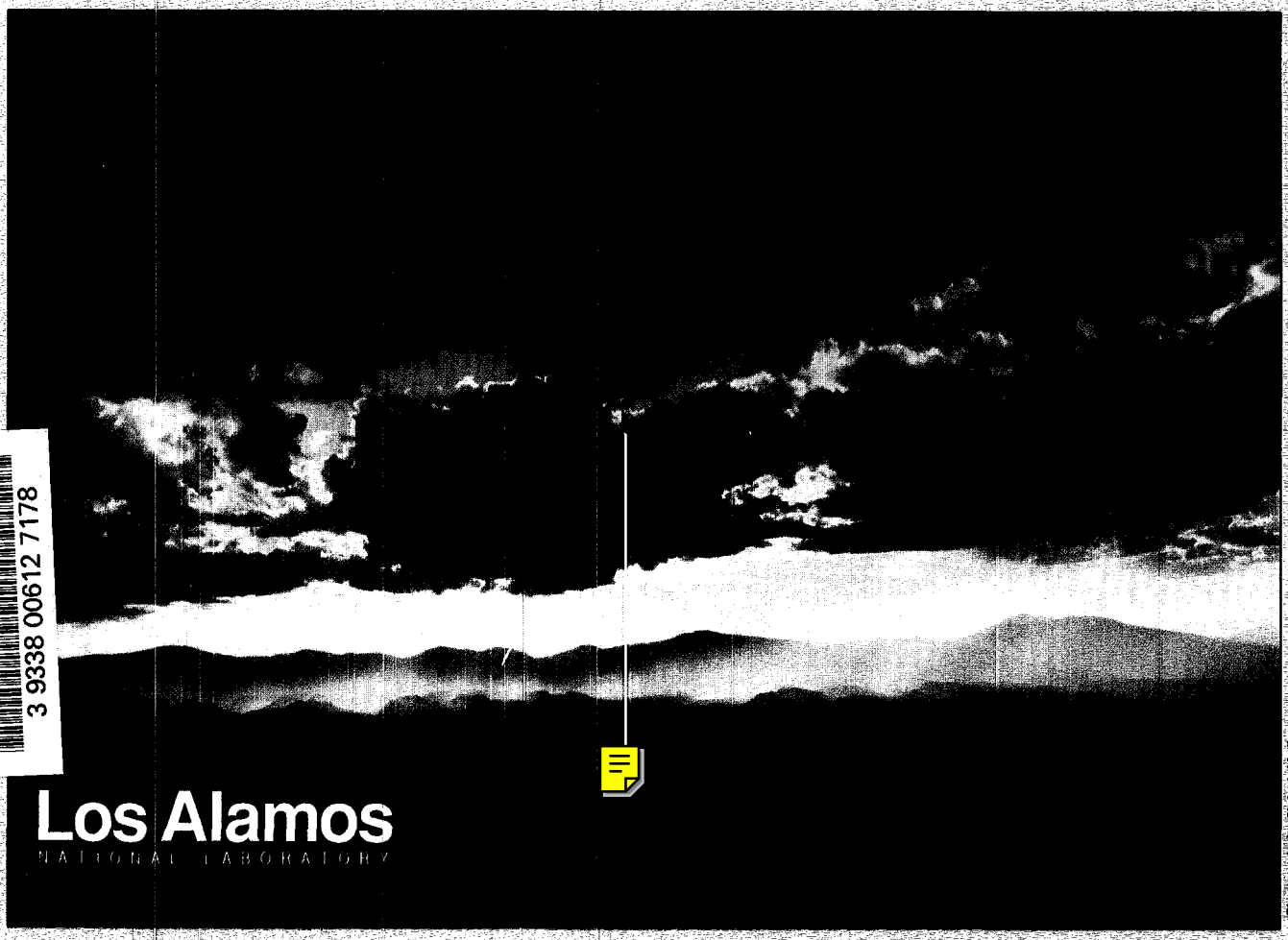
LA-UR-92-3407

SESAME: THE LOS ALAMOS NATIONAL LABORATORY EQUATION OF STATE DATABASE



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SESAME: THE LOS ALAMOS NATIONAL LABORATORY EQUATION OF STATE DATABASE

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Publications

Editors: Stanford P. Lyon, James D. Johnson, Group T-1

SECTION 1

INTRODUCTION

INTRODUCTION

THE SESAME DATABASE

The SESAME Equation-of-State (EOS) Library is a standardized, computer-based library of tables for the thermodynamic properties of materials with FORTRAN subroutines for the use of the library. All are developed and maintained by the Mechanics of Materials and Equation-of-State Group (T-1) of the Theoretical Division at Los Alamos National Laboratory.

The Library currently contains data for about 150 materials, including simple elements, compounds, metals, minerals, polymers, mixtures, etc. The EOS's for existing materials in the Library are upgraded when appropriate, and EOS's for new materials are added frequently. The Library is used by many researchers, both inside and outside the Laboratory; external users include scientists at various institutions in the United States and in other countries. The Library is presently being offered to all interested users free of charge.

The thermodynamic data stored in the Library include tables of pressure P and energy E (and also in many cases, of Helmholtz free energy A), each as a function of density ρ and temperature T. Besides total P, E, and A tables, often separate P, E, and A tables of thermal electronic and ion (including zero point) contributions are available. Some materials also have vaporization, melt and shear tables. The typical density and temperature ranges are from 10^{-6} to 10^{4} gm/cc and 0 to 10^{5} ev respectively.

There also exist SESAME Libraries for opacity and conductivity data. The lower limit on the opacity data is about 1ev. The opacity library includes Rosseland and Plank mean opacities, electron conductive opacity and mean ion charge for elements with atomic number $Z \leq 30$. The conductivity library contains tables of mean ion charge, electrical and thermal conductivity, thermoelectric coefficient and electron conductive opacity for elements $Z = 1$ through $Z = 96$.

THEORETICAL MODELS AND METHODS

Because of the large ranges of density and temperature, and because of the very diverse kinds of phases and materials encountered in the Library, the global EOS's in the Library are formed using various combinations of different theoretical models in different regions with interpolation between, usually thermodynamically consistent.

Most often these models include a Thomas-Fermi-Dirac theory for thermal electronic contributions to the EOS. A few EOS's incorporate the INFERNO

model for an atom embedded in an electron gas at finite temperature; electron-band structure models, including augmented plane-wave, LMTO, KKR, and Gaussian orbital approaches; or a Saha model for ionization equilibrium.

Other models include Einstein, Debye, Cowan, Chart-D and generalized Chart-D models for lattice vibrations in solids; hard-sphere perturbation approaches for fluids; and rigid-rotator and harmonic-oscillator methods for molecular rotational and vibrational terms, respectively.

