LA-7130
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Issued: February 1978

Recent Developments in the Sesame Equation-of-State Library

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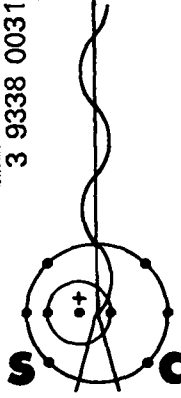

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UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36

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

Printed in the United States of America. Available from
National Technical Information Service
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RECENT DEVELOPMENTS IN THE SESAME EQUATION-OF-STATE LIBRARY

by

B. I. Bennett, J. D. Johnson, G. I. Kerley, and G. T. Rood

ABSTRACT

The Sesame library is a computer file of tabular equations of state and other material properties, developed in Group T-4 of the Los Alamos Scientific Laboratory. This report describes some of the theoretical models used in the library, the structure of the data storage and acquisition system, and the computer routines that have been developed to access and use the tables in practical applications. It also discusses how non-LASL users can obtain the Sesame data and subroutine libraries.

I. INTRODUCTION

The Sesame library is a file of equation-of-state (EOS) tables and other material properties that can be accessed by computer programs for a variety of applications. It has been in use at the Los Alamos Scientific Laboratory (LASL) for several years. Now LASL offers this library, together with interpolation programs and utility routines for manipulating the data files, to other laboratories and research groups. In this report, we will give an overview of the Sesame library and discuss some new developments that should be of interest to users.

During the past 30 years, remarkable achievements have been made in numerical hydrodynamics calculations.[1] Modern computer codes, which include the effects of material strength, fracture, viscosity, chemical reactions, heat conduction, and radiation transport, can be used to make realistic predictions for complicated hydrodynamic flow problems. These numerical codes have become essential tools to workers in many fields, including weapons effects, reactor safety analysis, and laser fusion.

To make accurate hydrodynamics calculations, it is necessary to have realistic EOS and other properties. However, the study of an EOS is a big project in itself. Even when data are readily available, a researcher may have difficulty finding a way to represent them in his code.

The Sesame library was developed to store the best EOS data in a tabular form, which is useful for hydrodynamics codes and other applications. A key feature of the library is that the codes can access the tables directly, instead of using approximate analytic fits to the data. Although analytic formulas can be useful, they cannot represent a complicated EOS table accurately over a wide range of temperatures and densities. We have designed computer subroutines that search the tabular library for a list of materials and calculate the thermodynamic functions by interpolation from the tables. These routines are modular and are written in standard FORTRAN, so that they can be incorporated into user codes with relative ease. Using these techniques, we have found the tabular EOS formulation to be very feasible and useful.

In Sec. II, we discuss some of the theoretical models used in generating Sesame EOS tables. The structure of the data storage and acquisition system is presented in Sec. III. In Sec. IV we describe the subroutine library that has been written for users to access the data for applications.

To obtain additional information about the Sesame library or to be placed on the mailing list for documents, write to

Sesame Library, MS-925
Los Alamos Scientific Laboratory
Los Alamos, NM 87545.

To obtain Sesame tables, a user should mail his own magnetic tapes and a list of the materials required to the above address. One tape will be written with a copy of the Sesame FORTRAN subroutine library, and the other tapes will be written with tabular data in a BCD card image format. One tape can hold data for up to 25 materials. A set of instructions will be enclosed when the tapes are returned.

II. MODELS FOR CALCULATING EOS

There exists no universal method for calculating the EOS that is valid for all pressures, temperatures, and chemical compositions. Many models can be used,

and studies should be conducted to determine which approach is best for a particular material. It is our goal that the Sesame library should provide the best theoretical and experimental data available. Therefore, the EOS tables can come from any source, including laboratories other than LASL.

In this section, we will discuss some of the models that have been developed at LASL for generating Sesame tables and give a general idea of the concepts involved. It is rarely possible to apply these methods to a specific problem in a straightforward way. For an example of a problem in which more theoretical work is required, the reader should refer to our study of the deuterium EOS.[2,3]

It is common to write the EOS as a sum of three contributions.[4] The pressure is given by

$$P(\rho,T) = P_c(\rho) + P_N(\rho,T) + P_e(\rho,T) \ , \tag{1}$$

where ρ is the density and T is the temperature. $P_c(\rho)$ is the cold curve, or contribution from electronic cohesive and repulsive forces at T = 0 K. $P_N(\rho,T)$ is the contribution from nuclear motion, and $P_e(\rho,T)$ is the thermal electronic term. Expressions for the internal energy, the Helmholtz free energy, and the other thermodynamic functions are similar to Eq. (1).

