, but it cannot answer these kinds of questions. It cannot provide the background knowledge the modeler needs and show him/her what options to choose.

In recent years, *ab initio* numerical calculations have become increasingly popular and are sometimes regarded as a replacement for the kind of modeling done with EOSPro. In practice, the numerical methods are still approximate and will require much more development before they can be used to construct a global EOS.¹ However, numerical calculations are a very valuable resource for some parts of EOSPro models, especially zero-Kelvin isotherms and phase transition behavior.

EOSPro offers a wide variety of EOS modeling options, ranging from very simplistic to very sophisticated. Construction of a *good* EOS model is a time-consuming process, requiring months and even years of work.² In the real world, the modeler is often restricted by schedules that only allow time for use of the simplistic options. But it should not be thought that the crude models are “just as good” as the sophisticated ones, that there is some way to squeeze a good modeling job into a short period of time (regardless of what program managers choose to believe).

In constructing an EOS model, one should make numerous comparisons with whatever data can be found. It is a mistake to use some subset of the data for calibration purposes. Experience shows that fitting a small region of the EOS surface with high precision often results in poor results for the rest of the surface, sometimes even pathological behavior. It is wise to examine many plots of the EOS surface, both global plots and plots over small regions, to ensure that the behavior is reasonable everywhere. Such plots will sometimes identify problems with the model, even when data are not available for comparison. EOSPro provides tools for generating files for plotting with programs like Gnuplot [4].

CODE EXECUTION

To start a session: Enter the code name, with a list of optional parameters (using a namelist format):

```
eospro    out=outfile in=infile plot=plotfile id=identifier
```

Here *eospro* is the name of the executable or an alias to it. User-specified names, given in italics above, are:

outfile is the name of the output file, i.e., record of the session (defaulted to out.pro),

infile is the name of the input file (no input file if not specified),

plotfile is the name of the plot file (defaulted to plot.pro),

identifier is a tag that will appear on the output and plot files (defaulted to “none”).

If *outfile* = “none” there will be no output file. Other input and plot files can be defined during the course of a session, using commands discussed below. Terminate a session by the command END, QUIT, or EXIT.

Commands: Input to the code is specified by giving a COMMAND, followed by a parameter list. In most cases, the parameter list can be omitted, in which case the code will issue a prompt. Most commands require additional input. Therefore, the code has two kinds of prompts:

-
1. To the best of my knowledge, none of the EOS tables in existing databases for hydrocode calculations and other applications have been constructed using *ab initio* numerical methods.
 2. Water and silica are two of the most important materials on the earth’s surface. Yet satisfactory EOS models for these materials still do not exist after *decades* of work.

eospro> indicates that the code is waiting for a command, while
 > indicates that the code is waiting for parameters for the *last* command.

Abbreviations: Many commands can be abbreviated. Here, and also in the command summary, asterisks are used to indicate the minimum set of required characters in a command. In the example

```
mod*el sol*id
```

all characters after the asterisk are ignored; they can be omitted or included, as the user prefers.¹

Tokens: Commands and parameter lists consist of numerical and character “tokens” delineated by any combination of blanks, equal signs, commas, left and right parentheses, and left and right brackets. (Equal signs, commas, parentheses, and brackets are converted to blanks on input, except in comments, and so are used only for readability.) Each token can consist of up to 50 characters.

Continuations: An ampersand (&) can be used to continue an input line. (However, the total number of characters in an input line must not exceed 300.)

Comments: Comments are denoted by an exclamation point (!) or “pound sign” (#). The ! or # can come at the beginning of a line, after a command/parameter string, and even after an ampersand. Comments are allowed in keyboard input as well as input files.

Marker lines: Markers are lines having a colon (:) as the first non-blank character, followed by an alphanumeric name. They are used in input files for branching with a GOTO command, as discussed below. (They are treated as comments when entered at the keyboard.)

Case sensitivity: Input is case-insensitive except for file names, symbol names, and the values of character symbols, as discussed below. (All input is converted to upper case except in these three instances.)

Defaults: Many input variables, both numerical and character, can be defaulted; the default is normally obtained by entering a - or * character in the field corresponding to that variable, or leaving fields blank when they are on the end of the input line.

File names: File names can be up to 50 characters in length and may include the full path (as defined by the computing system). File names must *not* be enclosed in quotes *except* when defining character symbols, as discussed below.

Date, CPU time: EOSPro acquires the current date; it does not have to be entered by the user, as was required by PANDA. EOSPro also furnishes the CPU time of each session.

CONTROL COMMANDS

Also refer to the command summary [2] for information about syntax.

Plotting: The PLOT command directs the code to open a plot file send data to it for plotting with a graphics utility. The format of this file is that recognized by the Gnuplot program [4], organized into blocks of data with # signs as comments. (Subsequent commands prompt the user to enter the comments for this file.) The command NO PLOT stops sending data to the file.

Command files: The command @*fname* directs the code to take input from a text file, called *fname*, until an end-of-file (EOF) is encountered. These input files can be nested, one file calling other files; when an EOF is encountered, control will revert to the last file called, eventually reverting to the keyboard.

1. Note that variations like “modeler solide” or “modellare solido” would also work in this example. More fancy “translations” could be made using the SYM*BOLS option.

Symbols: The SYM*BOLS command is used to preassign numerical and character values to symbols that can be used as tokens in subsequent commands. Character symbols are enclosed in single quotes to distinguish them from numerical symbols. Symbol names are case sensitive. The following example,

```
sym    r0 = 2.65  T0 = 2460  File = '/User/smith/library'  SETUP = 'mod'
```

defines four symbols. The symbols “r0” and “T0” (sans quotes) can be used in subsequent commands requiring numerical tokens, but “R0” and “t0” will not be recognized because of case sensitivity. The symbols “File” and “SETUP” (again sans quotes) can be used in subsequent commands requiring character tokens. (For example, note that the command “SETUP SOL” will now be equivalent to “MOD SOL”).¹

The command SHOW SYM*BOL *s1 s2 ...* will display the values of the symbols listed. If no symbols are listed, all defined symbols will be displayed.

Arithmetic: Five operations—addition, subtraction, multiplication, division, and exponentiation—can be used in numerical tokens, including definitions of numerical symbols. (No spaces are allowed between operators and operands.) In the following example,

```
sym    x = 1.0e2  y = -40  a = x+y  b = -2*x  c = y/4  d = a^2
```

the symbols a, b, c, and d will have the values 60, -200, 10, and 3600, respectively.

Branching: The command GOTO *mark* tells the code to branch to the marker line beginning with *:mark*. This command can be used either in input files or after a PAUSE statement, as discussed below. (GOTO must always be a single word.)

Pauses: The PAUSE command causes code execution to wait for input from the keyboard before continuing. It may be followed by a simple carriage return, directing the code to resume execution, or by a GOTO statement, directing the code to branch within the current input file. (GOTO statements after pauses only have meaning while commands are being taken from an input file containing the specified markers.)