Other approaches include molecular-dynamics (MD) computer simulations of metals, of rigid diatomic and triatomic molecules, and of nonrigid diatomic molecules. Pseudopotentials and melting in metals have been studied by MD. The capacity also exists in the T-1 Group to study glasses and solid-solid transitions by MD.

Various somewhat empirical methods are also used: virial expansions; analytic fits of data to various intermolecular potentials, including Lennard Jones (6,12), Buckingham (exp-6), and modified Morse potentials; multi-parameter functional fits of data; Mie-Grüneisen equation of state; etc.

The aim of the SESAME Library is to have thermodynamically self-consistent EOS's that are made with the best possible physics and the best possible agreement with available experimental data-given realistic time constraints. Most EOS's in the SESAME Library have been generated by the T-1 Group, but the Library does include some EOS's originally constructed by researchers at other institutions (such as the National Bureau of Standard and Lawrence Livermore National Laboratory and adapted by the T-1 Group for the SESAME Library). The T-1 Group uses its own versions of some externally developed theoretical models to generate EOS's, but also develops its own new models and methods.

Other features of various EOS's in the SESAME Library include treatments of shock data, incorporation of various phase transitions (including Maxwell constructions or van der Waals' loops for first-order phase transitions), modeling of foams or porous materials, and calculation of dilute gas mixtures.

Of recent interest is the inclusion of better theoretical models and methods for (1) melting and (2) nonideal mixtures in the mechanisms used to generate the global EOS's. Many of these improved models and methods have been developed by various T-1 Group members and can be used now for calculations of individual thermodynamic points or of small regions in phase space. Still other models and methods are being developed in these areas, as well as in many other areas of interest in the calculation of EOS's for a variety of diverse materials.

SESAME SOFTWARE

SESAME Subroutine Library

The SESAME subroutine library was developed to simplify use of tabular EOS data. SESAME tables are transmitted to users on magnetic tapes in a card image format that can be read and interpreted by the user's computing system. The user is also supplied with FORTRAN subroutines that preprocess the data into a compact binary file and update this file as needed. The user is supplied with subroutines that search this file for a given material, load data into a local array, and compute thermodynamic functions by search and interpolation. Linear and rational function interpolation schemes are available for one and two dimensions.

Routines are available to compute P and E (and their first derivatives) as a function of ρ and T and also to compute P and T (and their first derivatives) as a function of ρ and E. Other EOS data that can be computed include isotherms, isochores, adiabats, Hugoniots (shock velocities and particle velocities), vapor-liquid coexistence curves, thermodynamic behavior of foams, phase transitions, and melt and shear modulus tables.

Display Codes

The T-1 Group has a number of in-house display codes that combine various subroutines mentioned in the preceding section to provide tabular and graphical representation of the EOS data. SES2D and SES3D are two- and three-dimensional graphics codes using DISSPLA graphics which plot tabulated data. SES2D plots isotherms, isochores, Hugoniots and adiabats. (See the end of this section for sample output from SES2D.) The SHIP code displays the library data in tabular form and the DSPLX code is used to calculate Hugoniots, isentropes, and other quantities which it also displays in tabular form. Finally, SESLIST is used to generate a catalog of materials in a SESAME library along with a description of methods used to calculate each table and its density-temperature range.

OBTAINING THE SESAME LIBRARY

To obtain the SESAME EOS data and subroutine library either mail or FAX your request to

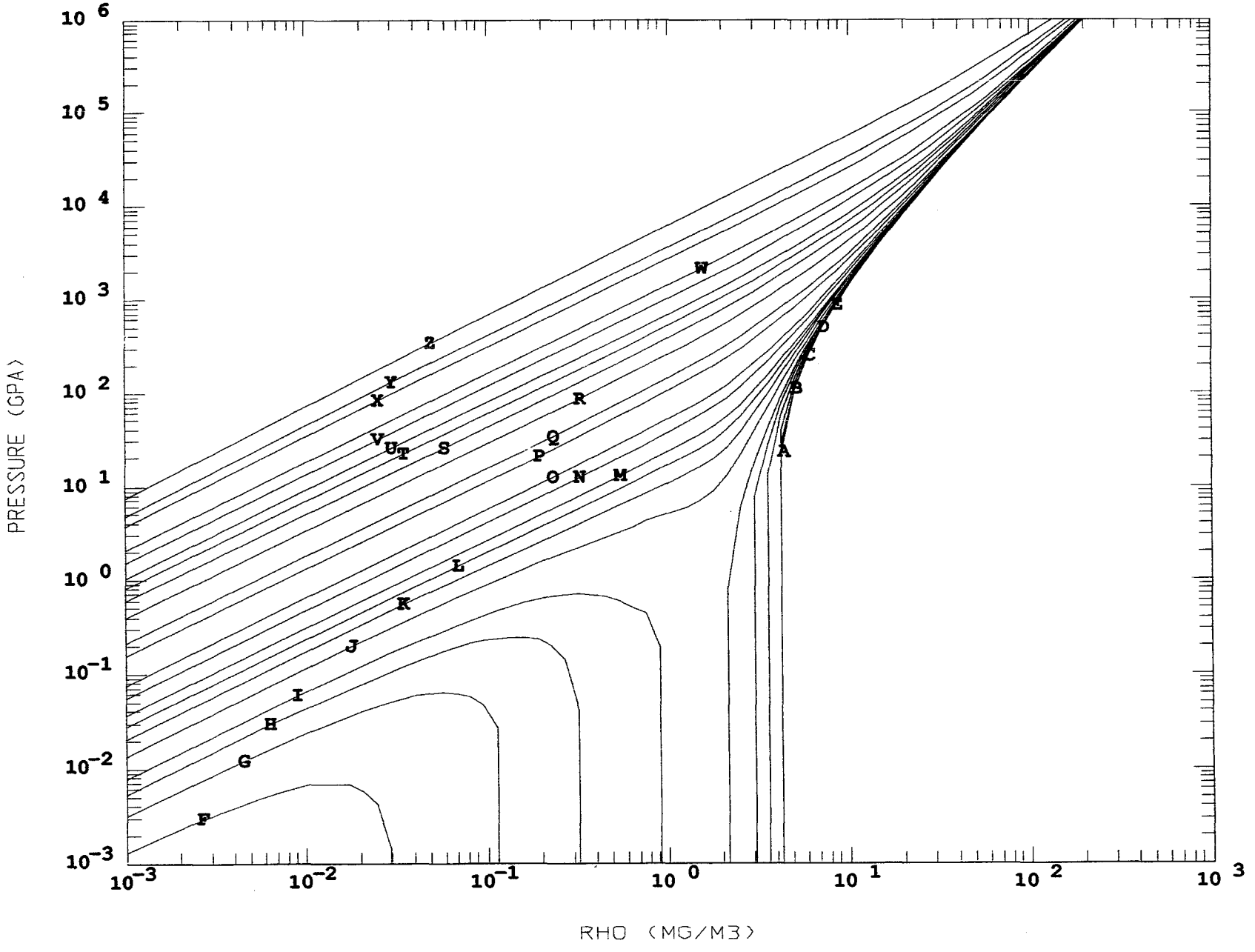
SESAME Library, T-1, MS-B221
Los Alamos National Laboratory
Los Alamos, NM 87545

Fax No: 505-665-5757. Please include your choice of storage media and format. For a standard 2400 ft. magnetic tape specify either ASCII or EBCDIC character set and either 1600 or 6250 BPI.