A. The Cold Curve

For most practical applications, the cold curve must be determined by empirical methods and phenomenological theories. However, prospects for improving this situation are good. Some calculations for compressed solids have been made using band-theoretical methods,[5-7] although these computations are too difficult and expensive to perform on a routine basis. Recently, Liberman has developed a relativistic and quantum-mechanical compressed atom model that may be useful for many applications.[8] Sometimes these more sophisticated techniques can be used to check and improve upon the empirical methods discussed below.

The Thomas-Fermi-Dirac (TFD) theory[9] and other statistical theories of the atom give reasonable results for the EOS at high densities. Many methods for calculating the cold curve are based upon empirical corrections to the TFD results.

Barnes[10] has found that the cold curve for many materials can be described by

$$P_c(\rho) = a\eta^{2/3}\left(\eta e^{b_r\nu} - e^{b_a\nu}\right), \tag{2}$$

where $\eta = \rho/\rho_o$, $\nu = 1 - \eta^{-1/3}$, and ρ_o is the normal density of the solid. The constants a and b_r are obtained by fitting the TFD data at high densities, and b_a is determined from the experimental bulk modulus, B_o, using the relation

$$B_o = \left(\rho dP_c/d\rho\right)_{\rho_o} = \frac{1}{3}\, a\, \left(3 + b_r - b_a\right). \tag{3}$$

Equation (2) has been used in generating many of the Sesame EOS tables. For materials having phase transitions that involve large volume changes, a separate cold curve is calculated for each phase, and the transition pressure is determined from experiment.

Rice, McQueen, and Walsh showed that the cold curve can be determined from the shock Hugoniot, if a Mie-Grüneisen EOS is assumed.[11] Using the Dugdale-MacDonald relation for the Grüneisen function,[12] they calculated cold curves for 25 metals. Vaidya and Kennedy have made static compressibility measurements up to 45 kbar on 18 metals,[13] and the results agree well with the shock wave predictions.[14] To illustrate the procedure, let us write the Mie-Grüneisen EOS in the form[15]

$$P_c(\rho) - \rho\,\gamma(\rho)E_c(\rho) = P_H(\rho) - \rho\,\gamma(\rho)E_H(\rho)\ . \tag{4}$$

P_H and E_H are the pressure and internal energy on the Hugoniot, which are obtained from experiment. The Grüneisen function, $\gamma(\rho)$, is related to the Debye temperature, $\theta(\rho)$, by

$$\gamma = \frac{d\ \ln\ \theta}{d\ \ln\ \rho}\ . \tag{5}$$

The cold curve pressure, P_c, and internal energy, E_c, are related by

$$P_c = \rho^2\,\frac{dE_c}{d\rho}\ . \tag{6}$$

With these relationships, Eq. (4) can be integrated, as follows:

$$E_c(\rho) = \theta(\rho) \left[E_c(\rho_o)/\theta(\rho_o) + \int_{\rho_o}^{\rho} \frac{P_H(x) - x\,\gamma(x)E_H(x)}{x^2\theta(x)}\,dx \right] . \qquad (7)$$

If the functions $\gamma(\rho)$ and $\theta(\rho)$ are known explicitly, the cold curve can be determined quite easily from Eq. (7). If $\gamma(\rho)$ is expressed in terms of $P_c(\rho)$, as in the Dugdale-MacDonald formula, the procedure of Rice et al.[11] may be used.

The above procedure is used in generating Sesame EOS tables as an alternative to Eq. (2). The technique is augmented by a high-density extrapolation, which defines the cold curve at densities that cannot be obtained by shock wave methods or in regimes where the Mie-Grüneisen EOS is not valid. An expression similar to Eq. (2), based upon the TFD EOS, is used in most cases.

