

LA-8737-MS

C.3

CIC-14 REPORT COLLECTION²

REPRODUCTION
COPY

**EOSSCAN: A Program to
Display Equation-of-State Data**

University of California



LOS ALAMOS SCIENTIFIC LABORATORY

Post Office Box 1663 Los Alamos, New Mexico 87545

An Affirmative Action/Equal Opportunity Employer

This report was not edited by the Technical Information staff.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

**UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36**

LA-8737-MS

UC-32

Issued: March 1981

EOSSCAN: A Program to Display Equation-of-State Data

B. I. Bennett



ABSTRACT

EOSSCAN is a program to interactively compute various equation-of-state quantities from either the Los Alamos tabular library SESAME or from a variety of analytic formulae commonly used by Lawrence Livermore Laboratory. The results can be presented as printed output, or the program will generate a set of data files that can be manipulated and graphically displayed by several utility programs provided by Los Alamos National Laboratory Group T-4.

EOSSCAN: A PROGRAM TO DISPLAY EQUATION-OF-STATE DATA

by

B. I. Bennett

The program EOSSCAN was originally written to examine the various analytic formulae used by Lawrence Livermore Laboratory¹ for equations of state and tabulate them so that they could be included in the SESAME 2 library². This provided users of hydrodynamics programs at Los Alamos a new choice of being able to use the same equations of state as were used at Livermore Lab. EOSSCAN's capability has been extended to include materials already on the SESAME 2 library file. The input data for this program is in NAMELIST format on the file COFIN. A sample deck is shown in Table I. The program may also accept input data via NAMELIST from the computer teletype. These data will be described later.

The program is available on the Los Alamos Common File System under the node /SESAME/EOSSCAN and is executed on the CDC-7600 LTSS system by typing the name EOSSCAN.

THE CONTROLLING KEY WORDS

The program expects the input from a file COFIN in NAMELIST format. This file may be prepared ahead of time by using any of the text editor programs available on LTSS. Immediately upon execution, the program will read in the first set of data from the file and then prompt the user for any changes. If there are no changes, the user may type in, beginning in column 2:

\$RED \$

After the data is entered, the program is controlled by a series of key words. These words and their meaning are described below.

EOS	(Equation of State) Given a density and energy, find the pressure.
ABT	(Adiabat or Isentrope) Given an initial density and energy, find the pressures and energies for a set of densities.
HUG	(Hugoniot) Given the initial density, pressure, and energy of the material, compute the shock pressure, energy, shock velocity and particle velocity for a series of densities.

COLD (T=0 curve) Given a density find the pressure and energy for that density and zero temperature.

TABLE Generate a SESAME 1 table of pressure and energy vs density and temperature plus a file which can be used to update or add to the SESAME 2 library.

NEWMAT Start a new case by reading the NAMELIST file.

END Stop

The general way to exit from a given mode of computation is to enter a negative value for the first variable (a density). This will cause the code to prompt you for a new option key word. The specific form of the input for each of these key word options will be given later.

THE NAMELIST INPUT

The NAMELIST input assumes there is a total of 5 general types of equations of state available. These are designated by the variable IEQ. For values of IEQ = 1 to 4, the program expects a set of parameters for Livermore Lab's analytic forms. These analytic forms treat the density and internal energy as independent variables. If IEQ = xxxx, where xxxx represents a 4 digit SESAME material number, then the program will look for an equation of state table from the file SES2L (which may reside as a public or a local file). The SESAME tables usually treat the density and temperature as independent variables.

For the analytic forms, referring to Reference 1 and the following tables, one may see the correspondence between the parameters and the internal variables, CA1, CA2, etc. for each value of IEQ. There are two special cases, IEQ = -1 and -3 which are described in Reference 1 and are indicated below.

EQUATION 1

JWL equation of state for HE detonation products

$$\text{IEQ} = 1$$

$$P = A\left(1 - \frac{\omega}{R_1 V}\right)e^{-R_1 V} + B\left(1 - \frac{\omega}{R_2 V}\right)e^{-R_2 V} + \frac{\omega E}{V}$$

where, $V = \rho_0/\rho$

<u>parameter</u>	<u>variable</u>
A	CA1
B	CA2
R_1	CA3
R_2	CA4
ω	CA5
ρ_0	RHOZRO

$$\text{IEQ} = -1$$

$$P = (A_3 V^{-A_3})e^{-A_2 V}\left(1 - \frac{B_1}{V}\right) + \frac{B_2 E}{V}$$

<u>parameter</u>	<u>variable</u>
A_1	CA1
A_2	CA2
A_3	CA3
B_1	CA4
B_2	CA5
ρ_0	RHOZRO

EQUATION 2

Linear Polynomial Form for Solids

$$\text{IEQ} = 2$$

$$P = A_0 + A_1 \mu + A_2 \mu^2 + A_3 \mu^3 + (B_0 + B_1 \mu + B_2 \mu^2)E$$

where, $\mu = \rho/\rho_0 - 1$

<u>parameter</u>	<u>variable</u>
A_1	CA1
A_2	CA2
A_3	CA3
B_0	CA4
B_1	CA5
ρ_0	RHOZRO

For materials which include a term proportional to μ^{**4} , enter the coefficient as CA6.