Users interested in opacity data should contact

Group T-4, MS B212
Los Alamos National Laboratory
Los Alamos, NM 87545

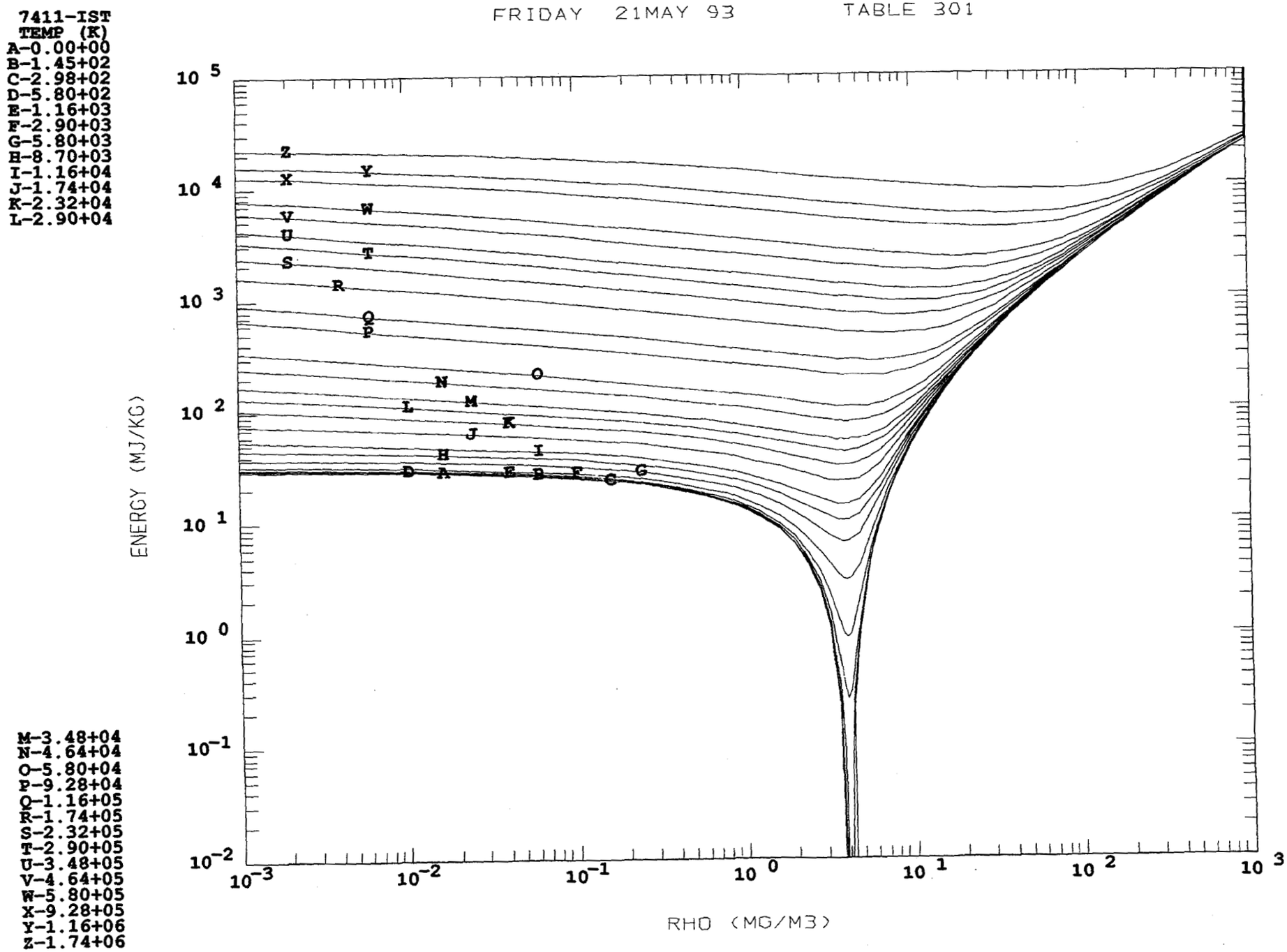
7411-IST
TEMP (K)
A-0.00+00
B-1.45+02
C-2.98+02
D-5.80+02
E-1.16+03
F-2.90+03
G-5.80+03
H-8.70+03
I-1.16+04
J-1.74+04
K-2.32+04
L-2.90+04



M-3.48+04
N-4.64+04
O-5.80+04
P-9.28+04
Q-1.16+05
R-1.74+05
S-2.32+05
T-2.90+05
U-3.48+05
V-4.64+05
W-5.80+05
X-9.28+05
Y-1.16+06
Z-1.74+06