System commands: SYS*TEM *command_list* can be used to run commands from the operating system (OS) without exiting EOSPro or opening another window. The *command_list* must, of course, follow the syntax of the OS being used. For a Unix or Linux system, the following example,

```
sys    cp file1 file2; vi file2; gnuplot; vi file3
```

would copy *file1* to *file2*, invoke the vi editor on *file2*, run a Gnuplot session, and edit *file3* before continuing the EOSPro session. If SYS*TEM is called from within an input file, control switches to the keyboard while running the system commands, e.g., as in running Gnuplot. The cd (change directory) command has no effect after the EOSPro session resumes. Symbols are not recognized in *command_list*.

Other features: OUT*PUT ON/OFF turns on/off messages to the output file. TERM*INAL ON/OFF turns on/off messages to the terminal. (These commands replace TTY ON/OFF, used in PANDA.) EOF, when inserted in an input file, has the same effect as reaching an actual end-of-file. RESET is used to start model input from scratch. PC VERSION, which was available in PANDA, is obsolete and has been removed.

SOLID-GAS & LIQUID-GAS MODELS

The MOD*EL SOL*ID and MOD*EL LIQ*UID commands are used to set up models for solids and liquids consisting of “one component,” i.e., a single phase of a single chemical species. (Models allowing phase transitions and mixtures of more than one chemical species are set up using the MOD TRN and MOD MIX commands, using EOS tables generated by the MOD SOL and MOD LIQ commands.)

1. Note that this feature allows one to redesign the command syntax or even translate it into another language. Accented Latin, Greek, and Cyrillic characters can be used, at least on a Mac, so there are many possibilities. However, symbols are case-sensitive, so one must be consistent.

MOD SOL and MOD LIQ contain “toggle switches” for terms in the model:

```
MOD SOL   CRV=i NUC=i TEL=i VRT=i TAB=i DIP=i RAD=i ESFT= $\Delta E$  VAC= $f_v$  WSL= $w_s$ 
MOD LIQ   CRS=i TEL=i VRT=i TAB=i DIM=i DIP=i RAD=i ESFT= $\Delta E$  WLQ= $w_l$ 
```

where $i=1$ to include a term, $i=0$ for terms not included. (See the command summary for definitions of the various toggle switches.)

Each term in the model must be defined using additional commands, e.g., COLD CURVE, SOL NUC, etc. However, the MOD SOL and MOD LIQ commands will invoke the necessary commands automatically, for any term that has not already been set up. The order for this additional input is the same as that used when specifying the toggle switches in the MOD command.¹

Usage of the MOD SOL and MOD LIQ commands in EOSPro is basically the same as in PANDA, as described in Sec. 2 of the manual. However, there have been a few changes and additions.

Porosity option: The SOL*ID TAB*LE option (invoked automatically if TAB=1 in MOD SOL) can be used to specify use of a p-alpha porosity model [5][6] with the solid table. After entering the material number and file name, append 1 (parameter IPOR). The code then prompts for seven parameters:

```
Enter P-Alpha parameters--R0,RP,PS,PE,CE,CS,XN
```

where	R0	TMD density—required
	RP	initial porous density—required, $RP < R0$
	PS	pressure for complete compaction—defaulted to 0.1 GPa
	PE	maximum elastic pressure—defaulted to 0
	CE	sound speed in elastic region—defaulted to 0
	CS	TMD sound speed—required if $CE > 0$
	XN	power of density term in compaction region (defaulted to 2)

This version of the p-alpha model is reversible—unloading occurs along the same path as loading. Note that this porosity model only applies to the *tabular* term in the solid EOS, so it should only be used when there are no other terms in the model. (Make a table from the solid model before using this option.)

Dipole term: The DIP*OLE command, which is new, is used to define a dipole-dipole interaction term for the solid and fluid models. (To obtain this term, set DIP=1 in the MOD commands.) The code prompts the user for three input parameters:

```
Dipole term--Enter DMU, RE, PWF
```

where	DMU	dipole moment in Debye (1.0E-18 esu)
	RE	charge separation distance (Å)
	PWF	parameter for high-density correction (default is PWF=1.0)

The dipole term is temperature-dependent. It goes to the value for a bcc lattice at 0K. The temperature dependence is a fit to unpublished Monte Carlo calculations. This model has not yet been documented or even used in any published EOS models. Further revisions are possible.

Radiation terms: Set RAD=1 to include radiation contributions to the EOS. (They can also be included in the MOD MIX and MOD TRN commands but should not be used again if already used in MOD SOL or MOD LIQ.) These terms are computed from the expressions given in Ref. [7] and require no additional input. Reference [6] discusses a case in which these terms were used.

1. Exceptions occur when the cold curve and Grüneisen function options are coupled, e.g. ICLD=1 and/or IGRUN=1. The simplest way to sort things out in such cases is to let the code prompt for the information needed and then keep the same order in subsequent input files.

SOL NUC option: The restriction on parameter TG for IGRN=4, described in Sec. 10.5 of the PANDA manual, has been removed.

Sample input files: Input files that use the MOD SOL and MOD LIQ options can be found in directory input/titanium. These files create four EOS tables that are then used in the phase transition model.

Other changes and additions to the solid and liquid terms are discussed in the next four sections.

COLD CURVE OPTIONS

Options for the zero-Kelvin isotherm, or cold curve, are discussed in Sec. 3 of the PANDA manual. There are several changes and additions to these options in EOSPro.

Hugoniot option (ICLD=1): The quadratic fit to the Hugoniot, Eq. (3.1), has been replaced by the formula

$$U_S = C_S(1 + S_1u + S_2u^2), \text{ where } u = u_p/U_S.$$

Note that this expression differs from the old one only in the quadratic term. This change has been made so that constants S_1 and S_2 are both unitless.

The Hugoniot option for the cold curve must be used with caution, because it assumes that the lattice-vibrational terms are represented by the Debye model. The EOS will not reproduce the specified Hugoniot if the VIB ROT option is used to include Einstein vibrational frequencies, if thermal electronic contributions are large, if the liquid model is used, or if other terms are included.

Birch-Murnaghan option (ICLD=6): The Birch-Murnaghan formula is

$$P_C(\rho) = \frac{3}{2}\beta_0(\eta^{7/3} - \eta^{5/3})[1 + \frac{3}{4}(\eta^{2/3} - 1)(\beta'_0 - 4)], \quad E_C(\rho) = \frac{9}{8}(\beta_0/\rho_0)(\eta^{2/3} - 1)^2[\frac{1}{2}(\eta^{2/3} - 1)(\beta'_0 - 4) + 1],$$

where $\eta = \rho/\rho_0$. This new cold curve option requires three input parameters—RZRO (ρ_0), BZRO (β_0), and DBDP (β'_0). This formula often gives an excellent description of the compressive behavior of a material from zero to high pressures, even without the TFD MATCH option. However, it cannot be expected to give satisfactory behavior in tension and should always be used with the LJ MATCH option.

