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ANEOS Analytic Equations of State for Shock Physics Codes Input Manual



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Samuel L. Thompson

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ANEOS
Analytic Equations of State
for Shock Physics Codes
Input Manual

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ABSTRACT

ANEOS is an in-line software package which provides thermodynamic information for shock physics codes. Solids, liquids, vapors, plasmas and phase mixtures are considered in a thermodynamically consistent and complete manner. The package is flexible and easy to use. This users manual contains input instructions, examples, and descriptions of user output.

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CONTENTS

Section	page
Introduction.....	1
Model Extensions and New Options.....	2
Thomas-Fermi Electronic Model.....	3
Low-Temperature Solid Model.....	4
Error Processing.....	5
Extensions for Reactive Chemistry Models....	6
References.....	7

APPENDICES

A. ANEOS Input Instructions.....	A-1
Option 2,3,4 Solid-Liquid-Gas.....	A-3
Option -1, Low-Temperature Solid.....	A-10
Option -2, Ideal Gas.....	A-17
Option -3, JWL High Explosive.....	A-24
Option -4, User Supplied Model.....	A-31
B. Summary of Model Parameters.....	B-1
Option 2,3,4 Solid-Liquid-Gas.....	B-2
Option -1, Low-Temperature Solid.....	B-6
Option -2, Ideal Gas.....	B-10
Option -3, JWL High Explosive.....	B-14
Option -4, User Supplied Model.....	B-18

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INTRODUCTION

ANEOS is a thermodynamically consistent analytic equation-of-state package used by CHARTD, CSQ, CTH, CKEOS and various wave propagation codes [1-6]. The package consists of a set of in-line routines that are flexible and easy to use. This document contains the input instructions for the various ANEOS equation-of-state models in Appendix A. Detailed descriptions of the models are given elsewhere [7,8,9,10]. The contents of the ANEOS storage arrays are given in Appendix B. These arrays are listed during the package set-up phase.

There have been a number of versions of the ANEOS package. The version described in this document has a date of February 1990. This manual will be updated to reflect additional options as they become available. A current version of this document can be obtained from the author or his computer document directory. Current documentation is distributed as an ASCII text file with the software and can be printed on any available printer. The intent is to have current on-line documentation on the same computer system where the package is used.

There are seven different ANEOS models. All seven models can now be used with all codes which use the ANEOS package.

The seven models with option numbers are

2. Gas with ionization
3. Solid-liquid-gas without ionization
4. Solid-liquid-gas with ionization
- 1. Low-Temperature Solid
- 2. Ideal Gas
- 3. JWL High Explosive with or without ionization
- 4. User Supplied Model

Previous versions of ANEOS had several options which could not be used with Eulerian wave codes. One major improvement in the current version is the -1 option which can now be used with any code with considerable execution time gains. Previous versions of ANEOS also had two other options (0 and 1) which were not particularly useful in most situation and have been removed from the input instructions.

Each of the above forms has many optional features. For example, ionization can be treated by the Saha ionization equilibrium model or the Thomas-Fermi model [11]. Detailed modeling of the melt phase change can be included at the user's option.

The -4 option allows the user to supply his own model in a convenient form. The author should be consulted if there is interest in using this feature.

MODEL EXTENSIONS AND NEW OPTIONS

There are a number of improvements in the current ANEOS code. Some of the improvements are numerical. For example, a vector interface to the package has been added and a considerable amount of code has been rewritten to allow for multiple CPU parallel processing. For workstation operation, the code can automatically be converted to double precision using CMP include decks [12].

There have also been several model extensions. Others are currently under development. The following sections give some details necessary to use the new options for a few selected models. Other new features are found in the input instructions. Detailed model descriptions are being written [9,10].

THOMAS-FERMI ELECTRONIC MODEL

Early in the development of ANEOS, a temperature-dependent Thomas-Fermi (TF) model was built by D. J. McCloskey based on the work of R. Latter [11]. In this implementation, the zero temperature terms were subtracted and the atomic weight and number were scaled out of the formal relations. A table was constructed in scaled density and temperature variables. By using a smooth interpolation routine, all interesting densities and temperatures could be computed for all materials.

The model was not included in the original ANEOS code because of the memory required to store the tabular data. By current standards the approximately 8500 CRAY words required for the tables and evaluation routines is acceptable and the model has been included in the new ANEOS.

In the models that include electronic terms (options -3, 2, 4), either the average atom ionization equilibrium or the Thomas-Fermi model can be selected by input. The two models will NOT give identical results. They do yield the same asymptotic behavior and generally are close in their predictions for most conditions though there are local variations. With regard to computational speed, the TF model is slightly slower than the single-element ionization equilibrium model, but it can be considerably faster than the multi-element ionization equilibrium model.

LOW-TEMPERATURE SOLID MODEL

The original ANEOS code contained a low temperature solid model (the -1 option). Unfortunately, this model could only be used in Lagrangian codes. The mixed-cell iterations required in Eulerian codes would sometimes fail because of unrealistic behavior at low or high densities.

The current version of ANEOS has several extensions to the model to allow use in Eulerian codes. To make the model usable, a "two-phase" extension has been developed for low densities. The P=0 curve is defined as the liquid-phase density with the vapor-phase boundary at a very small density. This allows the mixed-phase thermodynamic relations to be applied in a consistent manner.

The models developed in reference 8 are used only in the density range

$$RHO_{low} < RHO < RHO_{high} ,$$

where the bounds are input parameters and it is assumed that the reference density is within this range. For larger or smaller densities, where the model is not valid, an extrapolation is employed to allow mixed-cell iterations to converge. Default values of RHO_{low} and RHO_{high} are provided. RHO_{high} is selected at a Hugoniot pressure of three Mbars. If warning or fatal error messages are generated during the setup process, it might be necessary to define input values which are closer to the material reference density.

For temperatures below melt, the relations are treated in the same manner as the options 3 and 4 with a tension region [7]. For numerical reasons, the melt temperature must be sufficiently high so that the "triple point" is contained in the low density extrapolation region. If the user input does not satisfy this condition, the melt temperature is increased as required. If this is not satisfactory, then the user should increase the value of RHO_{low} .

There are three major additions to the relations in reference 7. The $Th(RHO)$ function in (III.4.6) is determined by numerical integration and stored as an interpolation table. For $RHO > RHO_{high}$, the cold compression pressure is given by

$$P_c = C(38) + C(39) * RHO^{**2}$$

and, for $RHO < RHO_{low}$,

$$P_c = C(49) + C(50) / RHO$$

where the indices of the C array refer to the values listed in appendix B. Additional details are available in reference [9].

This ANEOS model is completely vectorized. In codes that use the ANEOS vector interface, this option is by far the fastest model of a solid.

ERROR PROCESSING

The revised ANEOS package has improved error checking. This includes input processing and testing for unphysical behavior. Both "warning" and "fatal" messages can be produced during the set-up phase of ANEOS. Fatal errors will result in execution termination at the end of the set-up phase of ANEOS. Warning messages do not terminate the calculation but will point out features which do not seem to be realistic. The user should evaluate the problem and correct it if appropriate.