For most applications the cold curve must be defined in tension ($\rho < \rho_o$) as well as in compression. The binding energy of the solid, E_B, is related to the pressure on the cold curve by an integral over the tension region,

$$E_B = -\int_0^{\rho_o} P_c(\rho)\,\rho^{-2}\,d\rho \quad . \qquad (8)$$

For many materials, Eq. (2) gives reasonable values of the binding energy. This suggests that the Barnes form for the cold curve gives a realistic description for tension as well as compression. However, it is often desirable to attach another analytic form, such as one based upon a Lennard-Jones force law onto the cold curve at some density, and to adjust the constants so that the EOS agrees with experimental vaporization data. In this way, the experimental binding energy is usually matched exactly when generating a Sesame EOS.

B. Nuclear Contributions

For many solids the Debye model gives a reasonable estimate of the nuclear contributions to the EOS.

$$P_N = \rho\,\gamma(\rho)\,R\left[\frac{9}{8}\theta + 3D(\theta/T)\right] ,$$

$$D(X) = \frac{3}{X^3}\int_0^X \frac{y^3}{e^y - 1}\,dy , \qquad (9)$$

where R is the gas constant. Equation (9) includes both the zero point and thermal contributions to the pressure. As mentioned above, $\gamma(\rho)$ and $\theta(\rho)$ are frequently estimated from the cold curve, using the Dugdale-MacDonald formula or a similar approximation. Experimentally, information about these parameters can be obtained from thermodynamic data, from reflected shock experiments, from measurements of the sound speed in a shocked material, and from shock measurements on foams.[16] Sometimes simple analytic expressions for γ and θ may be adequate to fit the data.

At high temperatures or low densities, the nuclear term should approach the ideal gas limit.

$$P_N \to \rho RT \text{ as } T \to \infty \text{ or } \rho \to 0 . \qquad (10)$$

Many schemes for estimating the nuclear contributions to the EOS are just interpolation formulas between Eqs. (9) and (10). One method used in Sesame is that of Kormer et al.[17] A simplified version of this model has been used by Thompson and Lauson[4] and by Merts and Magee.[18] The reader should consult these references for discussion of the equations.

Barnes et al. have shown that a modified virial expansion of the nuclear term gives good results for the EOS of expanded materials.[19,20] In their approach, Eq. (9) is used for compressed states, $\rho \geq \rho_0$. For $\rho < \rho_0$, they write

$$P_N = RT\left[\rho + B(T)\rho^2 + C(T)\rho^3\right] , \qquad (11)$$

where the functions B(T) and C(T) are determined by matching Eq. (11) smoothly to Eq. (9) at $\rho = \rho_0$. In more recent work, we have added another term to the expansion; the extra coefficient can be determined from the requirement that the energy approach that for an ideal gas as $\rho \to 0$.

When the nuclear term is added to the cold curve, it is found that the calculated isotherms have a Van der Waals form below some critical temperature. Hence these models lead to the formation of a two-phase region in which the vapor coexists with the condensed phase.[20] In creating Sesame EOS tables, we attempt to vary the parameters in the model until the best fit to experimental vapor pressure measurements and other data is obtained.

In constructing a Sesame table, either the equilibrium or nonequilibrium results can be used in the mixed phase region. For problems in which a solid or liquid is heated rapidly and allowed to expand ("blowoff"), the correct treatment of vaporization can be essential in predicting hydrodynamic flow. Therefore, the equilibrium vapor pressures are normally used in constructing the high-temperature isotherms.

At low temperatures, however, vaporization may not occur on microsecond time scales. A solid can go into tension until critical stresses are exceeded, at which time spall (fracture) can take place. Therefore, some Sesame EOS tables are constructed with a negative pressure region at low temperatures, so that they can be used with spall models that are typical of hydrocodes.[21]

The mixed phase region is particularly important in the analysis of fast reactor safety. In the reactor analysis code, SIMMER, both equilibrium and nonequilibrium thermodynamic variables are used in computing evaporation and condensation.[22] We have developed a special Sesame EOS package for this code.

C. A Liquid Model - Melting

Although the empirical models discussed above can be made to match experimental vaporization data with good agreement, they do not predict a real melting transition. Melting is important, not only because it has an effect upon the EOS, but also because material strength disappears in the liquid phase. Consequently, the melting temperature at high pressures is needed for models of elastic-plastic flow.