Ionic cold curve: EOSPro offers a simple ionic model for the zero-Kelvin curve, available either as ICLD=7 or as a separate command, ION CURVE. The energy is given by

$$E_C(\rho) = E_{TFD}(\rho) - 1173.3Z_1Z_2\mu\xi^{1/3}/W^{4/3} \text{ MJ/kg, where } \xi = \rho/(1 + \rho/\rho_X).$$

$E_{TFD}(\rho)$ is the contribution from repulsive (electron overlap) forces to the EOS; it is computed from the TFD model. The second term is the attractive contribution from the Coulomb interaction between ions of charge Z_1 and Z_2 . μ is a "reduced Madelung constant," a unitless parameter typically on the order of 0.7-1.1 for most types of lattices, W is the molecular weight, and ρ_X is a parameter designed to "shut off" the Coulomb term at high densities, where the ion spheres overlap. The user is prompted to enter the four parameters Z1 (Z_1), Z2 (Z_2), FM (μ), and RX (ρ_X). Z_1 and Z_2 should both be entered as positive numbers. The TFD term and W are computed from the chemical formula, which is entered elsewhere.

Despite its simplicity, this ionic model has been found to give surprisingly good results for a number of ionic materials, particularly when parameters FM and RX are adjusted to match experimental data. The ION CURVE option is slightly better than the ICLD=7 option, in that it uses a more accurate expression for the TFD energy for ions of different sizes.

EXP6 command: This command, used to compute a cold curve from an EXP-6 potential (Sec. 3.9 of the PANDA manual), has been completely redone. The old option was not correct because it did not sum the repulsive term over all shells of neighbors. In the new version, the cold curve is summed over all neighbors and output as a table. The quantum terms and effective Einstein temperature are also calculated.

TFD match: This option, discussed in Sec. 3.7 of the PANDA manual, is used to ensure that the cold curve has reasonable asymptotic behavior at high densities. EOSPro uses an improved fit to the TFD curve for mixtures. The match density is specified by the user but is occasionally overridden; when that happens, the code prints out the new value.

LIQUID PERTURBATION THEORY (CRIS MODEL)

The CRIS model calculates the contributions to the EOS from *both* the intermolecular forces and the thermal motion of the molecular centers-of-mass. These two terms are the equivalent of the cold curve and lattice vibrational motion in the solid model. However, they are not additive as in the solid.¹ The CRIS model uses liquid perturbation theory (LPT) to compute the thermal motion and a solid-like cold curve to compute the energy of a molecule in the cage formed by its neighbors. The basic ideas are discussed in detail in Sec. 5 of the PANDA manual and references cited. EOSPro includes several changes and additions to the options discussed in the PANDA manual.

Quantum corrections: EOSPro uses a new model for calculating the quantum corrections to the CRIS model. It is based upon an idea, originally proposed by Rosenfeld [8], that relates the quantum terms to an Einstein oscillator frequency. The equations used in EOSPro are discussed in a report on the EOS of H₂ and D₂ [9] and were also used in computing and EOS for He [10]. The new option requires no additional user input. It is invoked by setting parameter QFAC=1 in the input for the CRIS model. (The old option, which can still be obtained by specifying a negative value for QFAC, is deprecated.)

New input parameters: Two new parameters, WX1 and WX2, can be entered after parameter XG (see page 48 of the Panda manual). They are factors that multiply the high-order corrections in the free energy expansion (the last two terms in Eq. 5.8 of the manual). These factors default to 1.0 if omitted or set to zero.

Transport properties: The command XPT LIQ can be used to calculate transport properties using the liquid model, as discussed in Sec. 5.5 of the PANDA manual. In EOSPro, the expression for the shear viscosity has been modified to go to the correct limit at low densities (Enskog expression). EOSPro also calculates the thermal conductivity, along with the viscosity and diffusivity.

VIBRATION-ROTATION MODEL

The VIB ROT command is used to define contributions to internal vibrational and rotational degrees of freedom to the EOS. The vibrational terms are also used to treat “optical modes” of vibrations in solids having more than one atom per unit cell. This command is discussed in Sec. 6 of the PANDA manual.

The old PANDA model used the rigid rotator-harmonic oscillator approximation, including a cutoff in the vibrational levels as a crude treatment of anharmonicity. Work on the H₂ & D₂ EOS [9] has shown that effects of density and vibration-rotation coupling can also be very important. EOSPro includes several changes to the simple model that can be used to treat these effects. These changes have not yet been documented, and additional revisions are expected.

The total number of vibrational and rotational terms should be 3N-3, where N is the number of atoms in the molecule. A separate input line is required for each rotational and each vibrational term.

Rotational terms: The rotational terms are defined first. The user is prompted as follows.

Rotational term--Enter IR,BE,SR,WR,D0,RE,WE

The first four parameters correspond to those in Sec. 6.2 of the PANDA manual: IR is the type of molecule (1 for linear, 2 for non-linear, 0 for no term), BE is the equilibrium rotational constant (cm⁻¹), SR is the sym-

1. Also note that the liquid EOS does *not* extrapolate to the solid cold curve at zero temperature.

metry factor, and WR is the weight of the rotational term. (The default, WR=1, corresponds to two degrees of freedom for a linear molecule, three for a non-linear molecule.)

The last three parameters are used for corrections to the rigid rotator expressions (Eqs. 6.1-6.8 of the PANDA manual). D0 is the energy (Kelvin) at which the rotational levels will be cut off. RE and WE are the equilibrium distance (Å) and vibrational frequency (cm⁻¹) for a vibrational level that is coupled to the rotational level. They are used, along with D0, to construct a Morse potential for modeling density effects and vibrational-rotational coupling.

Vibrational terms: The user is prompted as follows.

Vibrational term--Enter WE, GV, D0, GM, PV, TV, RE, BE

Parameters WE, GV, and GM are the frequency (cm⁻¹), degeneracy, and Grüneisen parameter of the vibrational mode. D0 is a dissociation energy (Kelvin) at which the vibrational levels will be cut off. (If D0 < 0, this parameter is interpreted as the number of allowed levels, the cutoff used in PANDA.)

Parameter PV describes the density-dependence of the Grüneisen parameter. If PV > 0, it is given by Eq. 6.13 of the PANDA manual. If PV < 0, It is given by

$$\Gamma = \Gamma_0 \eta (\eta - 1) / [1 + (\Gamma_0 / \Gamma_\infty) (\eta - 1)]^2, \text{ where } \Gamma_0 = \text{GM}, \Gamma_\infty = |PV|, \text{ and } \eta = \rho / \rho_0.$$

Parameter TV is used to treat the temperature-dependence of the vibrational level, Eq. 6.14 of the PANDA manual.