T1 SES2D CRAY 02

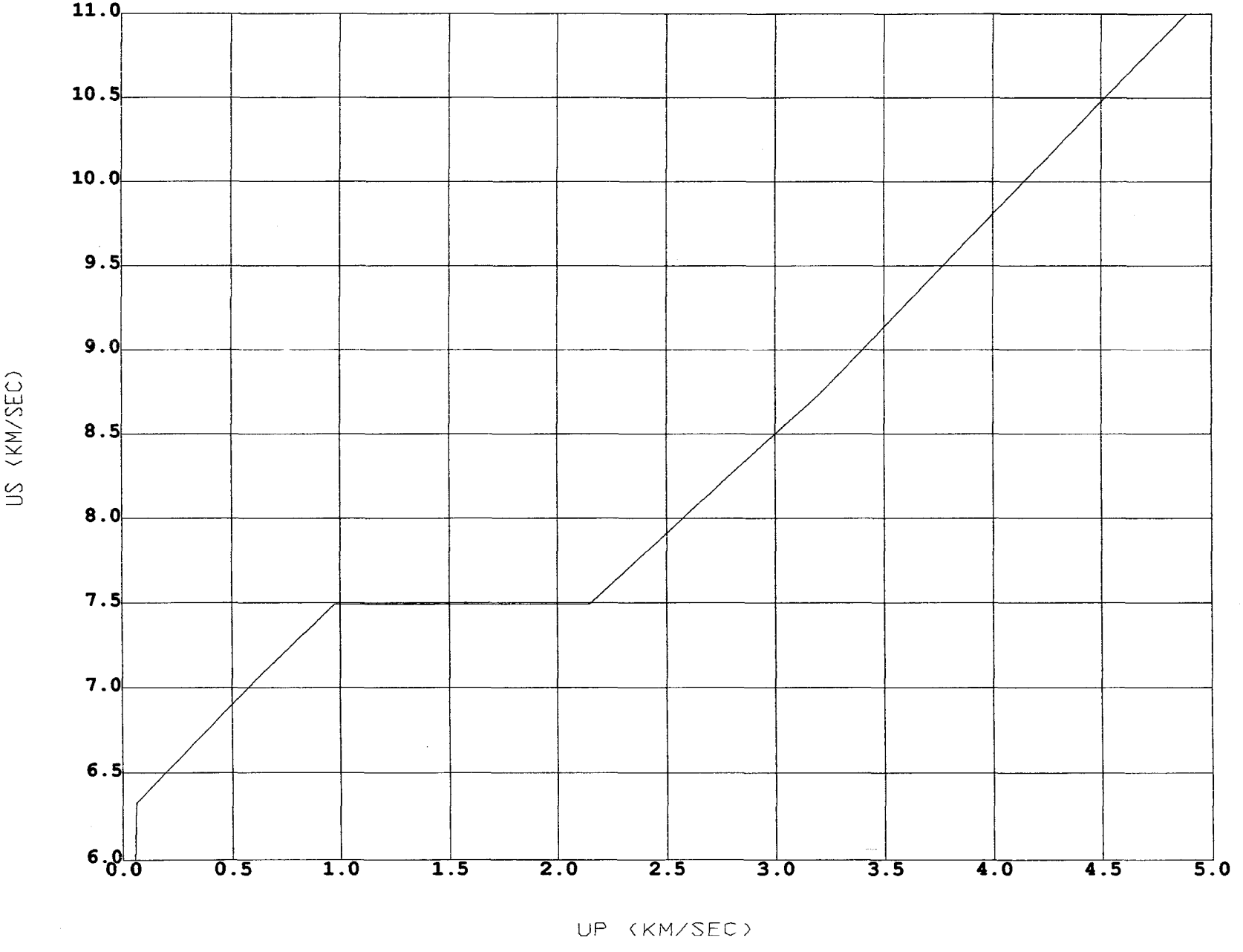
FRIDAY 21MAY 93 TABLE 301



T1 SES2D CRAY 02

7440-HU1
E0 MJ/KG
0.00+00

FRIDAY 21MAY 93 TABLE 301



T1 SES2D CRAY 02

SECTION 2

BASELINE EOS THEORY

BASELINE EOS THEORY

Almost all of the equations of state being produced for SESAME are now being done with one method, one set of models. Also, over the years by far most of the EOS's have been created by similar modeling. In this section we will outline this baseline method. We will also mention a couple of more elaborate methods that are sometimes used, especially for metals. Finally, we have discontinued using a number of techniques that produced a few EOS's that are in the Library. Report LA-10160-MS should be consulted for those.[1]

The standard thinking for SESAME is that an EOS is composed of three parts; the zero temperature isotherm (cold curve), the thermal ionic, and thermal electronic. We model each separately and construct the total EOS, the 301 table, by summing the three. Other tables, 304, 305, and 306, come from the individual parts. By convention we put the zero point motion of the ions in with the thermal ionic contribution.

The thermal electronic contribution is calculated using finite temperature Thomas-Fermi-Dirac (TFD) theory. Our current model for this is due to Liberman[2] and is the same as that of Cowan and Ashkin[3] but treats exchange and correlation with a local density approximation. The thermal part is produced by running TFD everywhere including zero temperature and then subtracting the TFD cold curve from the whole table. For a few materials the INFERNO model[4] for the finite temperature electronic structure has been used. Here the Dirac equation is solved for the single particle quantum levels in the self-consistent field of an atom in a constrained spherical cell. INFERNO obtains structure from the electron ionization while TFD smoothes through such.

Our ionic models have been very similar with the current one having more details of melting.[5] The solid region is treated with Debye theory. The location of melting is determined by the Lindemann formula. Above melting an interpolation is made, going smoothly to ideal gas at high temperatures. For these models it is necessary to know the Debye temperature as a function of density. This we obtain from simple analytic forms fit to data.

For the cold curve we look at three different density regions. We usually have shock wave data from the ambient density of the solid to some high density. Over this range we use the shock data and the above fit for the Debye temperature

to calculate the cold curve from Mie-Grüneisen theory.[6] For higher densities an interpolation is made to TFD theory with a smooth connection to the Mie-Grüneisen region. For low densities a simple analytic form is again smoothly merged into the Mie-Grüneisen region. The other parameters for expansion are selected to obtain the correct cohesive energy and gas-liquid critical point. In a few special cases the Mie-Grüneisen procedure has been replaced by *ab initio* band-structure calculations.

The above method gives us our basic EOS tables. We also pull out the details of melting and vaporization and place those in special tables, 401, 411, and 412, for these phase transitions. Most recently we have included a zero temperature shear modulus table. It is sometimes appropriate to create an EOS that is a mixture. We use simple mixing rules such as additive volume and partial pressure.[7]

While the above is our standard procedure and does account, by far, for most of our database, we have and still attempt to serve the users' special needs. This includes using models and limited regions with increased accuracies as well as going to material data other than equation of state. We hope to continue this expansion of what is treated in the Sesame Library.

REFERENCES

(1) K. S. Holian, LANL report LA-10160-MS (1984).

(2) D. A. Liberman, unpublished notes.

(3) R. D. Cowan and J. Ashkin, Phys. Rev. 105, 144 (1957).

(4) D. A. Liberman, Phys. Rev. B 20, 4981 (1979).

(5) J. D. Johnson, High Pressure Research 6, 277 (1991).

(6) G. I. Kerley, LANL report LA-8833-M (1981).

(7) J. Abdallah, Jr., LANL report LA-10244-M (1984).