We have developed a variation theory of liquids, which uses the hard sphere EOS with perturbation terms to correct for the effect of realistic interatomic forces.[23] Our model is similar to that of Mansoori and Canfield.[24] However, the interatomic interactions are obtained from the cold curve, instead of from pair potentials. The reader should consult Ref. 23 for details. This theory gives good results for hydrogen, deuterium, and argon.[2,3,23] In particular, the predicted melting curve for argon was in good agreement with experiment. We are

working with this model to generate new Sesame EOS tables for metals, and the preliminary results are encouraging. Some calculations of the lead EOS are discussed in Sec. II.E.

D. Thermal Electronic Contributions

The term $P_e(\rho,T)$ in Eq. (1) represents contributions from thermal excitation and ionization of the electrons to the EOS. These effects become appreciable at temperatures above 10^4 K, and they can be significant at much lower temperatures in special cases.

At the present time, most of the Sesame EOS tables are based upon the temperature-dependent TFD theory, using a code written by R. D. Cowan.[9,25] Although the TFD theory neglects effects that result from discrete atomic levels and band structure, we believe it is adequate for reproducing some of the gross features of electronic excitation. Better theoretical methods are becoming available, and we intend to use them in generating Sesame tables in the future.

The calculations of Huebner et al. take the discrete atomic levels into account by solving the Schrödinger equation for the perturbed and thermally excited atoms.[26] For temperatures less than 10^6 K, experimental level data are used for those states that have been measured. At higher temperatures and for the highest densities, a mean ion model is used. Ion-ion correlations, which are neglected in these calculations, become important at high densities and low temperatures. For this region, we are investigating a new model, which has been proposed by Liberman.[8]

E. An Example - Lead EOS

Shock Hugoniot data for lead[27] provide some confirmation of the models. In Fig. 1, the experimental shock velocity (U_s) vs particle velocity (U_p) curve is compared with three calculations. The curve for the solid phase, based upon the Debye model, exhibits a linear U_s, U_p relationship which is typical of metals. For strong shocks, there is a marked change of slope, which suggests that melting has occurred.[28] Our calculated curve for the liquid agrees well with the experimental data. For still stronger shocks, there is sufficient thermal energy to cause significant electronic excitation and ionization. When this effect is included, even better agreement with experiment is obtained.

In summary, Sesame EOS tables are constructed from many different models and obtained from a variety of sources. When new theoretical and experimental results become available, the tables are revised or replaced, so that the best data is accessible to users.

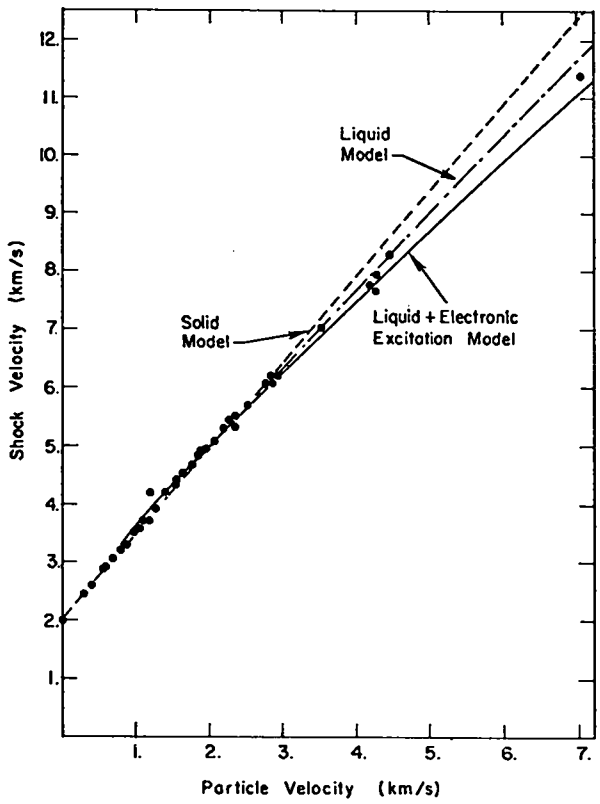


Fig. 1.
Comparison of experimental shock data (circles) with theoretical calculations for lead.

III. STRUCTURE OF THE SESAME DATA LIBRARY

The Sesame library is a general purpose system for storing and accessing processed material property data. At the present time, Sesame only offers tables of thermodynamic properties, which is the purpose for which it was originally developed. However, it uses a flexible scheme for storing and cataloguing data, so that it can be adapted to other applications. We plan to add opacity tables to the library soon.