The new parameters RE and BE are the equilibrium distance (Å) and rotational constant (cm⁻¹). They are used, along with D0, to model density destabilization of the vibrational level and vibrational-rotational coupling. Note that different values of D0, RE and BE can be used for each rotational and vibrational level and that D0 and RE do not have to agree with those for the rotational levels.

Rotational constant: The BROT command is used to compute the rotational constant from its structure, i.e., the X-Y-Z coordinates of its atoms, as described in Sec. 6.4 of the PANDA manual. EOSPro will compute the rotational constant for linear molecules as well as nonlinear.

THERMAL ELECTRONIC TERM

The ELEC command is used to define the thermal electronic contribution to the EOS of the one-component solid or liquid. As explained in Sec. 8 of the PANDA manual, there are three options for this term—the TFD model, specified energy levels, or a table of the electronic entropy as a function of density and temperature, read from a file. In the latter case, the pressure and internal energy are computed from the entropy by a thermodynamically-consistent procedure.

Thermal broadening: A thermal broadening option has been added to the tabular option. The user is prompted as follows.

Electronic term--file name or option, XB, Q0

If XB > 0, the input entropy is averaged over volume fluctuations using a temperature-dependent Gaussian distribution [11]. (The same broadening option is also offered in the IONEQ model, discussed below.)

Thermal broadening *increases* with *decreasing* XB. A nominal value for this parameter is XB=60*AW*C0**2, where AW and C0 are the atomic weight and sound speed of the material [11]. Hence broadening effects should be greatest in regimes of the EOS surface where the sound speed is smallest. In the current version of the code, however, the same value of XB is used everywhere.

Interpolation and extrapolation: The tabular entropy routines extrapolate to T=0 when the tables do not already include a T=0 point. In this case, it is necessary to enter Q0, the electronic statistical weight at zero

temperature and density, i.e., the degeneracy of the ground state of the neutral atom. (Q0 can be determined using the LEVELS DATA command that is part of the IEQ model, discussed below.) Except for T=0, EOSPro now uses the TFD model when the density or temperature is off the entropy table.

IONIZATION EQUILIBRIUM MODEL

The IONEQ command is used to compute a table of the thermal electronic entropy using the EOSPro ionization equilibrium (IEQ) model. Additional commands—LEVELS DATA, LEVELS FILE, and PART*ITION FUNC*TION—can be used to compute energy levels and partition functions for atomic ions. This model can be applied to any single element in the periodic chart, both low and high atomic numbers. (The thermal electronic contributions for compounds and mixtures are automatically included when MOD MIX is employed with EOS tables including the electronic term for individual elements in the mixture.)

The EOSPro IEQ model has never been fully documented and is, in fact, still a research model. A basic outline of the original model is given in Sec. 9 of the PANDA manual. There have been many subsequent changes and improvements, most of which are discussed in Sec. 4 of Ref. [11]. Section 8 of Ref. [9] also gives an overview of the model. The overview given below is very brief.

Overview: The EOSPro IEQ model employs a simple approximation for making a very fast computation of the ionization potentials and energy levels of atomic ions, using a tabulation of orbital data [12], together with approximations for treating the free electrons and the effects of continuum lowering. All stages of ionization, and excited states, with up to four electron-hole excitations, are treated explicitly.¹ This approach avoids the “average configuration” approximation that is made in most other electronic theories and which gives significant errors in the treatment of localized bound states.

The original model did, however, use the “average atom” approximation, in which each atom is located within an identical, electrically neutral, spherical cell. The current version of the model includes two corrections to this approximation: charge fluctuations, which account for variations in electrical neutrality of the ion spheres, and thermal broadening, which accounts for fluctuations in the size of the ion cells.

Charge fluctuations: As explained in [9] and [11], the effects of charge fluctuations are important primarily at low densities and at low temperatures where the ground state and first excited state are present. These corrections can be included by setting input parameter F3 > 0. (A value in the range 0.1 to 1.0 is appropriate.)

Thermal broadening: The thermal broadening option in IONEQ is similar to that in ELEC, described above, and is obtained by setting input parameter XB > 0. In that case, the calculated entropy is averaged over volume fluctuations using a temperature-dependent Gaussian distribution [11]. Broadening *increases* with *decreasing* XB, and a nominal value is $XB=60*AW*C0**2$. Broadening can be included in either the IONEQ or ELEC command, or even in both.

Sample input file: The EOSPro input directory contains a commented input file for generating an electronic entropy table, using nitrogen as an example. This file can be edited and used for other elements. It also shows how to use the LEVELS DATA command.

Restart capability: IONEQ calculations can be very time-consuming, especially for high-Z elements with MX=4. At times it may be necessary to stop a calculation before it is finished (e.g., using Control-C). EOSPro provides a restart file (ieqrst) that enables one to pick up the calculation at the last ionization state completed. To make use of this option, enter RES*TART as the fourth parameter in the first input line, following the element name, orbital data file, and output entropy file.

1. Note that the atomic energy level model does *not* use the hydrogenic approximation as do other models.

Ionization state: The IEQ model calculates the number of free electrons, as a function of density and temperature, in addition to the entropy. Preliminary studies show that this calculation, when used with the Lee-More model of electronic conductivity, gives much better results than obtained with the default Thomas-Fermi model [13]. (This capability is not presently an option in EOSPro but may be added later on.)

Problem areas: The main difficulty with the IEQ model—the reason why it must still be regarded as a research model—is that it gives discontinuities in the thermodynamic properties at densities where bound states cross over into the continuum. These jumps can be reduced by using the thermal broadening option. However, problems generally still remain, especially for high-Z elements. In several cases, notably hydrogen [9], helium [10], and carbon [11], it was possible to use the IEQ model for constructing the EOS over the entire density-temperature range. In other cases, it has been necessary to construct a merged entropy table, using IEQ at the lower densities and a (revised) version of Liberman’s INFERNO model [14] at high densities. Examples of this approach are shown in Refs. [15]-[18]. Unfortunately, the INFERNO code, and the special merging programs that were used in [15]-[18], are not part of the EOSPro package.

None of the problems with the IEQ model are unsolvable. One reason that they haven’t been solved already is that time (i.e., funding) has never been allocated to work on them. In fact, virtually all model development thus far has been made by taking time from programmatic projects to make incremental improvements. (Like everything else in PANDA and EOSPro!) It remains to be seen whether or not this situation will change in the future, allowing the IEQ model to graduate from being a research model to being a tool for production EOS modeling.

MIXTURE MODEL

The EOSPro mixture/chemical equilibrium model is used to compute EOS for materials consisting of two or more chemical species. It uses a modified form of ideal mixing to construct the mixture EOS from EOS tables for the individual species, and their various phases, created with the MOD SOL and MOD LIQ commands. (An analytic option is also available for simple cases and for sensitivity studies.) The mixtures can be either “reactive,” in which the composition, calculated by minimizing the free energy, varies as a function of density and temperature, or “inert,” in which the composition is fixed. The mixture model is discussed in Sec. 10 of the PANDA manual. The EOSPro version includes important changes and improvements.