SECTION 3

STRUCTURE OF THE SESAME LIBRARY

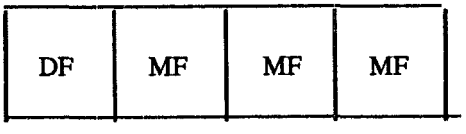
STRUCTURE OF THE SESAME LIBRARY

The SESAME library is a fileset consisting of a directory file and one or more material files. The directory file consists of two records described on page 3-2. Each material file corresponds to a specific material and consists of an index record followed by a variable number of data records or tables. The structure of the index record appears on page 3-2. The various types of SESAME data records and their structure are shown on pages 3-3 to 3-6.

The SESAME library may be constructed with either a sequential or random I/O format. The sequential version has a one-word record mark at the end of each record, a one-word file mark at the end of each file and two end of file marks at the end of the library. The random version has an address array in the second record of the directory file with address that can be used to locate the beginning of each material file and an address array in the index record of each material file containing the addresses of the data records for that material. The random and sequential versions may be read by the TABRAN and TABSEQ subroutines found in the SESAME subroutine package described in Section 4.

The SESAME libraries maintained by T-1 on the CRAY machines at LANL have random I/O format.

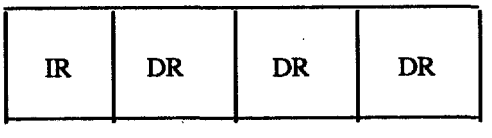
Library



DF - directory file

MF - material file

Material File



IR - index record

DR - data record

STRUCTURE OF THE DIRECTORY FILE FOR THE SESAME LIBRARY

Record 1. N, DATE, VERS.

N - Number of material files in the library (real number).

DATE - Date of current version.

VERS - Version number.

Record 2. (MATID(I), I = 1, N), (NWDS(I), I = 1,N), (IADR(I), I = 1, N).

MATID - Table of material id numbers, in the same order as the material files in the library (real number).

NWDS - For each material file MATID(I), NWDS(I) is the number of words in the index record (real number).

IADR - IADR(I) is the address of each index record (random format).

STRUCTURE OF THE INDEX RECORD FOR A SESAME MATERIAL FILE

Record 1. MATID, DATE1, DATE2, VERS, NREC, (TBLID(I), I = 1, NREC), (NWDS(I), I = 1 NREC), (IADR(I), I=1,NREC).

MATID - Material id number (real number).

DATE1 - Date of creation of material.

DATE2 - Date when material file was last updated.

VERS - Version number of most recent update.

NREC - Number of data records (real number).

TBLID - Table id numbers for the data records in the same order as they are stored in the material file.

NWDS - For each TBLID(I), NWDS(I) is the number of words in the data record (real number).

IADR - IADR(I) is the address of each data record (random format).

TYPES OF SESAME DATA RECORDS

Table 101	Comments
Table 102	Comments
Table 201	Atomic Number, Atomic Mass, Normal Density
Table 301	Total EOS (304 + 305 + 306)
Table 303	Ion EOS Plus Cold Curve (305 + 306)
Table 304	Electron EOS
Table 305	Ion EOS (Including Zero Point)
Table 306	Cold Curve (No Zero Point)
Table 401	Vaporization Table
Table 411	Solid Melt Table
Table 412	Liquid Melt Table
Table 431	Shear Modulus Table
Table 501	Opacity Grid Boundary: Calculated vs. Interpolated
Table 502	Rosseland Mean Opacity ($cm^2\ g^{-1}$)
Table 503	Electron Conductive Opacity[1] ($cm^2\ g^{-1}$)
Table 504	Mean Ion Charge[1] (free electrons per atom)
Table 505	Planck Mean Opacity ($cm^2\ g^{-1}$)
Table 601	Mean Ion Charge[2] (free electrons per atom)
Table 602	Electrical Conductivity (sec^{-1})
Table 603	Thermal Conductivity ($cm^{-1}\ sec^{-1}$)
Table 604	Thermoelectric Coefficient ($cm^{-1}\ sec^{-1}$)
Table 605	Electron Conductive Opacity[2] ($cm^2\ g^{-1}$)

[1]Opacity Model (Hubbard-Lampe)

[2]Conductivity Model (Ziman)

STRUCTURE OF THE SESAME DATA RECORDS

Table 201

Word	Description	
1	ZBAR	Mean atomic number
2	ABAR	Mean atomic mass
3	RHO0	Normal (solid) density
4	B0	Solid bulk modulus
5	CEX	Exchange coefficient

Table 301-305

Word		
1	NR	Number of densities
2	NT	Number of temperatures
3	(R(I), I=1,NR)	Density array (Mg/m^3)
NR+3	(T(I),I=1,NT)	Temperature array (K)
NR+NT+3	((P(I,J),I=1,NR),J=1,NT)	Pressure array (GPa)
NR+NT+3+NR*NT	((E(I,J),I=1,NR),J=1,NT)	Energy array (MJ/kg)
NR+NT+3+2*NR*NT	((A(I,J),I=1,NR),J=1,NT)	Free energy array (MJ/kg)

Table 306

Word		
1	NR	Number of densities
2	NT (=1)	Number of temperatures
3	(R(I),I=1,NR)	Density array (Mg/m^3)
NR+3	T (=0)	Temperature (K)
NR+4	(P(I),I=1,NR)	Pressure array (GPa)
2*NR+4	(E(I),I=1,NR)	Energy array (MJ/kg)
3*NR+4	(A(I),I=1,NR)	Free energy array (MJ/kg)

Table 401

Word		
1	NT	Number of temperatures
2	(P(I),I=1,NT)	Vapor pressure (GPa)
2+NT	(T(I),I=1,NT)	Temperature (K)
2+2*NT	(RG(I),I=1,NT)	Vapor density on coexistence line (Mg/m^3)
2+3*NT	(RL(I),I=1,NT)	Density of liquid or solid on coexistence line (Mg/m^3)
2+4*NT	(EG(I),I=1,NT)	Internal energy of vapor on coexistence line (MJ/kg)
2+5*NT	(EL(I),I=1,NT)	Internal energy of liquid or solid on coexistence line (MJ/kg)
2+6*NT	(AG(I),I=1,NT)	Free energy of vapor on coexistence line (MJ/kg)
2+7*NT	(AL(I),I=1,NT)	Free energy of liquid or solid on coexistence line (MJ/kg)

Table 411

Word		
1	NR	Number of densities
2	NT (=1)	
3	(RS(I),I=1,NR)	Density of solid on melt line (Mg/m^3)
NR+3	T (=0)	
NR+4	(TM(I),I=1,NR)	Melt temperature (K)
2*NR+4	(PM(I),I=1,NR)	Melt pressure (GPa)
3*NR+4	(ES(I),I=1,NR)	Internal energy of solid on the melt line (MJ/kg)
4*NR+4	(AS(I),I=1,NR)	Free energy of solid on the melt line (MJ/kg)