During the run phase of the calculation, ANEOS may produce fatal error messages for a few situations. These result in immediate termination of the execution. Examples might be a request to evaluate properties of an undefined material or a material with a negative density. There are no warning messages during this phase of the calculation.

EXTENSIONS FOR REACTIVE CHEMISTRY MODELS

Reactive chemistry calculations are becoming increasingly important in the type of codes which employ the ANEOS package. While these are not envisioned to be an integral part of the ANEOS package, they do add requirements which ANEOS data must satisfy.

The basic formulation of the thermodynamics used in ANEOS has two arbitrary constants. These can be used to add offsets to the absolute energy and entropy. For example, if ρ is the density, T is the temperature and $F(\rho, T)$ is a description of the Helmholtz free energy of a material, then

$$F'(\rho, T) = F(\rho, T) + E_{\text{shift}} - T * S_{\text{shift}}$$

is an equally good description. The two constants E_{shift} and S_{shift} do not alter the hydrodynamic behavior. They are important only in reaction models where one material is converted to another. The shifts are used to control reaction chemistry and energy release.

The details of how these constants should be selected depend on the reaction model employed and will be addressed with the model.

— —

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ANEOS Input Manual

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APPENDIX A

ANEOS INPUT INSTRUCTIONS

There are five complete sets of input instructions for the seven options. The first and last records in the set are the same for all options. There are three or five intermediate records depending on the information on the first record. Older versions of ANEOS used only three intermediate records. The extended input format is allowed in the current version to provide for model extensions. The physical meanings of input parameters on the intermediate records vary for the different options.

ANEOS has its own input processor which is compatible with the free form processors used in most wave codes. Each input record begins with an identification field (RID=Record ID) which must be ANEOS. User identification characters can be added after the "S". Positional parameter locations are indicated by (number) following the variable name. Except for the first record, all input is in the positional format with blank separators. Trailing zeros can be omitted. The keyword parameters on record 1 (form KEYWORD=VALUE or KEYWORD) are optional and must follow positional parameters. Records with an * in column 1 are comments.

Inputs units are cgs with temperature in ev (1 ev = 11605.333 K) unless otherwise noted. All printed output is also in these units.

The numbers in square brackets [] refer to the reference with section or equation numbers. For example [8,7.3] refers to equation 7.3 in reference 8.

On the first input record there is a parameter NEOS which is the equation-of-state number. This parameter is normally referenced in the wave code input to link a given wave code material to this data; for example, to tell the code that material 3 uses ANEOS number -5. This number must be unique in the data input set and ranges from -1 to -n, where n is the maximum number of materials allowed in this code application. For CHARTD, n is 20; for CSQ and CTH, n is 10; and for CKEOS, n is 5. Positive equation-of-state numbers have traditionally been reserved for tabular data forms.

ANEOS equations of state have been created for nine materials and have been added to the code as a library. These examples are intended to illustrate the input and features [7]. They are probably not the best data for the given materials. The program CKEOS [6,10] can be used to analyze any ANEOS equation of state constructed for use with any of the wave codes.

ANEOS Input Manual

Examples of ANEOS Input Records

```

ANEOS -1 'Aluminum from library' LIB=6 TYPE=4
*
* * * * *
ANEOS1 -2 'Iron with 130 Kbar phase change' THUG=-1 RHUG=-1
*   V1   V2   V3   V4   V5   V6   V7   V8
ANEOS2  1   3   7.85  0   0   1.93E12  1.75  0
*   V9   V10  V11  V12  V13  V14  V15  V16
ANEOS3  0   2   7.3E10  0.282  0   0   0   0
*   V17  V18  V18  V20  V21  V22  V23  V24
ANEOS4  0   8.36  8.75  1.12E11  2.3E12  5.E12  0   0
*   Z   FRACTION
ANEOS5  26   1
*
* * * * *
aneos -3 'JWL PBX 9404 with Saha electrons'
* detonation velocity = 8.8e5 Pcj = 3.7e11
*   V1   V2   V3   V4   V5   V6   V7   V8
aneos  4   -3   1.84  0   0   1   0.38  0
*   V9   V10  V11  V12  V13  V14  V15  V16
aneos  0   0   6E11  .04  0   0   0   0
*   V17  V18  V18  V20  V21  V22  V23  V24
aneos  0   8.524  0.1802  4.6  1.30  1   0   0
*   Z   FRACTION
aneos  1 .293177
aneos  6 .149254
aneos  7 .270789
aneos  8 .286780
*
* * * * *
ANEOS -4 'Lead with Thomas-Fermi and Melt' LONG
*   V1   V2   V3   V4   V5   V6   V7   V8
ANEOS  1   4   11.35  0   0 -2.051E5  2.77  0.0076
*   V9   V10  V11  V12  V13  V14  V15  V16
ANEOS  1.46  2   9.5E9  -4.08E8  2.E12  0   4.E10  0
*   V17  V18  V18  V20  V21  V22  V23  V24
ANEOS  9.94  0   0   0   0   0   2.3E8  0.967
*   V25  V26  V27  V28  V29  V30  V31  V32
ANEOS  0
*   V33  V34  V35  V36  V37  V38  V39  V40
ANEOS  1
*   Z   FRACTION
ANEOS  82   1

```

Inputs for ANEOS options 2,3,4

Record 1

RID (1) ANEOS

NEOS (2) Equation-of-state number (negative number).
 For CHARTD, -1 to -20.
 For CSQ and CTH, -1 to -10.
 For CKEOS, -1 to -5.

TITLE (3) Character string name of material.
 Enclose in single quotes (') if more than one word.

LIB=number Library equation-of-state number if desired.

TYPE=number Used only with a library equation of state (LIB=).
 Number determines the type of analytic calculation
 (see V2, record 2 below). If outside of the range 2
 to 4 or if the library information is only for a gas,
 this input is ignored.

RHUG=value Value is the initial density for an in-line Hugoniot
 calculation. If not present, the calculation is skipped.
 If value < 0, the initial density is taken to be
 the reference density (V3, record 2 below).

THUG=value Value is the initial temperature for an in-line
 Hugoniot calculation. If not present, the calculation
 is skipped. If value < 0, the initial temperature is
 taken to be the reference temperature (V4, record 2
 below).

LONG This parameter is optional. If not present, the model
 uses 24 input parameters on records 2 through 4; if
 present, the model used 40 input parameters on records
 2, through 6.

```

* * * * *
*   If a library equation of state is requested, no   *
*   more data records are required for this material. *
* * * * *
    
```

Record 2

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=1,8. If a gas-only form is requested, V5 to V8 are ignored.

RID (1) ANEOS

V1. (2) The number of elements in this material.

V2. (3) Switch for type of equation of state.

- =2. Gas with ionization.
- =3. Solid-liquid-gas without ionization.
- =4. Solid-liquid-gas with ionization.

V3. (4) ρ_{00} - Reference density.

V4. (5) T_0 - Reference temperature.
If $T_0 \leq 0$, code sets $T_0 = 0.02567785$ ev (298 K).

V5. (6) P_0 - Reference pressure (normally 0).

V6. (7) B_0 - Reference bulk modulus (positive number) [7,III-3].
or
- S_0 - Reference sound speed in linear shock-particle velocity relation (negative number) [7,VIII-1].