Setup: The MOD MIX command is used to set up the EOSPro mixture model. The command line can be used to specify six parameters, all of which are optional. A namelist format is used:

	MOD MIX	EZRO= ΔE PSFT= $\Delta\phi$ TLO= T_L RLO= ρ_L TFLR= T_0 RAD= i
where	EZRO	energy shift (added to internal energy)—defaulted to zero
	PSFT	shift used for the pseudopressure (see below)—defaulted to zero,
	TLO,RLO	limits of the tension region (see below)—both defaulted to zero,
	TFLR	lowest temperature for free energy minimization—defaulted to 10K,
	RAD	toggle switch for including the radiation contribution.

The MOD MIX command line is followed by two lines of input for each chemical species in the mixture: The first line supplies the chemical formula, e.g., H[2]O[1], C[1]O[2], Ca[1]C[1]O[3], etc. The second line supplies the EOS parameters, the number of moles in the “initial” composition, the “miscibility” parameter (PTY), and a name for the species (used in output). The code uses the chemical formulas and the initial composition to determine the chemical constraints used in the minimization procedure for determining the chemical composition. (Specification of a “reaction path” is not required.)

Input parameters for the individual chemical species are the same as given in Secs. 10.3-10.5 of the PANDA manual, with two exceptions. First, the MASS parameter can be used, in lieu of the MOLES parameter, to specify the initial mass (in grams) of any species. (This parameter is ignored if the number of moles is entered.) Second, EOSPro uses a new treatment of the pseudopressure that is described below.

Once the mixture model has been set up, the CONC*ENTRATION PLOT command can be used to compute the composition of the mixture as a function of density and temperature. This option is discussed in Sec. 10.5 of the PANDA manual. One change in EOSPro is that the concentrations of all species (up to 30) are now output to the plot file.

Pseudopressure: In ideal mixing, all chemical species are taken to have the same temperature and pressure (thermal and mechanical equilibrium). Satisfying this condition requires searching each EOS table for density as a function of pressure. Special problems arise when the pressure is not a monotonic function of density, a common situation when the EOS surface has “van der Waals loops.” This difficulty can be eliminated by making the “Maxwell constructions,” in which the loops are replaced by the equilibrium vapor pressure, with a small positive slope to the pressure vs. density in the coexistence region. However, that approach does not allow construction of a tension region in the EOS.

In order to construct a tension region when using the mixture model, EOSPro constructs a “pseudopressure” that is used to find the densities in regions where the pressure is not monotonic. EOSPro now offers two options for constructing the pseudopressure. The old method, described in Sec. 10.4 of the PANDA manual, requires specification of the parameter PFLR in the parameter list for each species. This option is still available but is no longer recommended.

The new option, which is preferred in most cases, is to add a constant shift (input parameter PSFT on the MOD MIX command line) to the pressures of all species, so that equilibration of the pseudopressures is completely equivalent to equilibration of the pressures. Since this procedure does not eliminate the van der Waals loops, it must be used, together with input parameters TLO and RLO, to specify an excluded region of the EOS surface ($\rho \leq \rho_L, T \leq T_L$) in which the thermodynamic functions are replaced by an artificial region—like that discussed in Sec. 13.5 of the PANDA manual.

Application of these tools to produce a satisfactory EOS surface will often require some experimentation. To summarize the main points: The EOS for each chemical species should generally include Maxwell constructions above the lowest temperature (TLO) at which tension will be allowed. The pressure shift (PSFT) should be the maximum tensile pressure (absolute value) that will be allowed in the EOS for any chemical species that will be present in this temperature range. The lowest allowed density (RLO) should then be the density for the maximum tensile pressure of the mixture.

Energy zero: The default energy zero for the mixture EOS is determined by the energy zero used in constructing the EOS for the individual species. When constructing these EOS, using either the tabular or analytic option, *it is essential to use a consistent energy zero for all species*. One way to do that is to require that the enthalpy of each species equal its heat of formation at its standard state, normally 298K and 1 bar (10^{-4} GPa). In that case, the default energy zero for the mixture EOS will correspond to the heat of formation of the material in *its* (unreacted) standard state. The EZRO parameter can then be used to shift the entire EOS table for the mixture to whatever energy zero is desired.

For reactive materials, it is important to recognize that the mixture model describes the EOS of the reaction products, *not* the EOS of the unreacted material. Hence it will *not* generally reproduce the enthalpy of a unreacted material in its standard state. This situation is especially evident when the model is applied to explosives. In that case, the mixture model EOS, i.e., the reaction products, should predict a higher pressure and *lower* internal energy than that of the unreacted explosive at RTP.

Sample input files: The EOSPro input directory contains two commented input files for setting up and running calculations using the mixture model. One example (directory input/tntpr) constructs an EOS for the reaction products of TNT explosive, using tabular EOS from the species library (splib) in the data directory. The other example (directory input/air) constructs an EOS for air, using the analytic option for the chemical species.

Problem areas: When using the mixture model, one must have a set of EOS tables for all chemical species and phases to be allowed. Most of the work of developing a mixture model goes into creating these tables. A library of standard CHNO species is provided with the code, but users will have to create their own tables for other cases. (More work is also needed on some CHNO species, especially H₂O and HCOOH.)

The mixture model sometimes fails to converge. An obvious problem arises when a ρ - T state of the mixture is outside the range of the input EOS tables; those states must either be excluded or the input tables must be extended. Other cases can sometimes be handled by choosing the ρ - T mesh to avoid problem regions. In some cases, it may be necessary to generate several tables over different ρ - T regions, excluding species that are causing problems, then merging all of the tables together with the MOD MRG option.

The mixture model allows a given phase to be miscible (PTYP=1) or immiscible (PTYP~0.01). Certain species, such as liquid carbon, must be treated as immiscible (e.g., with H₂O, N₂, etc.) at low temperatures but should become miscible at high temperatures. EOSPro does not yet have an option to treat the transition between immiscibility and miscibility.

PHASE TRANSITION MODEL

The EOSPro phase transition model is used to compute EOS for materials consisting of two or more phases. The user first creates separate EOS tables for each phase, using the MOD SOL, MOD LIQ, and MOD MIX commands. These tables are then supplied to the phase transition model, which locates the phase boundaries and constructs the multiphase EOS. The basic approach is the same as described in Sec. 11 of the PANDA manual. However, the EOSPro version includes several important changes and additions, making it more accurate, more robust, and more powerful.