For efficient storage and rapid data acquisition, the library is kept as a binary (unformatted) file on a disk or other mass storage device. Such a file is not portable, because binary files have different structures on different computing systems. To transmit the library to users, we have developed a procedure for writing the data onto a magnetic tape in a BCD card image format, which can be read and interpreted by most systems. This tape is preprocessed by the user at his own installation, using FORTRAN routines from the Sesame subroutine library. The result is a binary file, created by the local system, that is saved for future use. From time to time, the user can add or replace data on the library with update tapes from LASL.

A. Data Records

The fundamental unit of information on the Sesame library is a data record. One record contains a data string of arbitrary word length, written onto the file with an unformatted FORTRAN WRITE or similar output command. A description of the data records used in Sesame is given in Table I.

The type of data and specific format with which it is tabulated in a record is identified by a catalog number. For example, a 301 data record is used to tabulate pressure and internal energy as functions of density and temperature.

TABLE I

STRUCTURE OF THE SESAME DATA RECORDS[a]

No. 201. Basic Data: five real words.

- Z - average atomic number
- A - average atomic weight
- ρ_o - solid density
- B_o - solid bulk modulus
- C_{ex} - exchange coefficient (not always used)

No. 301. EOS Tables: pressure and internal energy as functions of density and temperature.

NR, NT, (R(I), I = 1, NR), (T(J), J = 1, NT), ((P(I,J), I = 1, NR), J = 1, NT), ((E(I,J), I = 1, NR), J = 1, NT)

- NR - number of points on density mesh (real number)
- NT - number of points on temperature mesh (real number)
- R - density mesh
- T - temperature mesh
- P - pressure
- E - internal energy

No. 302. Inverted EOS tables: pressure and temperature as functions of density and internal energy.

NR, NE, (R(I), I = 1, NR), (ET(J), J = 1, NE), (EC(I), I = 1, NR), ((P(I,J), I = 1, NR), J = 1, NE), ((T(I,J), I = 1, NR), J = 1, NE)

- NR - number of points on density mesh (real number)
- NE - number of points on thermal energy mesh (real number)
- R - density mesh
- ET - thermal energy mesh (ET = E - EC)
- EC - internal energy at 0 K
- P - pressure
- T - temperature

TABLE I (cont)

No. 401. Vaporization Tables: thermodynamic quantities on the vapor-liquid and vapor-solid coexistence curve.

NT, (P(I), I = 1, NT), (T(I), I = 1, NT), (RG(I), I = 1, NT), (RL(I), I = 1, NT), (EG(I), I = 1, NT), (EL(I), I = 1, NT)

NT - number of temperatures (real number)

P - vapor pressure

T - temperature

RG - vapor density on coexistence line

RL - density of liquid or solid on coexistence line

EG - internal energy on coexistence line

EL - energy of liquid or solid on coexistence line

- When interpolating on a 401 data string, all quantities except EG can be used as independent variables.
- T(NT) is the critical temperature.

---

[a]Units used in the Sesame library are

pressure - GPa

energy - MJ/kg

density - Mg/m^3

temperature - K.

$$P = f_1(\rho,T) \ , \qquad (12)$$

$$E = f_2(\rho,T) \ .$$

A 302 data record is used to tabulate the "inverted" EOS, pressure and temperature as functions of density and energy.

$$P = g_1(\rho,E) \ ,$$

$$T = g_2(\rho,E) \ . \qquad (13)$$

Equations (13) could be calculated from a 301 data record, but note that the formats are different in the two cases. At the present time, the 302 data records are not kept on the library, because they are easy to generate from the 301 form when they are needed.

When a new data form is added to the library, a format is worked out and it is assigned a catalog number. Hence the library will become more general in time. There are only two restrictions on the formats that can be used. Each record must be all Hollerith, all real, or all integer, and all Hollerith records must be assigned a catalog number from 100-199.