Table 412

Word		
1	NR	Number of densities
2	NT (=1)	
3	(RL(I),I=1,NR)	Density of liquid on melt line (Mg/m^3)
NR+3	T (=0)	
NR+4	(TM(I),I=1,NR)	Melt temperature (K)
2*NR+4	(PM(I),I=1,NR)	Melt pressure (GPa)
3*NR+4	(EL(I), I=1,NR)	Internal energy of liquid on the melt line (MJ/kg)
4*NR+4	(AL(I),I=1,NR)	Free energy of liquid on the melt line (MJ/kg)

Table 431

Word		
	NR	Number of densities
2	NT (=1)	
3	(R(I),I=1,NR)	Density array (Mg/m^3)
NR+3	T (=0)	
NR+4	(G(I),I=1,NR)	Shear modulus array (GPa)

Table 501

Word		
1	N	Number of temperature-density pairs
2	(T(I),R(I),I=1,N)	$LOG_{10}T_1$,$LOG_{10}R_1$,
		...
		$LOG_{10}T_N$,$LOG_{10}R_N$

Table 502-505,601-605

Word		
1	NR	Number of densities
2	NT	Number of temperatures
3	(R(I),I=1,NR)	LOG_{10} density array (g/cm^3)
NR+3	(T(I),I=1,NT)	LOG_{10} density array (eV)
NR+NT+3	((X(I,J),I=1,NR,)J=1,NT)	LOG_{10} quantity

SECTION 4

USE OF THE SESAME LIBRARY

USE OF THE SESAME LIBRARY

In addition to the SESAME Equation of State database, the user will also receive the subroutine library SESPACK. SESPACK consists of two distinct subroutine packages. The first is composed of the basic subprograms needed to implement SESAME tables in a computer program which uses equation of state data. The second is the HYDSES subroutine package for use in hydrodynamic codes. This package is described in "HYDSES: A subroutine package for using SESAME in hydrodynamic codes" (LA-8209). In particular, we emphasize that SESPACK contains two versions of the routines ISRCHK, INV301 and RATFN1. The first version is for general EOS work. The second in each case is the HYDSES version. Note that parameters bracketed by $ signs in dimension, common and data statements are dummy symbols to be replaced by the appropriate integer values.

There is no standard density-temperature grid for Sesame EOS tables. Each grid can be constructed to give the best representation of the EOS with as few points as possible. Consequently, storage requirements vary from material to material. At the present time, no table requires more than 15000 words. In most cases, a Sesame EOS table covers a much larger density and temperature range than is needed for a particular application. The file SESPACK provides a routine, WDW301, which reduces the size of the EOS tables by deleting data outside of specified density and temperature limits. Some users may want to call this routine from within S2GET or S2GETI. We expect that use of this option could decrease storage requirements by an order of magnitude in many cases.

The routines in the basic subroutine package are classified into several types, as shown below. These routines are written in ANS FORTRAN so that users should not have to adapt them to their local compilers. However, there may be certain exceptions to this rule. Input and output may be system dependent, so it is confined to the routines listed under A.

A. GENERALIZED INPUT/OUTPUT.

These routines call system I/0. The user is expected to check and modify them, if necessary.

INBUF binary read and end file test
OUTBUF binary write or end file mark
INBUFR random read
OUTBFR random write

OUTBUF is used to create or update the EOS Library. INBUF is used to read the library and should be compatible with OUTBUF.

B. LIBRARY PREPROCESSOR.

Subroutine UPDATE either creates or adds data tables to a binary library file from a data tape written in ASCII/EBCDIC card image format. Although this routine is system independent, the user must provide the library file, a scratch file and a file on which the new library (created or updated) will be returned. If the user specifies the creation of a new library, the old library file is not used. If the user specifies an update to the existing library, that library remains intact after the update. It is the responsibility of the user to save the new library after execution. Usage:

CALL UPDATE (DATE, NCPW, FMT, INEW, LUP, LIB, LM, LNEW, LP)

DATE	date of updating library (a six digit real number)
NCPW	number of characters per word
FMT	format for reading Hollerith data
INEW	0 (create a new library), 1 (update an existing library)
LUP	unit number of coded update file
LIB	unit number of original library
LM	unit number of scratch file
LNEW	unit number of new (created/updated) library
LP	unit number of printer file for diagnostic messages

Externals: INBUF, OUTBUF, RDCARD, S2BLDM, RETMAT, BDINDX, S2SRTM, S2BLDL, S2UPDT, SKIPMF, COPMAT, COPMTS, S2MOD, ASORT2, UPSUM, COMPAK, UPTPGM, COMBIN, TBFCH.

Because different computing machines have different word lengths for character data, the user must supply the appropriate format for reading 80 coded characters. For example, CDC machines permit up to 10 characters per word, while IBM machines allow a maximum of 4. In these two cases, the appropriate parameters would be as follows.

CDC: NCPW = 10, FMT = "(8A10)"
IBM: NCPW = 4, FMT = "(20A4)"

C. PACKAGED EOS ROUTINES FOR HYDRO CODES.

S2GET, S2EOS - These routines are intended for hydro codes which use density and temperature as the independent variables and pressure and internal energy as the dependent variables.

S2GET: Subroutine S2GET is used to get data from the library. S2GET reads in the 201 and 301 tables for the material specified.

The user must allocate an array for storage of the EOS tables and provide a COMMON block for a directory to this array. The COMMON block has the form

COMMON/S2DIR/LCMX, NRS, LCFW (10)

LCMX	length of the array
NRS	number of material regions (see below)
LCFW	an array used as a directory, initialized to zero by the user

Usage of S2GET is as follows:

CALL S2GET (IR, IDS2, TBLS, LCNT, LU, IFL)

IR	material region number
IDS2	Sesame material number
TBLS	name of array designated for storage of tables
LCNT	current word in array TBLS
LU	unit number for library
IFL	error flag

Each "region" corresponds to a different material. Regions should be numbered consecutively, whether or not a Sesame EOS is used. The same EOS may be requested for more than one region -- the routine will load a given table only once. S2GET must be called once for each region for which a Sesame EOS is required.

Data is loaded into the array TBLS, beginning with the word TBLS (LCNT). After successful execution of the routine, LCNT is set to the first word location following the data string which has been loaded. S2GET can be called again, using this new value of LCNT. However, the user can load other data into the array and compute a new value of LCNT before calling S2GET

again. If the routine is successful, IFL = 1 is returned. If IFL = 0, S2GET was unable to locate the EOS tables on the file LU. If IFL <0, there is insufficient storage in the array TBLS, and the size of the array should be increased by at least |IFL| words. This feature will enable some users to allocate storage dynamically.