Setup: The MOD TRN command is used to set up the EOSPro phase transition model. The command line can be used to specify seven parameters, all of which are optional. A namelist format is used:

```
MOD TRN      PMIN= $P_M$  PFAC= $P_F$  ERR= $\epsilon$  RREF= $\rho_{ref}$  RCRT= $\rho_C$  TCRT= $T_C$  RAD= $i$ 
```

where

PMIN	lowest pressure in search for phase boundaries—defaulted to 0.1 GPa,
PFAC	pressure factor in coarse search for boundaries—defaulted to 1.02 (2%),
ERR	error parameter in search—defaulted to 10^{-6} ,
RREF	upper density bound in spinodal search—defaulted to 10^5 ,
RCRT, TCRT	lower density and upper temperature bounds—defaulted to 0 and 10^5 ,
RAD	toggle switch for including the radiation contribution.

RREF is the solid density, RCRT and TCRT are the critical density and temperature; they can be defaulted without any problems. The other search parameters should be changed when and if problems in finding the phase boundaries are suspected.

The MOD TRN command line is followed by one line of input for each phase in the model. This input has been expanded beyond that in the PANDA manual, using a namelist structure similar to that for the MOD MIX command. There are up to nine parameters for each phase, some of which can be defaulted:

```
MATID= $matid$  FILE= $fname$  NAME= $name$  ESHIFT= $\Delta E$  LIQ= $i$  &
RLO= $\rho_L$  RUP= $\rho_U$  TLO= $T_L$  TUP= $T_U$ 
```

where

MATID	material number for EOS table—required
FILE	file name for table—required for 1st phase, then defaults to last file name
NAME	name of phase (up to 10 characters)—optional, but useful for output
ESHIFT	shift in energy zero—defaults to 0
LIQ	set LIQ=1 for liquid (stable phase at low densities)
RLO, RUP	density bounds for region of stability—defaulted to range of table
TLO, TUP	temperature bounds for region of stability—defaulted to range of table

Search algorithm: EOSPro maps out the phase diagram by locating and tabulating the phase transition pressures while holding the temperature fixed. At each temperature, the code uses a coarse search grid, starting with pressure P_{MIN} and increasing the pressure by the factor PFAC, until a transition has been bracketed. It then does a binary search to locate the transition pressure. In this way, it continues to the highest possible pressure, making a table of the boundaries.

Specifying liquid phase: By default, the phase that is stable at its lower density limit or at its spinodal (at a given temperature) is defined to be the "liquid," i.e., the stable phase at all lower densities. In practice, it is best to specify the low-density phase by setting LIQ=1. (If more than one table is so designated, the last one will be chosen.) The vapor-liquid coexistence region for the multiphase table will be the same as that for the liquid phase. It is normally best to leave the Maxwell constructions until constructing the multiphase table.

Limiting range of tables: By default, a phase is included in the phase search only at densities and temperatures that fall within the range of its table. This range can be further restricted using the input parameters RLO, RUP, TLO, TUP.

Phase diagram: The PHASE DIAG*RAM command is used to construct a table of the phase transition points. The user enters a temperature mesh for tabulating the transitions, which are printed at the terminal and also sent to the plot file. The transitions are listed at increasing temperatures, transition pressure increasing within each temperature block. Each transition is identified by the names of the lower- and upper-density phases, the temperature and pressure, and the densities, energies, and entropies of each phase.

The output from PHASE DIAG is not always convenient for plotting. The new PHASE SORT command can be used to find all points corresponding to different pairs of phases and organizing them into separate blocks. The code prompts the user for the file generated with PHASE DIAG, an output file, and the names of all phases to be considered in the sorting. The output file sometimes requires further editing, especially in the vicinity of triple points.

Sample input files: An input file that uses the MOD TRN option can be found in directory input/titanium. This file calculates the phase diagram and constructs a multiphase EOS table from four EOS tables created with the MOD SOL and MOD LIQ options.

MERGE OPTION

The MOD MRG command, new to EOSPro, is used to merge EOS tables by specifying different EOS tables in different density-temperature regions. This option allows the use of several different models in construction of an EOS. However, it does not provide any algorithm for smoothing the transition between regions or ensuring thermodynamic consistency in regions of interpolation. MOD MRG can also be used to clean up numerical problems that have arisen in certain regions of the EOS surface.

Setup: No parameters are entered on the MOD MRG command line. The user is prompted to enter seven parameters for each EOS table: the material number, file name, energy shift, and density-temperature limits (RL, RU, TL, TU). A namelist format is *not* used in this case, and all parameters are required.

The order in which the tables are specified is very important. The EOS values at a given density-temperature point in the merged EOS will be computed from the first table for which the point falls within its limits. Each EOS table can be specified more than once, and regions can overlap, allowing the construction of complicated stability regions.

An application: In modeling reactive materials, it is best to construct separate EOS tables for the unreacted material and the reaction products, together with a time-dependent rate law for treating the transition, e.g., in a hydrocode. However, it is sometimes possible to construct a single EOS table by merging the

unreacted EOS, at low temperatures, with the reaction product EOS, at high temperatures. In such cases, it is usually necessary to leave out temperature points in the neighborhood of the transition, to eliminate pathological behavior (negative heat capacities, etc.). This procedure will *not* work for explosives, but it may give acceptable results for some polymers and other non-explosive materials. While not recommended as the *best* solution, it can be a useful expedient when time and/or experimental data are limited.

MODEL TESTING COMMANDS

EOSPro offers a number of commands for making calculations using the models discussed above. These commands are listed in the EOSPro command summary and discussed in Sec. 12 of the PANDA manual. There are several changes and improvements to the PANDA options.

Isentropes and adiabats: The ISEN*TROPE option is used to compute a constant-entropy curve. EOSPro also offers an ADIA*BAT command, which computes an adiabat without using the entropy, by integrating the equation $P = (\partial E / \partial \rho)_S$. The two commands are used in similar ways and should give similar results, but the ISEN option is generally more accurate. Both commands also allow material strength to be included in calculating release adiabats. The commands have the form:

ISEN*TROPE *modtyp* T1 R1 R2 NPTS MTYPE UP1 IEP

ADIA*BAT *modtyp* T1 R1 R2 NPTS MTYPE UP1 IEP

where

<i>modtyp</i>	model (SOL, LIQ, MIX, TRN, MRG)
T1, UP1	initial temperature and particle velocity (at density R1)
R1, R2, NPTS	density range and number of points
TYPE	1 for equal spacing, 2 for exponential spacing
IEP	0 for no strength, 1 to include strength (release behavior only)

Note that the SET STR command must be used to define the strength parameters before using IEP=1.

Detonation properties: The CJ (Chapman-Jouguet) command is used for computing the detonation properties of an explosive from the EOS of its reaction products. This option has been completely rewritten. It is much more accurate and can usually find the CJ state even in cases where there are multiple minima in the Hugoniot curves, which commonly occurs in high-carbon explosives like TNT. (Previously, these cases had to be analyzed by inspection of each point, using the HUGE option.)

Impedance matching: Impedance matching (sometimes called impedance *mismatching*) is a technique for using a standard material (the driver) to measure the shock properties of another material (the target). The experiment measures one shock property for both the driver and the target. The second shock property of the target is determined from the EOS of the standard, by locating the point at which the driver Hugoniot or release curve intersects the target Hugoniot. The EOSPro MATCH command offers four options for computing the shock state in the target, used in different conditions.