EQUATION 3

Ratio of Polynomials Form for Solids

IEQ = 3

$$P = \frac{F_1 + F_2E + F_3E^2 + F_4E^3}{F_5 + F_6E + F_7E^2} (1 + A_{80}\mu)$$

where, $F_n = A_{n0} + A_{n1}\mu + A_{n2}\mu^2 + A_{n3}\mu^3$ and, $\mu = \rho/\rho_0 - 1$

<u>parameter</u>	<u>variable</u>
A ₁₀ to A ₁₄	CA1(I), I=1,5
A ₂₀ to A ₂₄	CA2(I), I=1,5
A ₃₀ to A ₃₃	CA3(I), I=1,4
A ₄₀ to A ₄₃	CA4(I), I=1,4
A ₅₀ to A ₅₃	CA5(I), I=1,4
A ₆₀ to A ₆₃	CA6(I), I=1,4
A ₇₀ to A ₇₃	CA7(I), I=1,4
A ₈₀	CA8
ρ_0	RHOZRO

For those equations of state where $A_{12}\mu^2$ becomes $A_{12}\mu|\mu|$, when μ is less than 0, IEQ = -3.

EQUATION 4

Gruneisen Equation of State with Cubic Shock Velocity - Particle Velocity

TEQ = 4

$$P = \rho_0 C^2 \mu \frac{[1 + (1 - \frac{\gamma_0}{2})\mu - \frac{a}{2}\mu^2]}{[1 - (S_1 - 1)\mu - S_2 \frac{\mu^2}{\mu+1} - S_3 \frac{\mu^2}{(\mu+1)^2}]^2} + (\gamma_0 + a\mu)E$$

and $P = \rho_0 C^2 \mu + \gamma_0 E$, when $\mu < 0$

where $\mu = \rho/\rho_0 - 1$

<u>parameter</u>	<u>variable</u>
C	CA1
S ₁	CA2
S ₂	CA3
S ₃	CA4
γ ₀	CA5
a	CA6
ρ ₀	RHOZRO

COMMAND FORMATS FOR THE OPTIONS

The various options made available by the key words described above, will cause the program to prompt the user for particular input data. The data, unless explicitly noted will be expected to be entered with the following units and quantities printed will also be in these units.

Density - grams per cubic centimeter.

Pressure - megabars.

Energy - megabars times cubic centimeters per gram.

Temperature - electron volts.

EOS option: This option will initially prompt the user to enter the density (RHO) and energy. The program will then print the density, pressure, and energy. It will then wait without prompting the user for another pair of values of density and energy.

ABT option: This option will prompt the user for the density and energy of the initial state from which the adiabat will start, and a density step size and limiting pressure. The program will then compute an adiabat for a series of densities starting at the initial value and incrementing this density by the density step size until either 50 values have been printed or the limiting pressure has been reached. The density step size can be a negative number. In this case the limiting pressure serves as a lower bound. The negative step size enables one to compute a release adiabat from some compressed state of the material, for example, a point on an Hugoniot. After receiving these options, the program will compute the pressure of the initial state and print the initial state variables. Then it will print the density, pressure, and energy along the adiabat. After the printing is finished, the program will wait for a new set of input data.

HUG option: This option will prompt for the density, pressure, and energy of the initial state of the material to be shocked, the lowest density for which results are desired, a scale factor for this density, and a limiting pressure. The program will then print values of density, compression, pressure, energy, shock velocity, and particle velocity (the latter two quantities have units of kilometers per second) for either 50 values of the density or until the limiting pressure is reached. The values of density used are obtained by multiplying the current value (starting at the first density) by the density scale factor. After this case is printed, the program will wait for a new set of data to be entered.