B. Material File

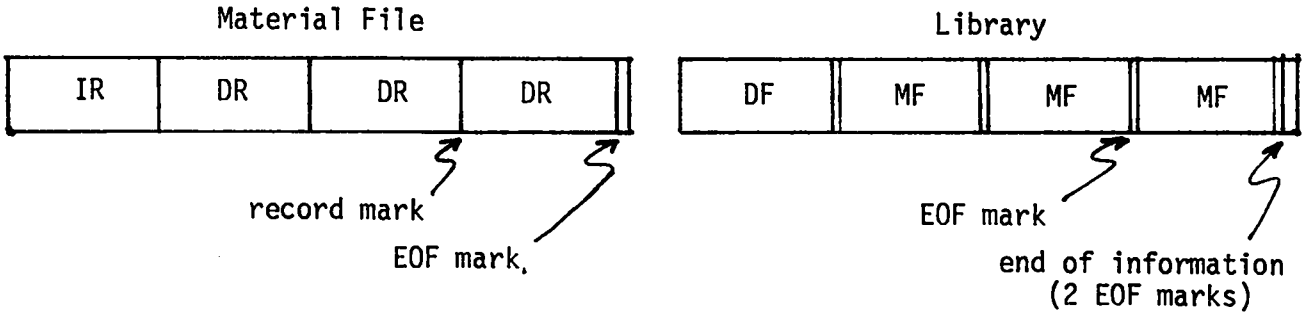
A collection of several data records, together with an index record, forms a material file, as illustrated in Fig. 2. Each file contains data for a particular material, which is identified by a material number from 1000-9999. A list of the Sesame materials presently available in the library is given in Table II. Those materials identified as "reactor safety" were generated for the SIMMER-II code, and they cover a more limited density-temperature range than the others. Materials 5760, 7150, and 7151 were obtained from Lawrence Livermore Laboratory (LLL).[29,30] The other tables were generated at LASL. Some of these tables are being revised, and new materials will be added continually to the library.

The index record to a file gives the material number, the number of data records in the file, and the catalog number and word length of each record. The structure of an index record is described in Table III.

C. Structure of the Library

The library is a collection of material files, preceded by a directory, as illustrated in Fig. 2. Files are separated by END FILE (EOF) marks, which can be used to search through the library for a particular material. On IBM, and on other systems for which multiple file-sets are cumbersome, the EOF marks can be replaced by one-word ASCII records. Directions for making this simple change are included in the instructions that are enclosed with the Sesame subroutine library.

The directory file, described in Table IV, gives the number of material files in the library and the material I.D. number of each.



IR - index record (see Table III)
DR - data record (see Table I)
DF - directory file (see Table IV)
MF - material file (depicted at right)

Fig. 2.
Structure of the Sesame data library.

IV. THE INTERPOLATION ALGORITHM AND SUBROUTINE LIBRARY

The Sesame subroutine library was developed to simplify use of the tables. It contains routines to preprocess the magnetic BCD data tape, to load data from the library into local storage, and to search and interpolate on the data. With the exception of binary input/output, which has been localized in only two routines, all subprograms are written in standard FORTRAN, so that no system conversion should be required. Use of the subroutines is discussed in comment cards and in the instructions that are provided with the subroutine library. Hence we will discuss only general concepts in this report.

A. Rational Function Interpolation

Considerable work has been done to develop an interpolation algorithm suitable for EOS data.[31] In some applications where accuracy can be sacrificed, linear interpolation is attractive because it is simple and computationally fast. Consequently, we provide users with a linear scheme as one of the options.

However, we found that it was necessary to develop a higher order method as well. The Sesame tables often cover wide temperature and density ranges, and the mesh is often much too coarse for a linear algorithm. Moreover, many users require derivatives of the functions (sound speed, specific heat), and linear methods give poor estimates of these quantities.

Our rational function method of interpolation is particularly useful for functions having a rapid or discontinuous change in the derivatives.[31] This feature is important in working with EOS data, which may have phase transitions.

TABLE II

UNCLASSIFIED SESAME MATERIALS AS OF DECEMBER 1977

1540 - Uranium[a]	5760 - Helium[b]
2020 - Beryllium[a]	7081 - Boron Carbide (reactor safety)
2140 - Iron[a]	7111 - Nevada Alluvium[a]
2145 - Iron (reactor safety)	7150 - Water[b]
2448 - Sodium (reactor safety)	7151 - Steam[b]
2700 - Gold[a]	7170 - CH_2 (polyethylene)[a]
2980 - Molybdenum[a]	7240 - ^6LiD[a]
3100 - Nickel[a]	7370 - ^6LiH[a]
3200 - Lead[a]	7380 - SiO_2 (quartz, sand)[a]
3330 - Copper[a]	7390 - Westerly granite[a]
3710 - Aluminum[a]	7410 - Al_2O_3 (alumina, sapphire)[a]
3730 - Platinum[a]	7432 - UO_2 (reactor safety)
4100 - Brass[a]	7510 - Vermiculite (mica)[a]
4270 - Stainless Steel[a]	7560 - Urethane[a]
5263 - Deuterium	7590 - CH (polystyrene)[a]
5410 - Neon[a]	8180 - High Explosive (XO-290)[c]

[a]Generated by J. F. Barnes.
[b]Obtained from LLL.
[c]Generated by C. L. Mader.