Depending on the option to be used, Hugoniot and/or release curves for the driver and target are first computed using the HUG, HUGE, ISEN, and/or ADIA commands. The option is then selected using

MATCH *opt*

where

<i>opt=0</i>	code issues a list of the four options
<i>opt=1</i>	find shock state for given impact velocity from driver & target Hugoniot
<i>opt=2</i>	find shock state for given target shock velocity from driver velocity & Hugoniot
<i>opt=3</i>	find shock state from target Hugoniot and driver release curve
<i>opt=4</i>	find shock state for given target shock velocity and driver release curve

An input file that uses the MATCH option can be found in directory input/match. This file determines the shock state when an Al driver impacts a D₂ target. It first finds the shock state from the driver release curve and target Hugoniot calculated from existing EOS tables (*opt=3*). It checks the result by using the driver isentrope with the calculated target shock velocity (*opt=4*).

TABULAR EOS COMMANDS

The EOS models in EOSPro are much too complicated to be incorporated and used “in-line” in hydrocodes and other programs. The Sesame EOS library was developed to enable the use of such models in tabular form. EOSPro offers a number of commands that are used for generating, storing, and accessing the EOS tables in a Sesame data base. These commands are listed in the command summary and discussed in Secs. 13 and 14 of the PANDA manual. Only a few additional comments are needed here.

Maxwell constructions: In constructing tables, the standard, recommended procedure is to make the so-called Maxwell constructions at high temperatures, e.g., above the boiling point, and leave a tension region at low temperatures, for use with spall (tensile fracture) models in hydrocodes. This procedure is described in Sec. 13.5 of the PANDA manual. When the user elects to include Maxwell constructions, the following prompt is issued:

```
Enter TSPALL, guess of RSPALL, and DPDR
```

where TSPALL and RSPALL are the boundaries of the tensile region. The last parameter, DPDR, is the derivative of the pressure with respect to density in the coexistence region. A very small positive slope (0.001) is useful for making tables for the MOD MIX option. The modifications to the EOS in tension can be skipped by specifying RSPALL=0.

MISCELLANEOUS

MOD USE: The PANDA code allowed users to construct a new model by replacing two routines in the code (Sec. 15.1 of the manual). The mechanics for this option have been retained in EOSPro, but the option is presently deactivated because the source code is not being made available to users.

SHOCK DATA: This command is used to enter Hugoniot data or retrieve data from a file having a specific format, as described in Sec. 15.2 of the PANDA manual. The only change in EOSPro is to enter KEYB*OARD, instead of TTY, when entering data from the keyboard.

Strength model: The SET STR command is used to define material strength parameters for use in the HUG, HUGE, ISEN, and ADIA commands. The command syntax and equations are given in the command summary. Input differs from that given in Sec. 15.3 of the PANDA manual in that the initial density R0 must also be specified as the first parameter. One other minor change is that the yield strength and shear modulus are not allowed to go negative. The model presently does not provide for melting; that option could be added in the future.

MONTE CARLO: This command, discussed in Sec. 15.4 of the PANDA manual, uses the well-known numerical method to generate an EOS for a finite system of particles interacting with specified two-body potentials. In EOSPro, the first-order quantum mechanical correction to the free energy is computed for the EXP-6 potential. The units are MJ-kg/(kg-mole)**2; divide this term by the molecular weight W to obtain MJ/kg-mole or by W**2 to obtain MJ/kg.

Recentering Hugoniot data: The term “recentering,” when applied to Hugoniot data, means estimating how the data would shift if the material were shocked from a different initial density, pressure, and energy. This technique can be useful in analyzing shock data for porous materials, because porosity not only shifts the Hugoniot, in the $U_s - u_p$ plane, but also distorts it at low shock pressures. It can also be used to clean up noise due to variations in initial density, and to analyze the effects of shock-induced phase transitions. Some assumption about the Grüneisen parameter must be made to apply this method.

The RECEN*TER command is used to perform this analysis in EOSPro. The code prompts the user:

```
Enter parameters for new initial state--R0,P0,E0,G0,GN,GL,SR
--> Gruneisen function is GAMMA = G0*(R0/RHO)**GN+GL
```

where R_0 , P_0 , and E_0 are the density, pressure, and energy for the *new* initial state; G_0 , G_N , and G_L are the parameters for the Grüneisen function (as indicated in the formula); and SR is an optional density scaling factor to be applied to the original data (defaulted to $SR=1$).

The code then prompts for one line of input for each shock point to be recentered, containing five items of data: R_0 , UP , US , P_0 , E_0 —the initial density, the particle and shock velocities, and the initial pressure and energy. Output is sent to the terminal and the plot file, with the same format as in SHOCK DATA.

MIX PROP: This command can be used to compute the chemical composition, thermodynamic properties, and Hugoniot of an *unreacted* mixture, using the properties of the individual mixture components. Note that this option is completely different from the MIX MOD option; MIX PROP gives a less accurate prediction of the mixture EOS but is much simpler and quicker to use for making rough estimates.

The command form is MIX PROP *PMX*, where *PMX* is an optional upper pressure on the estimated Hugoniot (defaulted to 50 GPa). The code then prompts the user for two lines of input for each component of the mixture. The first line is the chemical formula, entered the same way as in the SET BAS and MIX MOD commands. The second line consists of up to eight parameters. The code prompt is:

Enter WT,RO,HF,CS,S1,S2,G0,CV for this component

where	WT	weight (or weight fraction)—required
	RO, HF	density and heat of formation (MJ/kg)—required
	CS, S1, S2	coefficients in US-UP fit—optional, same fit as cold curve option ICLD=1
	G0, CV	Grüneisen parameter and heat capacity (MJ/kg/K)—optional

The code computes the elemental composition, density, and heat of formation of the mixture, at ambient pressure and temperature, assuming thermal and mechanical equilibrium between the components. It also estimates the Hugoniot at 25 pressures from 0 to *PMX*, by assuming additive volumes at equal shock pressures (a crude approximation); it also gives a rough quadratic fit to the results. It also estimates the Grüneisen parameter and heat capacity of the mixture using simple averages.

The MOD MIX option is especially useful for determining the properties of unreacted explosives and other reactive materials that contain varying amounts of additives, binders, elastomers, fillers, etc. The chemical formula and heat of formation of the mixture can then be used as input to the MOD MIX command for the reaction products. The Hugoniot, Grüneisen parameter, and heat capacity can also be used as rough estimates for the EOS of the unreacted material; though admittedly crude, these estimates are often more reliable than those obtained by trying to fit experimental data, which are frequently very hard to find, sparse, and of low precision for these kinds of materials. A sample input file that applies this option to an aluminumized HMX explosive composition can be found in directory input/mixprop.