V7. (8) GAMMA - Reference Gruneisen coefficient [7,III].

V8. (9) Theta - Reference Debye temperature [7,IV;8,III-1].
If theta = 0, code sets theta = 0.025.
If theta > 0, use high temperature approximation form.
If theta < 0, use complete Debye functions for solid model.

Record 3

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=9,16. If a gas-only form is requested, V9 to V14 are ignored.

RID (1) ANEOS

V9. (2) TG - Model selection parameter [7,III-1].

TG = -1, Slater theory,
TG = 0, Dugdale and MacDonald theory,
TG = 1, free-volume theory,
or

S1 - Constant in linear Hugoniot shock-particle
velocity relation [7,VIII-1].

Input variable is defined in relation to V6 on record 2.
(TG if V6 = Bo and S1 if V6 = So)

V10. (3) (3C24) - three times the limiting value of the Gruneisen
coefficient for large compressions, usually 0 or 2.
When a value of 2 is input, C24 = 2/3 [7,IV-1].

V11. (4) Es - Zero temperature separation energy [7,III-2].

If Es > 0, input is in ergs/gm.

If Es < 0, input is in ev/atom.

V12. (5) Tmelt - Melting temperature [7,V-1],

or

-Em - Energy to the melting point at zero pressure from
the reference point [7,V-1].

V13. (6) C53 - Parameter for low-density Pc modification to move
critical point (normally zero) [7,III-2].

V14. (7) C54 - Parameter for low-density Pc modification to move
critical point (normally zero) [7,III-2].

V15. (8) Ho - Thermal conductivity coefficient. If zero, thermal
conduction is not included. Note that the units of
H = Ho*T**C41 are ergs/(cm sec ev) [7,VII-2].

V16. (9) C41 - Temperature dependence of thermal conduction
coefficient (see V15) [7,VII-2].

Record 4

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=17,24. If a gas-only form is requested, all parameters are ignored.

RID (1) ANEOS

V17. (2) RHOMin - Lowest allowed solid density [7,V-3].
 If RHOMin \leq 0, code sets RHOMin = 0.8 * RHOo.

V18. (3) Parameter D1	\	Solid-solid phase transition parameters. If not used, enter 0. > See model descriptions in [7,V-7]
V19. (4) Parameter D2		
V20. (5) Parameter D3		
V21. (6) Parameter D4		
V22. (7) Parameter D5		

V23. (8) Hf - Heat of fusion for melt transition [7,V].
 If Hf = 0, melt transition is not included.
 If Hf < 0, code sets Hf=1.117E12 Tmelt/A (ergs/gm)
 where A is the average atomic weight.

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

V24. (9) Ratio of liquid to solid density at melt point [7,V],
 or
 - (Density of liquid at melt point),
 or
 (1 + Dvolume) where Dvolume is change in volume at melt.

Note: In the first option, the input number is between 0 and 1; in the second, it is negative; and in the third, it is greater than one.
 If Hf \neq 0 and V24 = 0, code sets V24 = 0.95.

Record 5

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=25,32. If a gas-only form is requested, all parameters are ignored.

RID (1) ANEOS

V25. (2) Upper bound of the term $B_{00}/(\rho_{00} \cdot E_s \cdot G_{hat}^{**2})$ in the cold compression relation for expanded states [7,3.30].
If input = 0, the default is one. In general, smaller values will decrease critical point temperature.

V26. (3) Lower bound of the term $B_{00}/(\rho_{00} \cdot E_s \cdot G_{hat}^{**2})$ in the cold compression relation for expanded states [7,3.30].
If input = 0, the default is zero.

V27. (4) Alpha of liquid EOS correction [7,5.22]. If input Alpha = Beta = Gamma = 0, the older defaults of Alpha = 0.3, Beta = 0.1 & Gamma = 0.2 are used. Parameter range is 0-1. Adjustment of these parameters is sometimes required to match vapor pressure data and boiling points.

V28. (5) Beta of liquid EOS correction [7,5.22]. If input Alpha = Beta = Gamma = 0, the older defaults of Alpha = 0.3, Beta = 0.1 & Gamma = 0.2 are used. Parameter range is 0-1. Beta and Gamma can not be equal.

V29. (6) Gamma of liquid EOS correction [7,5.22]. If input Alpha = Beta = Gamma = 0, the older defaults of Alpha = 0.3, Beta = 0.1 & Gamma = 0.2 are used. Parameter range is 0-1.

V30. (7) Not used in current model, enter zero.

V31. (8) Not used in current model, enter zero.

V32. (9) Not used in current model, enter zero.

Record 6

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=33,40. If a gas-only form is requested, all parameters except 33, 34 and 35 are ignored.

RID (1) ANEOS

V33. (2) Flag for form of ionization model.
Used only for V2 options 2 and 4.
= 0, Saha model.
= 1, Thomas-Fermi model.

V34. (3) Eshift - Energy shift for reactive chemistry modeling.

V35. (4) Sshift - Entropy shift for reactive chemistry modeling.

V36. (5) Not used in current model, enter zero.

V37. (6) Not used in current model, enter zero.

V38. (7) Not used in current model, enter zero.

V39. (8) Not used in current model, enter zero.

V40. (9) Not used in current model, enter zero.

Record Set 7

There is one set of the following records for each element in variable 1, record 2. (I = 1, number of elements).

- RID (1) ANEOS
- Z(I) (2) Atomic number of element.
- f(I) (3) Unnormalized atomic number fraction of element,
or
- (Unnormalized atomic weight fraction of element.)
- All elements should be defined in the same way.

Example Input

```

ANEOS1 -1 Copper THUG=-1 RHUG=-1
ANEOS2 1 3 8.94 0 0 -3.94E5 1.99 0.271
ANEOS3 1.489 2 5.25E10 -4.637E9 6.E12 0.7 4.4E11 0
ANEOS4 0 0 0 0 0 0 2.055E9 -8.217
ANEOS5 29 1
*
ANEOS -4 'Mostly lead with TF and Melt' LONG
* v1 v2 v3 v4 v5 v6 v7 v8
ANEOS 2 4 11.35 0 0 -2.051E5 2.77 0.0076
* v9 v10 v11 v12 v13 v14 v15 v16
ANEOS 1.46 2 9.5E9 -4.08E8 2.E12 0 4.E10 0
* v17 v18 v18 v20 v21 v22 v23 v24
ANEOS 9.94 0 0 0 0 0 2.3E8 0.967
* v25 v26 v27 v28 v29 v30 v31 v32
ANEOS 0
* v33 v34 v35 v36 v37 v38 v39 v40
ANEOS 1
* z fraction
ANEOS 82 0.99
ANEOS 29 0.01
    
```

Inputs for ANEOS option -1

Low Temperature Solid

Most features of this EOS model is described in [8,III.4-1]. This form should not be used in energy flow calculations unless the material is isolated from any high temperature regions.

Record 1

RID (1) ANEOS

NEOS (2) Equation-of-state number (negative number).
 For CHARTD, -1 to -20.
 For CSQ and CTH, -1 to -10.
 For CKEOS, -1 to -5.