COLD option: This option needs only the desired density along the zero temperature isotherm. For examination of a SESAME table, the program simply interpolates on the tables for zero temperature. In the case of the analytic formulae, the program solves a differential equation for the energy at zero temperature and then evaluates the pressure formula for that energy and density. It is here that the namelist input variables RELERR, and ABSERR are needed. These are the relative and absolute error criterion used by the subroutine ODE (Ordinary Differential Equation solver). These variables have default values of 10^{-5} . The density, pressure, and energy are then printed and the program waits for a new value of the density.

TABLE option: This option can operate in two different modes. The first one allows one to obtain printed values of the pressure and energy for desired values of the compression and temperature. The second enables one to generate two types of files containing pressures and energies as a function of density and temperature. One file that is produced is called EOSTAB which is in the so-called SESAME 1 format. This file can be accessed directly by a variety of existing utility routines written by group T-4. The format of this file is shown in Table II. The second file is called SESUP and is an update file to be used by the T-4 utility S2M to modify or update the SESAME 2 library file⁴, SES2L.

For SESAME type equations of state, namely those which already exist in tabular form, this option could be used to extract just a portion of the existing table (However, there exists alternate methods to do this in the HYDSES package, described in Reference 3.) or one could retabulate a table on a coarser mesh to save storage space.

For the Livermore Lab's analytic formulae, the tabulation of the pressure and energy as functions of density and temperature is artificial, since these formulae are intended to give pressure as a function of density and energy alone. Therefore, no temperature is defined by these equations. However, the tabulation can be accomplished by choosing simple models for the relationship between the internal energy and a temperature. The models adopted assumed that the total energy is composed of a contribution from the binding energy (the cold or T=0 isotherm), the nuclear motion (ignoring the zero point motion), and a Saha like model for electronic excitations. These are described in References 5 and 6.

With the option TABLE the code will request the following variables.

Z	Atomic Number
AW	Atomic Weight
RHOZRO	Density to which the compressions are relative. This is usually the density for which the pressure and energy are zero.
POTI	An ionization potential in ev's for a simple Saha model for electronic excitations. This can be taken to be

the 1st ionization potential for the atom. This has no meaning for a retabulation of a SESAME table.

ITABFG A flag to tell what sort of calculation is to be done in the "TABLE" mode. If it is set to zero, one may enter values of compression and temperature (in ev's) to print selected EOS points. If it is set to 1 the program will proceed to generate the tables.

With ITABFG = 1, the program will prompt the user for information about the range of compressions and temperatures and the type of grid on which these are to be provided for the tables. Both of these prompts expect data in the following general form.

A, B, N, ITYPE

where:

A is the minimum value of compression or temperature in the table.
B is the maximum value of compression or temperature in the table.
N is the total number of points in the mesh from A and B, inclusive.
ITYPE is a parameter which controls the spacing between mesh points.
ITYPE can take on the following values.

ITYPE = 0, Equidistant mesh between A and B.
= 1, Logarithmic mesh, where
 $X(I) = A + (B-A) * \text{ALOG10}(I) / \text{ALOG10}(N)$.
= 2, Exponential mesh, where
 $X(I) = B * 10.0^{(I-N)/S}$, and
 $S = (N-1) / \text{ALOG10}(B/A)$.
= 3, Randomized equidistant mesh, where
 $X(I) = A + (I-1-T) * (B-A) / (N-1)$, and
 T is a random variable on the interval (0,1).

The most commonly used values of ITYPE are 0 and 2. After entering the input data for either the compressions or the temperatures, the program will enquire if a list of the mesh is desired. If no list is required, the program will proceed. If such a tabulation is produced, the user may choose to repeat the mesh generation for that variable, add additional points to the mesh, or delete selected points from the mesh. The program

will give the appropriate messages to enable the user to make these choices.

In generating the meshes in compression and temperature, the program will allow the user to add additional isotherms for the same set of compressions. This is convenient if the user wishes to have a series of equally spaced isotherms followed by some exponentially spaced isotherms. There are two restrictions imposed upon this procedure. The additional groups of temperatures must be sequentially greater than the previous temperatures, and the temperatures and/or compressions must satisfy the following inequality for the present program dimensions.

$$Y \leq \text{INT}\left\{\frac{12625 - X}{2X + 1}\right\}$$

where INT is the integer part of the expression in the brackets. For example, if 100 compressions are chosen, the maximum number of temperatures allowed is 62.

As the program continues, it will prompt the user for a material number, the number of compressions, and the maximum number of temperatures to be used in constructing the final table. The material number is usually, but not restricted to be a four digit number, and the maximum number of compressions and temperatures must satisfy the above inequality. After the program has generated the two files EOSTAB and SESUP, it will prompt the user for a new option key word.