PLANET: This option computes the structure of Jovian-like planets, using the third-order perturbation method (“theory of figures”), developed by Zharkov and Trubitsyn (ZT) [19]. The method, and its application to the structures of Jupiter and Saturn, is described in Ref. [20]. The key points are summarized below.

- In the ZT method, all points in the planetary interior lie on a single density-pressure curve, usually called the “planetary adiabat,” which starts at the density-temperature state at the outer radius and proceeds to higher densities.
- The adiabat is constructed before calling the PLANET option, using the ISEN or ADIA command. The mixture model is normally used, because the planetary atmospheres consist of several chemical elements. Separate adiabats are used for the envelope and the core. The envelope adiabat can also be created in sections, to treat changes in chemical composition with depth [20].
- After calling PLANET, the user specifies the adiabat information, the planetary mass, equatorial radius, rotation period, a guess of the flattening parameter, and the computational mesh.
- The code calculates the gravitational moments, J_2 , J_4 , and J_6 , the central core pressure, the “equidistance” (inverse transit time for a sound wave) and various other parameters related to the shape.

Directory input/jupiter includes a sample input file in which the PLANET command is used to compute the structure of Jupiter, using the model described in Ref. [20].

RETAB*ULATE: This command is used to map the columns of a file onto a new mesh and send the results to the plot file. The user is prompted to enter the name of the data file and the number of columns to be read. (The file can include comment lines (starting with #) and even blank lines, as in an EOSPro plot file.) The user selects one column in the file that is to be treated as the independent variable and then interpolates all the columns onto a new mesh. By following the prompts, the user can:

- reverse the order of the data on the file,
- specify the new mesh and the column to be used as the independent variable,
- choose certain columns to be treated using logarithmic interpolation.

This option is useful adding or removing points for plotting. It is also useful for locating specific points on curves, e.g., specific pressures on a Hugoniot.

REFOR*MAT: This command is used to reorder columns of data in a file, apply scale factors and shifts, and send the results to the plot file. The user is prompted to enter the name of the data file and the numbers of the columns to be included, specified in the order they are to appear in the output file. (This file must not include any comments or blank lines.) The user is then prompted to specify the columns to be modified, along with the scale factor and shift. This option is useful for certain editing tasks, e.g., for plotting or setting up input to other EOSPro commands.

FSPLIT: This command is used to split a text file into a number of smaller files. It is similar to the command, available on some Unix systems, that splits a Fortran program into individual subroutine units. The EOSPro version looks for blocks in the file that begin with one of four keywords—PROGRAM, MODULE, SUBROUTINE, or FUNCTION—followed by a name for that block. Each block ends when another keyword is detected. The code constructs a separate file for each block, assigning it the name following the keyword. (If no name follows the keyword, the routine makes one up.) The user also has the option to specify a suffix, e.g., .F, .f03, etc. FSPLIT is especially useful for code maintenance but occasionally comes in handy for splitting other kinds of text files.

OTHER UTILITIES

The util directory of the EOSPro code package contains some useful little programs that are not convenient to include in EOSPro itself. Only the source code is provided. Users should compile them on their own systems. They include:

- **udc.c**, written in C, changes text files between DOS and Unix formats: `udc opt file`, where *opt* is the option (*u2d* to convert from Unix to DOS, *d2u* to convert from DOS to Unix), and *file* is the name of the file to be converted.
- **ulc.c**, written in C, changes text files between lower and upper case: `ulc opt file`, where *opt* is the option (*l2u* to convert from lower to upper, *u2l* to convert from upper to lower).
- **grun.f95**, written in Fortran, calculates the Grüneisen parameter from the volume coefficient of thermal expansion VTE (K⁻¹), the sound speed CS (km/s), and the constant pressure specific heat CP (J/g/K).
- **pois.f95** calculates Poisson's ratio from the bulk and shear moduli (GPa).
- **tmd.f95** calculates the theoretical material density (TMD) from the formula weight FW, the dimensions of the unit cell (three lengths and three angles), and the number of molecules per unit cell Z.
- **yhel.f95** calculates the yield strength (GPa) from the Hugoniot elastic limit HEL (GPa), the bulk modulus (GPa), and Poisson's ratio.

FINAL COMMENTS

In offering the user so many options for EOS modeling, EOSPro also offers many opportunities for making mistakes. The code is very robust. It traps many errors and prompts the user to take corrective action. It very seldom "crashes." One down side of this robustness is that a mistake or problem in an input file usu-

ally causes the rest of the file to be executed *incorrectly*. This situation is not always obvious, especially when error and warning messages scroll off-screen before they can be read. It is wise to scan output files for the words “ERROR” and “WARNING.” And, as already mentioned, one should make many plots.

Some common problems are:

- Opening and attempting to write to an existing file. The code will identify this situation and will ask the user what to do, requiring an extra line of input that may not be present in the file.
- Getting input lines out of sequence. It is wise to input from the keyboard, until the proper sequence has been nailed down, before relying exclusively on input files.
- Failing to terminate a block of input. Many commands continue to read lines of input until a blank line is entered.
- Misspelling or giving the wrong name for a namelist parameter. The code will issue a warning message if it encounters an unknown name, but it is easy to overlook this mistake.
- Typos in constructing meshes can lead to the omission of entire blocks of densities and temperatures when constructing EOS tables.

Many other problems can and will occur. One should expect and plan for them.

As already mentioned, the input directory of the code package contains sample input files that illustrate how to use various commands and options. It is important to recognize that these files show the results of the modeling process, not the process itself. The development of an EOS model should be regarded as a *research* problem—sometimes a little one, and sometimes a very big one.¹ It is not possible to reduce this kind of work to a set of step-by-step instructions, or even to a flow chart. One can only learn the process by doing it, by experience. But EOSPro should give you a lot of help. Also be sure to view the tutorials on the website and read the many reports that describe PANDA/EOSPro models. Good luck!

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- [3] <http://kerleytechnical.com>
- [4] Gnuplot is a powerful utility for plotting technical data on many different platforms. See <http://www.gnuplot.info/> for instructions on downloading, installation and use.
- [5] Equations for the p-alpha model are given in: E. S. Hertel, Jr. and G. I. Kerley, “CTH Reference Manual: The Equation of State Package,” Sandia National Laboratories report SAND98-0947, 1998. Distribution of this report is limited. See Ref. [6] for a more limited discussion.
- [6] G. I. Kerley, “Equation of State and Constitutive Models for Numerical Simulations of Dust Impacts on the Solar Probe,” Kerley Technical Services Report KTS09-1, August 2009.
- [7] D. A. McQuarrie, Statistical Mechanics (University Science Books, Sausalito, CA, 2000), Sec. 10-5.
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1. “Research” may be considered a bad word by those who are focused on programmatic objectives, but one can at least think it even if not allowed to use it when talking to management!

- EOSPro. A second file, named *orbmod*, tabulates orbital data for 16 elements that have been revised by hand, to give better agreement with experimental ionization potentials and energy levels.
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