S2EOS: Subroutine S2EOS is used to compute an EOS point. That is, it computes the pressure, energy, and their derivatives for a given density and temperature. Usage:

CALL S2EOS (IR, TBLS, R, T, P, E)

IR	material region number
TBLS	name of array which contains the EOS tables
R	density in Mg/m^3
T	temperature in degrees Kelvin
P, E	pressure, internal energy vectors

P(1), E(1)	pressure in GPa, internal energy in MJ/kg
P(2), E(2)	density derivatives, $(\partial P/\partial \rho)_T$, $(\partial E/\partial \rho)_T$
P(3), E(3)	temperature derivatives, $(\partial P/\partial T)_\rho$, $(\partial E/\partial T)_\rho$

Externals: INBUF, TBFCH, LA301A, ISRCH, RATFN2.

The parameters IR and TBLS should be identical to those which were used in calling S2GET. Note that the region number, not the Sesame material number, is used to identify the particular EOS table.

These programs are particularly useful for hydrodynamic codes. They provide for computations involving several Sesame tables, for the use of Sesame tables along with other EOS options, and for the specification of the same Sesame table in more than one region. All the necessary bookkeeping is internal to the routines.

S2GETI, S2EOSI - These routines are to be incorporated into a hydro code which uses the inverted form of an equation of state. Density and internal energy are the independent variables, and pressure and temperature are the dependent variables.

These routines are very similar to those described above. Usage of S2GETI is identical to S2GET. However, S2GETI reformats the EOS tables in order to

make the computations with S2EOSI more efficient. Usage of S2EOSI is as follows:

CALL S2EOSI (IR, TBLS, R, E, P, T)

IR	material region number
TBLS	name of array which contains the EOS tables
R	density in Mg/m^3
E	internal energy in MJ/kg
P, T	pressure, temperature vectors

P(1), T(1)	pressure in GPa, temperature in Kelvins,
P(2), T(2)	density derivatives, $(\partial P/\partial \rho)_E$, $(\partial T/\partial \rho)_E$
P(3), T(3)	energy derivatives, $(\partial P/\partial E)_\rho$, $(\partial T/\partial E)_\rho$.

Externals: INBUF, TBFCH, LA302A, INV301, ISRCH, ISRCHK, RATFN1, RATFN2.

For certain materials, the library also has tables of the pressure, temperature, density, and internal energy along the vapor-liquid coexistence curve. This information is needed in reactor safety problems. Routines S2GET and S2GETI can be modified to access the coexistence data, and routine LA401A can be used to compute the thermodynamic quantities.

D. AUXILIARY PACKAGED ROUTINES.

S2HUGI - Compute point on a Hugoniot
S2SHKI - Compute point on a Hugoniot
S2ABTI - Compute point on an Adiabat

E. SEARCH AND INTERPOLATION.

Basic routines to operate on data strings read in from library. Not usually called directly - LA301A, LA302A, WDW301, INV301, ISRCH, ISRCHK, RATFN1, RATFN2, LA401A, LA302B, LA302S.

RATFN1 and RATFN2 are the 1- and 2-dimensional rational function interpolation routines. RATFN2 also has a bilinear interpolation option.

F. LIBRARY MANIPULATION.

Basic routines to get data from a library. Not usually called directly - TBFCH, TABRAN, COPMAT, RDCARD, SKIPMF, COPMTS, LIBNIT. In the basic subroutine package, OUTBUF is used to create a sequentially formatted library. Tables are then fetched from this library using TBFCH which calls INBUF. A random formatted library may be created by using OUTBFR instead of OUTBUF. Tables may be fetched from the random library using TABRAN which calls INBUFR. (The routines TABSEQ and TABFCH in the HYDSES package may also be used to read SESAME tables. See LA-8209 for their usage.)

G. TEST PROBLEM.

To test the above procedures and to illustrate use of the Sesame library, we have constructed a test problem. - Subroutine TPRB1 accesses data for several materials specified by the user and computes and prints Hugoniot curves. Usage:

CALL TPRB1 (IDS2, N, LU, LP)

IDS2	An array, of dimension N, giving the material numbers selected by the user
N	number of materials specified
LU	unit number for library
LP	unit number for line printer

Externals: S2GETI, S2SHKI.

At the end of this section is a sample of the output from this routine, called with the following material numbers.

IDS2(1) = 3200 (lead),
IDS2(2) = 3332 (copper),
IDS2(3) = 3717 (aluminum).

(LCMX = 45000 in TPRB1)

The output variables are as follows.

R	density in Mg/m^3,
P	pressure in GPa,
E	internal energy in MJ/kg,
T	temperature in degrees Kelvin,
US	shock velocity in km/sec,
UP	particle velocity in km/sec.

shock hugoniot for sesame material number 3200

r mg/m3	p gpa	e mj/kg	t kelvin	us km/sec	up km/sec
0.158e+02	0.400e+02	0.500e+00	0.152e+04	0.353e+01	0.100e+01
0.190e+02	0.113e+03	0.200e+01	0.770e+04	0.497e+01	0.200e+01
0.217e+02	0.214e+03	0.450e+01	0.168e+05	0.628e+01	0.300e+01
0.242e+02	0.341e+03	0.800e+01	0.278e+05	0.753e+01	0.400e+01
0.264e+02	0.497e+03	0.125e+02	0.396e+05	0.876e+01	0.500e+01
0.284e+02	0.680e+03	0.180e+02	0.533e+05	0.999e+01	0.600e+01
0.301e+02	0.891e+03	0.245e+02	0.687e+05	0.112e+02	0.700e+01
0.318e+02	0.113e+04	0.320e+02	0.824e+05	0.124e+02	0.800e+01

shock hugoniot for sesame material number 3332

r mg/m3	p gpa	e mj/kg	t kelvin	us km/sec	up km/sec
0.109e+02	0.496e+02	0.500e+00	0.367e+03	0.555e+01	0.100e+01
0.125e+02	0.125e+03	0.200e+01	0.214e+04	0.699e+01	0.200e+01
0.137e+02	0.231e+03	0.450e+01	0.494e+04	0.863e+01	0.300e+01
0.147e+02	0.363e+03	0.800e+01	0.937e+04	0.102e+02	0.400e+01
0.157e+02	0.517e+03	0.125e+02	0.155e+05	0.116e+02	0.500e+01
0.166e+02	0.694e+03	0.180e+02	0.219e+05	0.130e+02	0.600e+01
0.175e+02	0.892e+03	0.245e+02	0.288e+05	0.143e+02	0.700e+01
0.184e+02	0.111e+04	0.320e+02	0.364e+05	0.156e+02	0.800e+01