TITLE (3) Character string name of material.
 Enclose in single quotes (') if more than one word.

LIB=number Library equation-of-state number if desired.

RHUG=value Value is the initial density for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial density is taken to be the reference density (V3, record 2 below).

THUG=value Value is the initial temperature for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial temperature is taken to be the reference temperature (V4, record 2 below).

LONG This parameter is optional. If not present, the model uses 24 input parameters on records 2 through 4; if present, the model used 40 input parameters on records 2 through 6.

```

* * * * *
*   If a library equation of state is requested, no   *
*   more data records are required for this material. *
* * * * *
    
```

Record 2

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=1,8.

RID (1) ANEOS

V1. (2) The number of elements in this material.

V2. (3) -1 = Switch for type of equation of state.

V3. (4) RHOo - Reference density.

V4. (5) To - Reference temperature.
If To \leq 0, code sets To = 0.02567785 ev (298 K).

V5. (6) Not used in current model, enter zero.

V6. (7) So - Reference point bulk sound speed.

V7. (8) GAMMA - Reference Gruneisen coefficient. Must be greater than zero. Default is one.

V8. (9) Not used in current model, enter zero.

Record 3

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=9,16.

RID (1) ANEOS

V9. (2) S1 - Constant in linear Hugoniot shock-particle velocity relation.

or

-100 - For power series representation of PH.
Enter variables 18 to 21.

V10. (3) Not used in current model, enter zero.

V11. (4) Cv - Heat capacity. If Cv <= 0, code sets Cv = 3*No*K.

V12. (5) Tmelt - Melting temperature.

or

-Em - Energy to the melting point at zero pressure from the reference point.

V13. (6) RHOlow - Low density limit for model extrapolation.
Enter zero for default.

V14. (7) RHOhigh - High density limit for model extrapolation.
Enter zero for default for Ph(RHOhigh)=3Mb.

V15. (8) Ho - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = Ho * T * C41$ are ergs/(cm sec ev) [7,VII-2].

V16. (9) C41 - Temperature dependence of thermal conduction coefficient (see V15) [7,VII-2].

Record 4

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=17,24.

RID (1) ANEOS

V17. (2) Not used in current model, enter zero.

V18. (3) Model parameter K1. \

V19. (4) Model parameter K2. | Used only if V9 = -100
> Otherwise enter zero

V20. (5) Model parameter K3. | See [8,III.4.23]

V21. (6) Model parameter K4. /

V22. (7) Not used in current model, enter zero.

V23. (8) Not used in current model, enter zero.

V24. (9) Not used in current model, enter zero.

— —

Record 5

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=25,32. All parameters are ignored.

RID (1) ANEOS

V25. (2) Not used in current model, enter zero.

V26. (3) Not used in current model, enter zero.

V27. (4) Not used in current model, enter zero.

V28. (5) Not used in current model, enter zero.

V29. (6) Not used in current model, enter zero.

V30. (7) Not used in current model, enter zero.

V31. (8) Not used in current model, enter zero.

V32. (9) Not used in current model, enter zero.

— —

Record 6

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=33,40. All parameters except 34 and 35 are ignored.

RID (1) ANEOS

V33. (2) Not used in current model, enter zero.

V34. (3) Eshift - Energy shift for reactive chemistry modeling.

V35. (4) Sshift - Entropy shift for reactive chemistry modeling.

V36. (5) Not used in current model, enter zero.

V37. (6) Not used in current model, enter zero.

V38. (7) Not used in current model, enter zero.

V39. (8) Not used in current model, enter zero.

V40. (9) Not used in current model, enter zero.

Record Set 7

There is one set of the following records for each element in variable 1, record 2. (I = 1, number of elements).

- RID (1) ANEOS
- Z(I) (2) Atomic number of element.
- f(I) (3) Unnormalized atomic number fraction of element,
 or
 - (Unnormalized atomic weight fraction of element.)

All elements should be defined in the same way.

Note: In this ANEOS model, the variables on record 7 are used only to determine the default value of heat capacity. If Cv is entered on record 3, the inputs on record 7 are read and ignored.

Example Input

```

ANEOS1 -1 'Be' THUG=-1 RHUG=-1
ANEOS2 1 -1 1.845 0 0 7.07e5 1.17 0
ANEOS3 1.091 0 0 0.134 0 0 0 0
ANEOS4 0 0 0 0 0 0 0 0
ANEOS5 4 1
    
```

Inputs for ANEOS option -2

Ideal Gas

This EOS model is described in [8,III.4-2]. This form should not be used in energy flow calculations unless the material is isolated from any high temperature regions.

Record 1

RID (1) ANEOS

NEOS (2) Equation-of-state number (negative number).
 For CHARTD, -1 to -20.
 For CSQ and CTH, -1 to -10.
 For CKEOS, -1 to -5.

TITLE (3) Character string name of material.
 Enclose in single quotes (') if more than one word.

LIB=number Library equation-of-state number if desired.

RHUG=value Value is the initial density for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial density is taken to be the reference density (V3, record 2 below).

THUG=value Value is the initial temperature for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial temperature is taken to be the reference temperature (V4, record 2 below).

LONG This parameter is optional. If not present, the model uses 24 input parameters on records 2 through 4; if present, the model used 40 input parameters on records 2 through 6.

```

* * * * *
*   If a library equation of state is requested, no   *
*   more data records are required for this material. *
* * * * *
    
```

Record 2

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=1,8.

RID (1) ANEOS

V1. (2) The number of elements in this material.

V2. (3) -2 = Switch for type of equation of state.

V3. (4) RHOo - Reference density.

V4. (5) To - Reference temperature.
If To \leq 0, code sets To = 0.02567785 ev (298 K).

V5. (6) K1 - Constant in Rosseland opacity expression.
Units are cm²/gm.

V6. (7) Not used in current model, enter zero.

V7. (8) (GAMMA-1) - Specific heat ratio minus one.

V8. (9) K2 - Constant in Rosseland opacity expression. Units are ev.
If K2 \leq 0, code sets K2 = .025 ev.

— —

Record 3

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=9,16.

RID (1) ANEOS

V9. (2) Not used in current model, enter zero.

V10. (3) Not used in current model, enter zero.

V11. (4) Cv - Heat capacity. If $Cv \leq 0$, code sets $Cv = 3/2 * No * K$.

V12. (5) Not used in current model, enter zero.

V13. (6) Not used in current model, enter zero.

V14. (7) Not used in current model, enter zero.

V15. (8) Not used in current model, enter zero.

V16. (9) Not used in current model, enter zero.

Record 4

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=17,24.

RID (1) ANEOS

V17. (2) Not used in current model, enter zero.

V18. (3) Not used in current model, enter zero.

V19. (4) Not used in current model, enter zero.

V20. (5) Not used in current model, enter zero.

V21. (6) Not used in current model, enter zero.

V22. (7) Not used in current model, enter zero.

V23. (8) Not used in current model, enter zero.

V24. (9) Not used in current model, enter zero.

Record 5

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=25,32. All parameters are ignored.

RID (1) ANEOS

V25. (2) Not used in current model, enter zero.