Finally, we have studied methods of optimizing the density and temperature mesh, and we feel that current storage requirements can be cut in half, eventually.

B. Accessing Data from the Data Library

The subroutine file contains a number of routines that search the data library for a material requested by the user, load data into a local array, and

TABLE III

STRUCTURE OF THE INDEX RECORD FOR A SESAME MATERIAL FILE

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

MATID - material I.D. 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 of catalog 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)

TABLE IV

STRUCTURE OF THE DIRECTORY FILE FOR THE SESAME LIBRARY

Record 1. Consists of three words.

N, DATE, VERS

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

DATE - date of current version

VERS - version number

Record 2. Consists of two arrays.

(MATID(I), I = 1, N), (NWDS(I), I = 1, N)

MATID - table of material I.D. numbers, in the same order as the material files in the library (real numbers)

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

compute thermodynamic functions, Eqs. (12) and (13), by search and interpolation. 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. These programs have been checked out and installed into the one-dimensional hydrocode SIN.[21] Sesame tables can be used with both LaGrangian and Eulerian codes, in problems that involve elastic-plastic flow, spall, foams, nonequilibrium phase transitions, and radiation flow.

For some reactor safety applications, EOS data is used in modeling multiphase fluid flow and phase transitions. The SIMMER code solves coupled sets of hydrodynamic equations for the solid, liquid, and a vapor mixture of varying chemical composition.[22] A special Sesame EOS package has been written for this problem. An algorithm was developed to calculate the EOS of the vapor mixture, as a function of its chemical composition, from EOS tables for the pure components. The tabular package also provides liquid-vapor coexistence quantities that are used in computing evaporation and condensation rates. These specialized routines are not available from the subroutine library, but interested users can send for them.

C. A Display Package

We have developed a new code to display Sesame EOS data graphically, in a variety of formats. The existing version of the code has several system-dependent features (primarily input/output) that limit its use to LASL computers. However, it is a modular code, designed to be adapted to other computer systems and display devices with minimum effort.

The heart of the display code is a plotting module that can produce graphs on three different output devices in use at LASL. Most of the plotting subroutines are independent of the hardware to be used in graphing. Those routines that refer to a specific output device are limited to elementary graphing operations (plotting a point or drawing a vector). Consequently, the code can be made to plot on new output devices without major revision.

The data to be graphed by the plotting module is generated by another module, which uses the interpolation routines discussed above. With relatively few commands, a user can generate isotherms, isentropes, and Hugoniot curves. Data can be plotted on either linear or logarithmic axes, and the user can zoom in on a

specific region of interest. Many curves can be plotted on the same figure, and each curve is labeled for identification.

Although the code is not yet available outside LASL, the subroutines that are used to calculate Hugoniots and isentropes are included in the Sesame subroutine library, for interested users.

V. SUMMARY AND CONCLUSIONS

In this report, we have given an overview of the Sesame library. Both the theory and the data handling procedures were described. We have not presented an evaluation of specific EOS tables and compared with experiment. Such studies will be reported elsewhere. Detailed discussion of computer programs has been avoided. However, users will be able to obtain much information from comment cards given in the routines themselves and from the instruction sheets that are enclosed with the listings and magnetic tapes.

As we continue to add new data and make improvements to the Sesame library, users will be kept informed by reports and newsletters.

ACKNOWLEDGMENTS

The authors are grateful to John F. Barnes, Jr., whose work formed the foundation of Sesame, and who generated many of the EOS tables in the library. We wish to thank Charles A. Forest, who contributed much useful advice in setting up the data storage and retrieval procedures. We are grateful to our colleagues at LLL, who have provided us with their data. There are many other individuals, too numerous to mention, who have aided us along the way.

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