ADDITIONAL OUTPUT

The program also produces a special file called PLTAPE. This file contains an assortment of summary information about the various calculations a user might have done exercising the variety of options (except TABLE). The file is in a format compatible with that required by the plotting utility CURVE, described in Reference 7. These data coupled with this utility provide the user with the capability of producing plots of the results of sufficient quality that they could be published directly.

TABLE I

Example of Format for File COFIN

\$RED CA1=0, 0.52135, 0.82727, 0.32358, CA2= 1.7657, 6.0678, 7.7968,
 3.4970, CA3= 1.1786, 1.7852, 0.61167, 7.6605E-4, CA4= 5.2155E-4, 6.674E-4,
 1.49E-4, 8.9924E-4, CA5= 1.0, 0.42455, 2.1084, 2.6901, CA6= 2.8317, 3.9254,
 1.1133, 1.2976E-3, CA7= 7.626E-4, 9.8247E-4, 2.2501E-4, 1.2462E-7, CA8=
 1.0, RHOZRO= 2.784, IEQ=3 \$

Note that \$RED begins in column 2 of the input line.

TABLE II

The SESAME 1 File Format

<u>WORD</u>	<u>DESCRIPTION</u>
1	Material Number (MATID)
2	Number of compressions (NR, also called MAXE)
3	Number of Temperatures (NT, also called MAXT)
4	Atomic Number (Z)
5	Atomic Weight (A)
6	Density by which compressions are scaled (ρ_0)
7 to 32	Miscellaneous data not needed for this application
32 to 32+NR	Compressions (NR values)
33+NR to 32+NR+NT	Temperatures in ev's. (NT values)

The next block of words consist of NR times NT values of pressure,
 arranged along isotherms.

The next block of words consist of NR times NT values of Energy,
 arranged along isotherms.

REFERENCES

1. D. J. Steinberg, "The Hydrodynamic Equations of State for the KOVEC Code" (U), Lawrence Livermore Laboratory Report, UCID-17046, Rev. 1 (SRD), (March, 15, 1978).
2. B. I. Bennett, J. D. Johnson, G. I. Kerley, G. T. Rood, "Recent Developments in the SESAME Equation-of-State Library, Los Alamos Scientific Laboratory Report, UC-34, (February, 1978).
3. J. Abdallah, Jr., G. I. Kerley, B. I. Bennett, J. D. Johnson, R. C. Albers, W. F. Huebner, "HYDSES: A Subroutine Package for using SESAME in Hydrodynamics Codes", Los Alamos Scientific Laboratory Report, LA-8209, (June, 1980).
4. S. P. Lyon, "New Version of SES2M", Los Alamos Scientific Laboratory Internal Memo, T-4, 11/26/79.
5. C. W. Cranfill and R. More, "IONEOS: A fast Analytic Ion Equation-of-State Routine", Los Alamos Scientific Laboratory Report, LA-7313-MS, (October, 1978). This is a description of an implementation of a model developed by R. D. Cowan, "Equations of State from The Thomas-Fermi-Dirac Theory of the Atom" (U), Los Alamos Scientific Laboratory Report, LA-2124 (SRD), (February, 1957). The subroutines which use this work are called PNCOW and GRUN.
6. G. I. Kerley, private communication. This model comprises the subroutine PELEC.
7. J. Abdallah, Jr., "CURVES", Los Alamos Scientific Laboratory Internal Memo, T-4, 1/21/81.

Printed in the United States of America
 Available from
 National Technical Information Service
 US Department of Commerce
 5285 Port Royal Road
 Springfield, VA 22161
 Microfiche \$3.50 (A01)

Page Range	Domestic Price	NTIS Price Code	Page Range	Domestic Price	NTIS Price Code	Page Range	Domestic Price	NTIS Price Code	Page Range	Domestic Price	NTIS Price Code
001-025	\$ 5.00	A02	151-175	\$11.00	A08	301-325	\$17.00	A14	451-475	\$23.00	A20
026-050	6.00	A03	176-200	12.00	A09	326-350	18.00	A15	476-500	24.00	A21
051-075	7.00	A04	201-225	13.00	A10	351-375	19.00	A16	501-525	25.00	A22
076-100	8.00	A05	226-250	14.00	A11	376-400	20.00	A17	526-550	26.00	A23
101-125	9.00	A06	251-275	15.00	A12	401-425	21.00	A18	551-575	27.00	A24
126-150	10.00	A07	276-300	16.00	A13	426-450	22.00	A19	576-600	28.00	A25
									601-up	†	A99

†Add \$1.00 for each additional 25-page increment or portion thereof from 601 pages up.