V26. (3) Not used in current model, enter zero.

V27. (4) Not used in current model, enter zero.

V28. (5) Not used in current model, enter zero.

V29. (6) Not used in current model, enter zero.

V30. (7) Not used in current model, enter zero.

V31. (8) Not used in current model, enter zero.

V32. (9) Not used in current model, enter zero.

— —

Record 6

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=33,40. All parameters except 34 and 35 are ignored.

RID (1) ANEOS

V33. (2) Not used in current model, enter zero.

V34. (3) Eshift - Energy shift for reactive chemistry modeling.

V35. (4) Sshift - Entropy shift for reactive chemistry modeling.

V36. (5) Not used in current model, enter zero.

V37. (6) Not used in current model, enter zero.

V38. (7) Not used in current model, enter zero.

V39. (8) Not used in current model, enter zero.

V40. (9) Not used in current model, enter zero.

— —

Record Set 7

There is one set of the following records for each element in variable 1, record 2. (I = 1, number of elements).

- RID (1) ANEOS
- Z(I) (2) Atomic number of element.
- f(I) (3) Unnormalized atomic number fraction of element,
or
- (Unnormalized atomic weight fraction of element.)

All elements should be defined in the same way.

Note: In this ANEOS model, the variables on record 7 are used only to determine the default value of heat capacity. If Cv is entered on record 3, the inputs on record 7 are read and ignored.

Example Input

```

ANEOSa -1 'He' THUG=-1 RHUG=-1
ANEOSb 1 -2 1.6154737e-4 0 0 0 0.6666667 0
ANEOSc 0 0 0 0 0 0 0 0
ANEOSd 0 0 0 0 0 0 0 0
ANEOSE 2 1
    
```

This EOS model is described in [8,III.4-3]. In this version of ANEOS, the JWL model is partially converted to ANEOS options 3 or 4 for the mixed-phase construction. The Van der Waals "loops" in the low-density, low-temperature region of the original Livermore formulation are not well suited for mixed-cell iterations. This causes slight differences in the calculated results for large expansions. See V22.

Tables of JWL constants are given in references 13 and 14. The following parameters from these tables should be entered as they appear in the tables without any unit conversion.

Record 1

- RID (1) ANEOS
- NEOS (2) Equation-of-state number (negative number).
 For CHARTD, -1 to -20.
 For CSQ and CTH, -1 to -10.
 For CKEOS, -1 to -5.
- TITLE (3) Character string name of material.
 Enclose in single quotes (') if more than one word.
- LIB=number Library equation-of-state number if desired.
- RHUG=value Value is the initial density for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial density is taken to be the reference density (V3, record 2 below).
- THUG=value Value is the initial temperature for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial temperature is taken to be the reference temperature (V4, record 2 below).
- LONG This parameter is optional. If not present, the model uses 24 input parameters on records 2 through 4; if present, the model used 40 input parameters on records 2 through 6.

```

* * * * *
*   If a library equation of state is requested, no   *
*   more data records are required for this material. *
* * * * *
    
```

Record 2

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=1,8.

RID (1) ANEOS

V1. (2) The number of elements in this material.

V2. (3) -3 = Switch for type of equation of state.

V3. (4) RHOo - Reference density.

V4. (5) To - Reference temperature.
If To \leq 0, code sets To = 0.02567785 ev (298 K).

V5. (6) Not used in current model, enter zero.

V6. (7) Flag which must be 1.

V7. (8) W - JWL parameter. (Enter in JWL table units)

V8. (9) Not used in current model, enter zero.

— —

Record 3

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=9,16.

- RID (1) ANEOS
- V9. (2) Not used in current model, enter zero.
- V10. (3) Not used in current model, enter zero.
- V11. (4) Cv - Heat capacity. If $Cv \leq 0$, code sets $Cv = 3/2 * No * K$. For most materials this default is too small; A value two to four times larger gives better results. Look at the calculated CJ point temperature T_{cj} and adjust as appropriate. Most explosives burn with a temperature in the range of 4000 K to 6000 K. (0.34 to 0.5 ev).
- V12. (5) Tmelt - Melting temperature. For this model, set to a value slightly above the reference temperature,
or
-Em - Energy to the melting point at zero pressure from the reference point.
- V13. (6) Not used in current model, enter zero.
- V14. (7) Not used in current model, enter zero.
- V15. (8) Ho - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = Ho * T * C41$ are ergs/(cm sec ev) [7,VII-2].
- V16. (9) C41 - Temperature dependence of thermal conduction coefficient (see V15) [7,VII-2].

Record 4

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=17,24.

RID (1) ANEOS

V17. (2) RHOMin - Lowest allowed solid density [7,V-3].
If RHOMin ≤ 0 , code sets RHOMin = 0.8 * RHOo.

V18. (3) Parameter A
V19. (4) Parameter B
V20. (5) Parameter R1
V21. (6) Parameter R2

\ | > | /
JWL Model Parameters
Enter in JWL table units.

V22. (7) Flag for form of ionization model.
= 0, Convert to type 3 - No electronic terms.
= 1, Convert to type 4 - Saha electronic model.
=-1, Convert to type 4 - Thomas-Fermi electronic model.
This parameter must be 1 or -1 if energy flow is to be calculated so that a Rosseland mean free path is returned.

V23. (8) Not used in current model, enter zero.

V24. (9) Not used in current model, enter zero.

Record 5

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=25,32. All parameters are ignored.

RID (1) ANEOS

V25. (2) Not used in current model, enter zero.

V26. (3) Not used in current model, enter zero.

V27. (4) Not used in current model, enter zero.

V28. (5) Not used in current model, enter zero.

V29. (6) Not used in current model, enter zero.

V30. (7) Not used in current model, enter zero.

V31. (8) Not used in current model, enter zero.

V32. (9) Not used in current model, enter zero.

Record 6

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=33,40. All parameters except 34 and 35 are ignored.

RID (1) ANEOS

V33. (2) Not used in current model, enter zero.

V34. (3) Eshift - Energy shift for reactive chemistry modeling.

V35. (4) Sshift - Entropy shift for reactive chemistry modeling.

V36. (5) Not used in current model, enter zero.

V37. (6) Not used in current model, enter zero.

V38. (7) Not used in current model, enter zero.

V39. (8) Not used in current model, enter zero.

V40. (9) Not used in current model, enter zero.

— —

Record Set 7

There is one set of the following records for each element in variable 1, record 2. (I = 1, number of elements).

- RID (1) ANEOS
- Z(I) (2) Atomic number of element.
- f(I) (3) Unnormalized atomic number fraction of element,
or
- (Unnormalized atomic weight fraction of element.)

All elements should be defined in the same way.

Example Input

```
* detonation velocity = 8.8e5  Pcj = 3.7e11
ANEOS -1 'PBX 9404 for radiation calculation'
ANEOS  4 -3  1.84  0  0  1  0.38  0
ANEOS  0  0  6E11  .04  0  0  0  0
ANEOS  0  8.524 0.1802  4.6  1.30  1  0  0
ANEOS  1 .293177
ANEOS  6 .149254
ANEOS  7 .270789
ANEOS  8 .286780
```

Inputs for ANEOS option -4

User Supplied Model

This EOS model uses user supplied code. Detailed coding interface instructions are available in subroutines ANUSET and ANUEOS.