shock hugoniot for sesame material number 3717

r mg/m3	p gpa	e mj/kg	t kelvin	us km/sec	up km/sec
0.318e+01	0.180e+02	0.500e+00	0.494e+03	0.667e+01	0.100e+01
0.360e+01	0.432e+02	0.200e+01	0.112e+04	0.800e+01	0.200e+01
0.399e+01	0.753e+02	0.450e+01	0.247e+04	0.930e+01	0.300e+01
0.434e+01	0.114e+03	0.800e+01	0.460e+04	0.106e+02	0.400e+01
0.467e+01	0.160e+03	0.125e+02	0.736e+04	0.119e+02	0.500e+01
0.497e+01	0.213e+03	0.180e+02	0.108e+05	0.131e+02	0.600e+01
0.525e+01	0.272e+03	0.245e+02	0.149e+05	0.144e+02	0.700e+01
0.552e+01	0.338e+03	0.320e+02	0.195e+05	0.157e+02	0.800e+01
0.577e+01	0.411e+03	0.405e+02	0.246e+05	0.169e+02	0.900e+01
0.601e+01	0.490e+03	0.500e+02	0.301e+05	0.182e+02	0.100e+02
0.624e+01	0.576e+03	0.605e+02	0.358e+05	0.194e+02	0.110e+02
0.647e+01	0.668e+03	0.720e+02	0.416e+05	0.206e+02	0.120e+02
0.668e+01	0.766e+03	0.845e+02	0.478e+05	0.218e+02	0.130e+02
0.688e+01	0.871e+03	0.980e+02	0.543e+05	0.230e+02	0.140e+02
0.707e+01	0.983e+03	0.112e+03	0.611e+05	0.243e+02	0.150e+02
0.726e+01	0.110e+04	0.128e+03	0.682e+05	0.255e+02	0.160e+02

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CURRENT LIST OF MATERIALS IN SESAME LIBRARY

Number	Material	Number	Material
1540	uranium	3210	indium
2020	beryllium	3280	gadolinium
2022	beryllium	3332	copper
2023	beryllium	3333	copper
2030	calcium	3334	copper
2110	europium	3510	cesium
2140	iron	3520	tantalum
2145	iron	3541	tungsten
2160	tin	3560	tungsten carbide
2290	lithium	3660	holmium
2291	lithium	3713	aluminum
2292	lithium	3715	aluminum
2293	lithium	3716	aluminum
2441	sodium	3717	aluminum
2448	sodium	3718	aluminum
2460	potassium	3719	aluminum
2550	vanadium	3730	platinum
2551	vanadium	3830	palladium
2680	cadmium	4100	brass
2700	gold	4270	stainless steel
2720	silver	4271	stainless steel
2740	niobium	5000	nitrogen
2810	rubidium	5001	nitrogen
2860	magnesium	5010	oxygen
2961	titanium alloy	5011	oxygen
2962	titanium alloy	5030	dry air
2980	molybdenum	5171	argon
2981	molybdenum	5172	argon
2982	molybdenum	5180	krypton
2983	molybdenum	5181	krypton
3050	rhodium	5190	xenon
3070	chromium	5210	carbon dioxide
3100	nickel	5250	hydrogen
3101	nickel	5251	hydrogen
3120	cobalt	5263	deuterium
3140	zinc	5271	d-t mixture
3180	zirconium	5272	d-t mixture
3200	lead	5280	ross-aller solar mix

Number	Material
5300	sr-xe mixture
5410	neon
5411	neon
5500	methane
5501	methane
5502	methane
5520	ammonia
5530	normal butane
5540	isobutane
5760	helium
5761	helium
5762	helium
7030	leaded glass
7081	boron carbide
7100	dry sand
7102	dry clay
7111	nevada alluvium
7112	nevada alluvium
7120	saturated tuff
7121	saturated tuff
7122	saturated tuff
7130	limestone
7150	water
7152	water
7153	water
7154	water
7160	deutero-polyethylene
7171	polyethylene (branched)
7180	polyethylene (marlex)
7190	teflon
7230	polytetradeutero-ethylene
7244	lithium(n)-deuteride
7245	lithium(6)-deuteride
7252	lithia-boria glass
7270	lithium fluoride
7281	salt
7282	salt
7283	salt
7330	calcium carbonate
7331	calcite
7371	lithium hydride
7380	quartz
7381	quartz
7383	polycrystal quartz
7385	polycrystal quartz
7386	fused quartz
7387	fused quartz
7390	westerly granite
7391	westerly granite
7410	alumina
7411	alumina
7432	uranium dioxide
7440	hematite
7450	calcium oxide
7460	periclase
7470	titanium dioxide
7480	niobium tritide
7510	dolomite
7520	mica
7521	muscovite (mica)
7530	basalt
7541	carbon phenolic
7452	carbon phenolic
7550	mylar
7560	polyurethane
7561	polyurethane
7570	phenolic
7580	phenolic refrasil
7590	polystyrene
7591	polystyrene
7592	polystyrene
7601	epoxy
7602	epoxy
7603	epoxy
7610	beryllium oxide
7611	beryllium oxide
7612	beryllium oxide
7660	peryphenylene sulfide
7740	polycarbonate

Number	Material
7741	polycarbonate (lexan)
7750	lucite
7760	garnet
7761	garnet sand
7770	parylene
7771	parylene
7830	diamond
7831	carbon liquid
7832	carbon (graphite)
7833	carbon (graphite)
7930	sylgard
7931	sylgard 184
8010	boron loaded silicone
8020	polyetheretherketone (peek)
8200	pbx-9502

MELT AND SHEAR TABLES

Number	Material
31540	uranium
32023	beryllium
32030	calcium
32140	iron
32160	tin
32292	lithium
32293	lithium
32441	sodium
32460	potassium
32551	vanadium
32680	cadmium
32700	gold
32720	silver
32740	niobium
32810	rubidium
32860	magnesium
32980	molybdenum
32983	molybdenum
33050	rhodium
33070	chromium
33100	nickel
33101	nickel
33120	cobalt
33140	zinc
33180	zirconium
33200	lead
33210	indium
33330	copper
33332	copper
33510	cesium
33520	tantalum
33540	tungsten
33541	tungsten
33710	aluminum
33717	aluminum
33830	palladium
34271	stainless steel 347

Number	Material
37030	leaded glass
37112	nevada alluvium
37270	lithium fluoride
37387	fused quartz
37470	titanium dioxide
37480	niobium tritide
37603	epoxy
37741	polycarbonate (lexan)
37770	parylene
37771	parylene
37832	carbon
37833	carbon