Record 1

- RID (1) ANEOS
- NEOS (2) Equation-of-state number (negative number).
 For CHARTD, -1 to -20.
 For CSQ and CTH, -1 to -10.
 For CKEOS, -1 to -5.
- TITLE (3) Character string name of material.
 Enclose in single quotes (') if more than one word.
- LIB=number Library equation-of-state number if desired.
- RHUG=value Value is the initial density for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial density is taken to be the reference density (V3, record 2 below).
- THUG=value Value is the initial temperature for an in-line Hugoniot calculation. If not present, the calculation is skipped. If value < 0, the initial temperature is taken to be the reference temperature (V4, record 2 below).
- LONG This parameter is optional. If not present, the model uses 24 input parameters on records 2 through 4; if present, the model used 40 input parameters on records 2 through 6.

```

* * * * *
*   If a library equation of state is requested, no   *
*   more data records are required for this material. *
* * * * *
    
```

Record 2

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=1,8.

RID (1) ANEOS

V1. (2) The number of elements in this material.

V2. (3) -4 = Switch for type of equation of state.

V3. (4) RHOo - Reference density.

V4. (5) To - Reference temperature.
If To <= 0, code sets To = 0.02567785 ev (298 K).

V5. (6) Available for user model input.

V6. (7) Available for user model input.

V7. (8) Available for user model input.

V8. (9) Available for user model input.

Record 3

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=9,16.

- RID (1) ANEOS
- V9. (2) Available for user model input.
- V10. (3) Available for user model input.
- V11. (4) Available for user model input.
- V12. (5) Available for user model input.
- V13. (6) Available for user model input.
- V14. (7) Available for user model input.
- V15. (8) Available for user model input.
- V16. (9) Available for user model input.

Record 4

Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=17,24.

- RID (1) ANEOS
- V17. (2) Available for user model input.
- V18. (3) Available for user model input.
- V19. (4) Available for user model input.
- V20. (5) Available for user model input.
- V21. (6) Available for user model input.
- V22. (7) Available for user model input.
- V23. (8) Available for user model input.
- V24. (9) Available for user model input.

— —

Record 5

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=25,32.

RID (1) ANEOS

V25. (2) Available for user model input.

V26. (3) Available for user model input.

V27. (4) Available for user model input.

V28. (5) Available for user model input.

V29. (6) Available for user model input.

V30. (7) Available for user model input.

V31. (8) Available for user model input.

V32. (9) Available for user model input.

Record 6

This record is present only if the "LONG" keyword is entered on record 1. Eight parameters are entered on this record. In the output listing, the input variables are echoed as IN(I), I=33,40.

RID (1) ANEOS

V33. (2) Available for user model input.

V34. (3) Eshift - Energy shift for reactive chemistry modeling.

V35. (4) Sshift - Entropy shift for reactive chemistry modeling.

V36. (5) Available for user model input.

V37. (6) Available for user model input.

V38. (7) Available for user model input.

V39. (8) Available for user model input.

V40. (9) Available for user model input.

Record Set 7

There is one set of the following records for each element in variable 1, record 2. (I = 1, number of elements).

- RID (1) ANEOS
 - Z(I) (2) Atomic number of element.
 - f(I) (3) Unnormalized atomic number fraction of element,
or
- (Unnormalized atomic weight fraction of element.)
- All elements should be defined in the same way.

Example Input

```

ANEOS -1 'MY EOS MODEL'
ANEOS  4 -4      1.84      0      0      0      0      0
ANEOS  0  0      0         0      0      0      0      0
ANEOS  0  0      0         0      0      0      0      0
ANEOS  1 .293177
ANEOS  6 .149254
ANEOS  7 .270789
ANEOS  8 .286780
    
```

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APPENDIX B

SUMMARY OF MODEL PARAMETERS

During the set-up phase of ANEOS, an array of numbers is generated for each defined EOS. This array can have up to 99 elements for each material. In the output listing these are echoed as C(I), I=1,99. This section gives short definitions of these values. More details are given in reference 9.

Model Parameters ANEOS options 2,3,4

1. ETA1 of [7,5.60] if defined for a solid-solid phase transition; otherwise, a large number.
2. ETA2 of [7,5.61] if defined for a solid-solid phase transition.
3. Boo of [7,3.7], Bulk modulus at zero temperature and pressure.
4. C4, Morse interatomic potential constant of [7.3.20].
5. C5, Morse interatomic potential constant of [7.3.20].
6. C6, Morse interatomic potential constant of [7.3.20].
7. Pctr of [7,V-7] if defined for a solid-solid phase transition.
8. Ec(ETA1) of [7,5.62] if defined for a solid-solid phase transition.
9. C9 of [7,5.65] if defined for a solid-solid phase transition.
10. Es of [7,3.23], Zero temperature separation energy. Also see variable 78.
11. RHOo, Reference point density.
12. To, Reference point temperature.
13. C13 of [7.4.20]
14. C14 of [7,4.26]
15. GAMMAo of [7,IV-1], Reference point Gruneisen coefficient.
16. C16 of [7,4.24]
17. C17 of [7,4.24]
18. Tn of [7,V-5], Melt temperature.
19. RH(oo of [7,III], Density at zero temperature and pressure.
20. Po, Reference point pressure.
21. Bo, Reference point bulk modulus.
22. C22 of [7,7.8]
23. RHomin of [7,V-3], Lowest allowed solid density.
24. C24 of [7,4.11]
25. THETAo of [7,4.12], Debye temperature. If negative, full Debye functions are used[8,III.1]; if positive, high temperature limits are

ANEOS Input Manual

used.

26. Zm of [7,6.5], Average atomic number.
27. No of [7,6.10], Number of atoms per gram.
28. Number of elements in this material.
29. Abar of [7,6.2], Average atomic weight.
30. EOS type flag, 2, 3 or 4 for this option.
31. Internal storage pointer.
32. C32 of [7,3.4]
33. C33 of [7,3.4]
34. C34 of [7,3.4]
35. C35 of [7,3.4]
36. C36 of [7,3.4]
37. C37 of [7,3.18]
38. C38 of [7,5.63]
39. C39 of [7,5.63]
40. C40 of [7,5.63]
41. C41 of [7,7.6]
42. C42 of [7,7.15]
43. C43 of [7,5.22]
44. C44 of [7,5.22]
45. C45 of [7,5.22]
46. RHOsm of [7,V-1]
47. RHOlm of [7,V-1]
48. C48 of [7,V-1]
49. C49 of [7,V-1]
50. C50 of [7,5.41]
51. C51 of [7,5.42]
52. C52 of [7,V-1]

ANEOS Input Manual

53. C53 of [7,3.33]

54. C54 of [7,3.33]

55. Input variable V25 or computed default. Upper bound of the term $Boo/(RHOo*Es*Ghat**2)$ in the cold compression relation for expanded states [7,3.30].

56. Input variable V26 or computed default. Lower bound of the term $Boo/(RHOo*Es*Ghat**2)$ in the cold compression relation for expanded states [7,3.30].

57. Input variable V27 or computed default. Alpha of liquid EOS correction. [7,5.22].

58. Input variable V28 or computed default. Beta of liquid EOS correction. [7,5.22].

59. Input variable V29 or computed default. Gamma of liquid EOS correction. [7,5.22].

60. Input variable V30, not used in current model.

61. Input variable V31, not used in current model.

62. Input variable V32, not used in current model.

63. Flag for ionization model determine from input variable V33.
= 0, No electronic model.
= 1, Saha model.
=-1, Thomas-Fermi model.

64. Eshift - Energy shift for reactive chemistry modeling.

65. Sshift - Entropy shift for reactive chemistry modeling.

66. Input variable V36, not used in current model.

67. Input variable V37, not used in current model.

68. Input variable V38, not used in current model.

69. Input variable V39, not used in current model.

70. Input variable V40, not used in current model.

71. Internal constant for liquid eos model.

72. Internal constant for liquid eos model.

73. Tcrit, Critical point temperature.

74. RHOcrit, Critical point density.

75. Tgamma for compressed states[7.3.10].

76. Tgamma for compressed states[7.3.25].
77. Value of $\text{Boo}/(\text{RH0o}*\text{Es}*\text{Ghat}**2)$ in the cold compression relation for expanded states [7,3.30].
78. Es of [7,3.23] in ev/atom, Zero temperature separation energy. Also see variable 10.
79. Not used in current model.
80. Not used in current model.
81. Not used in current model.
82. Not used in current model.
83. Not used in current model.
84. Not used in current model.
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94. Not used in current model.
95. Not used in current model.
96. Not used in current model.
97. Not used in current model.
98. Not used in current model.
99. Not used in current model.

1. Not used in current model.
2. Not used in current model.
3. E_0 of [8,III.4.13]
4. C_v of [8,III.4.1]
5. $RHO_0 * GAMMA_0 * C_v$, Frequently used combination of parameters.
6. Not used in current model.
7. Not used in current model.
8. Not used in current model.
9. Not used in current model.
10. Not used in current model.
11. RHO_0 , Reference point density.
12. T_0 , Reference point temperature.
13. Not used in current model.
14. Not used in current model.
15. $GAMMA_0$ of [8,III.4.1], Reference point Gruneisen coefficient.
16. Not used in current model.
17. Not used in current model.
18. T_m of [8,III.4], Melt temperature.
19. Not used in current model.
20. Not used in current model.
21. $RHO_0 * S_0^{**2}$, Frequently used combination of parameters.
22. C_{22} of [7,7.8]
23. RHO_{min} of [7,V-3], Lowest allowed solid density.
24. Not used in current model.
25. Not used in current model.
26. Z_m of [7,6.5], Average atomic number.

ANEOS Input Manual

27. No of [7,6.10], Number of atoms per gram.
28. Number of elements in this material.
29. Abar of [7,6.2], Average atomic weight.
30. EOS type flag, -1 for this option.
31. Internal storage pointer.
32. So of [8,III.4.19]
33. S1 of [8,III.4.19]
34. Number of points in numerical integration table for temperature along Hugoniot.
35. Tm of [8,III.4], Melt temperature.
36. $0.5 \cdot \text{RHOo}$
37. RHOhigh input parameter or default.
38. Constant for high density extrapolation.
39. Constant for high density extrapolation.
40. $\text{Ecold}(\text{RHOhigh})$ for high density extrapolation.
41. C41 of [7,7.6]
42. $\text{ETA}(\text{RHOLow})$, $\text{ETA}=1-\text{RHOo}/\text{RHO}$
43. $\text{ETA}(\text{RHOhigh})$, $\text{ETA}=1-\text{RHOo}/\text{RHO}$
44. K1 of [8,4.23]
45. K2 of [8,4.23]
46. RHOsm of [7,V-1]
47. RHOlm of [7,V-1]
48. RHOLow input parameter or default.
49. Constant for low density extrapolation.
50. Constant for low density extrapolation.
51. $\text{Ecold}(\text{RHOLow})$ for low density extrapolation.
52. Not used in current model.
53. K3 of [8,4.23]
54. K4 of [8,4.23]

55. Input variable V25, not used in current model.
56. Input variable V26, not used in current model.
57. Input variable V27, not used in current model.
58. Input variable V28, not used in current model.
59. Input variable V29, not used in current model.
60. Input variable V30, not used in current model.
61. Input variable V31, not used in current model.
62. Input variable V32, not used in current model.
63. Input variable V33, not used in current model.
64. Eshift - Energy shift for reactive chemistry modeling.
65. Sshift - Entropy shift for reactive chemistry modeling.
66. Input variable V36, not used in current model.
67. Input variable V37, not used in current model.
68. Input variable V38, not used in current model.
69. Input variable V39, not used in current model.
70. Input variable V40, not used in current model.
71. Not used in current model.
72. Not used in current model.
73. Zero, Used as critical point temperature.
74. Zero, Used as critical point density.
75. Value in numerical table for Hugoniot temperature.
76. Value in numerical table for Hugoniot temperature.
77. Value in numerical table for Hugoniot temperature.
78. Value in numerical table for Hugoniot temperature.
79. Value in numerical table for Hugoniot temperature.
80. Value in numerical table for Hugoniot temperature.
81. Value in numerical table for Hugoniot temperature.
82. Value in numerical table for Hugoniot temperature.

- 83. Value in numerical table for Hugoniot temperature.
- 84. Value in numerical table for Hugoniot temperature.
- 85. Value in numerical table for Hugoniot temperature.
- 86. Value in numerical table for Hugoniot temperature.
- 87. Value in numerical table for Hugoniot temperature.
- 88. Value in numerical table for Hugoniot temperature.
- 89. Value in numerical table for Hugoniot temperature.
- 90. Value in numerical table for Hugoniot temperature.
- 91. Value in numerical table for Hugoniot temperature.
- 92. Value in numerical table for Hugoniot temperature.
- 93. Value in numerical table for Hugoniot temperature.
- 94. Value in numerical table for Hugoniot temperature.
- 95. Value in numerical table for Hugoniot temperature.
- 96. Entropy of liquid at melt point.
- 97. Not used in current model.
- 98. Not used in current model.
- 99. Not used in current model.

1. Not used in current model.
2. Not used in current model.
3. GAMMA of [8,III.4.35]
4. Cv of [8,III.4.35]
5. (GAMMA-1)*Cv, Frequently used combination of parameters.
6. LOG(To*RHOo**(1-GAMMA))
7. Not used in current model.
8. Not used in current model.
9. Not used in current model.
10. Not used in current model.
11. RHOo, Reference point density.
12. To, Reference point temperature.
13. Not used in current model.
14. Not used in current model.
15. (GAMMA-1)
16. Not used in current model.
17. Not used in current model.
18. Zero, Used as melt temperature.
19. Not used in current model.
20. Not used in current model.
21. K1*K2**3 of [8,III.4.40]
22. Internal flag.
23. Internal flag.
24. Not used in current model.
25. K2 of [8,III.4.40]
26. Zm of [7,6.5], Average atomic number.

27. No of [7,6.10], Number of atoms per gram.
28. Number of elements in this material.
29. Abar of [7,6.2], Average atomic weight.
30. EOS type flag, -2 for this option.
31. Internal storage pointer.
32. Not used in current model.
33. Not used in current model.
34. Not used in current model.
35. Not used in current model.
36. Not used in current model.
37. Not used in current model.
38. Not used in current model.
39. Not used in current model.
40. Not used in current model.
41. Not used in current model.
42. Not used in current model.
43. Not used in current model.
44. Not used in current model.
45. Not used in current model.
46. Internal flag.
47. Internal flag.
48. Not used in current model.
49. Not used in current model.
50. Not used in current model.
51. Not used in current model.
52. Not used in current model.
53. Not used in current model.
54. Not used in current model.

ANEOS Input Manual

55. Not used in current model.
56. Not used in current model.
57. Not used in current model.
58. Not used in current model.
59. Not used in current model.
60. Not used in current model.
61. Not used in current model.
62. Not used in current model.
63. Not used in current model.
64. Eshift - Energy shift for reactive chemistry modeling.
65. Sshift - Entropy shift for reactive chemistry modeling.
66. Not used in current model.
67. Not used in current model.
68. Not used in current model.
69. Not used in current model.
70. Not used in current model.
71. Not used in current model.
72. Not used in current model.
73. Zero, Used as critical point temperature.
74. Zero, Used as critical point density.
75. Not used in current model.
76. Not used in current model.
77. Not used in current model.
78. Not used in current model.
79. Not used in current model.
80. Not used in current model.
81. Not used in current model.
82. Not used in current model.

ANEOS Input Manual

- 83. Not used in current model.
- 84. Not used in current model.
- 85. Not used in current model.
- 86. Not used in current model.
- 87. Not used in current model.
- 88. Not used in current model.
- 89. Not used in current model.
- 90. Not used in current model.
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- 93. Not used in current model.
- 94. Not used in current model.
- 95. Not used in current model.
- 96. Not used in current model.
- 97. Not used in current model.
- 98. Not used in current model.
- 99. Not used in current model.

1. Not used in current model.
2. Not used in current model.
3. Eoo of [8,III.4.52]
4. Cv of [8,III.4.51]
5. R1 of [8,III.4.49]
6. R2 of [8,III.4.50]
7. Not used in current model.
8. Not used in current model.
9. Not used in current model.
10. Not used in current model.
11. RHOo, Reference point density.
12. To, Reference point temperature.
13. Not used in current model.
14. Not used in current model.
15. W of [8,III.4.41]
16. Not used in current model.
17. Not used in current model.
18. Zero, Used as melt temperature.
19. RHOoo of [8,III.4..2]
20. Not used in current model.
21. Not used in current model.
22. Not used in current model.
23. RHOfmin of [7,V-3], Lowest allowed solid density.
24. Not used in current model.
25. Internal storage flag.
26. Zm of [7,6.5], Average atomic number.

ANEOS Input Manual

27. No of [7,6.10], Number of atoms per gram.
28. Number of elements in this material.
29. Abar of [7,6.2], Average atomic weight.
30. EOS type flag, -3 for this option.
31. Internal storage pointer.
32. A of [8,III.4.46]
33. B of [8,III.4.47]
34. Not used in current model.
35. Constant in [8,III.4.56]
36. Constant in [8,III.4.52]
37. Not used in current model.
38. Not used in current model.
39. Not used in current model.
40. Not used in current model.
41. Not used in current model.
42. Not used in current model.
43. Not used in current model.
44. Not used in current model.
45. Not used in current model.
46. Internal flag.
47. Internal flag.
48. Not used in current model.
49. Not used in current model.
50. Not used in current model.
51. Not used in current model.
52. Not used in current model.
53. Not used in current model.
54. Not used in current model.

ANEOS Input Manual

55. Not used in current model.
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59. Not used in current model.
60. Not used in current model.
61. Not used in current model.
62. Not used in current model.
63. Not used in current model.
64. Eshift - Energy shift for reactive chemistry modeling.
65. Sshift - Entropy shift for reactive chemistry modeling.
66. Not used in current model.
67. Not used in current model.
68. Not used in current model.
69. Not used in current model.
70. Not used in current model.
71. Not used in current model.
72. Not used in current model.
73. Tcrit, Critical point temperature.
74. RHOCrit, Critical point density.
75. Not used in current model.
76. Not used in current model.
77. Not used in current model.
78. Not used in current model.
79. Not used in current model.
80. Not used in current model.
81. Not used in current model.
82. Not used in current model.

ANEOS Input Manual

- 83. Not used in current model.
- 84. Not used in current model.
- 85. Not used in current model.
- 86. Not used in current model.
- 87. Not used in current model.
- 88. Not used in current model.
- 89. Not used in current model.
- 90. Not used in current model.
- 91. Not used in current model.
- 92. Not used in current model.
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- 94. Not used in current model.
- 95. Not used in current model.
- 96. Not used in current model.
- 97. Not used in current model.
- 98. Not used in current model.
- 99. Not used in current model.

1. Available for user code storage.
2. Available for user code storage.
3. Available for user code storage.
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5. Available for user code storage.
6. Available for user code storage.
7. Available for user code storage.
8. Available for user code storage.
9. Available for user code storage.
10. Available for user code storage.
11. ρ_0 , Reference point density.
12. T_0 , Reference point temperature.
13. Available for user code storage.
14. Available for user code storage.
15. Available for user code storage.
16. Available for user code storage.
17. Available for user code storage.
18. T_{melt} , melt temperature.
19. Available for user code storage.
20. Available for user code storage.
21. Available for user code storage.
22. Internal flag.
23. Internal flag.
24. Available for user code storage.
25. Internal flag.
26. Z_m of [7,6.5], Average atomic number.

ANEOS Input Manual

27. No of [7,6.10], Number of atoms per gram.
28. Number of elements in this material.
29. Abar of [7,6.2], Average atomic weight.
30. EOS type flag, -4 for this option.
31. Internal storage pointer.
32. Available for user code storage.
33. Available for user code storage.
34. Available for user code storage.
35. Available for user code storage.
36. Available for user code storage.
37. Available for user code storage.
38. Available for user code storage.
39. Available for user code storage.
40. Available for user code storage.
41. Available for user code storage.
42. Available for user code storage.
43. Available for user code storage.
44. Available for user code storage.
45. Available for user code storage.
46. Internal flag.
47. Internal flag.
48. Available for user code storage.
49. Available for user code storage.
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51. Available for user code storage.
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63. Available for user code storage.
64. Eshift - Energy shift for reactive chemistry modeling.
65. Sshift - Entropy shift for reactive chemistry modeling.
66. Available for user code storage.
67. Available for user code storage.
68. Available for user code storage.
69. Available for user code storage.
70. Available for user code storage.
71. Available for user code storage.
72. Available for user code storage.
73. Tcrit, Critical point temperature.
74. RHOcrit, Critical point density.
75. Available for user code storage.
76. Available for user code storage.
77. Available for user code storage.
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ANEOS Input Manual

- 83. Available for user code storage.
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- 99. Available for user code storage.

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