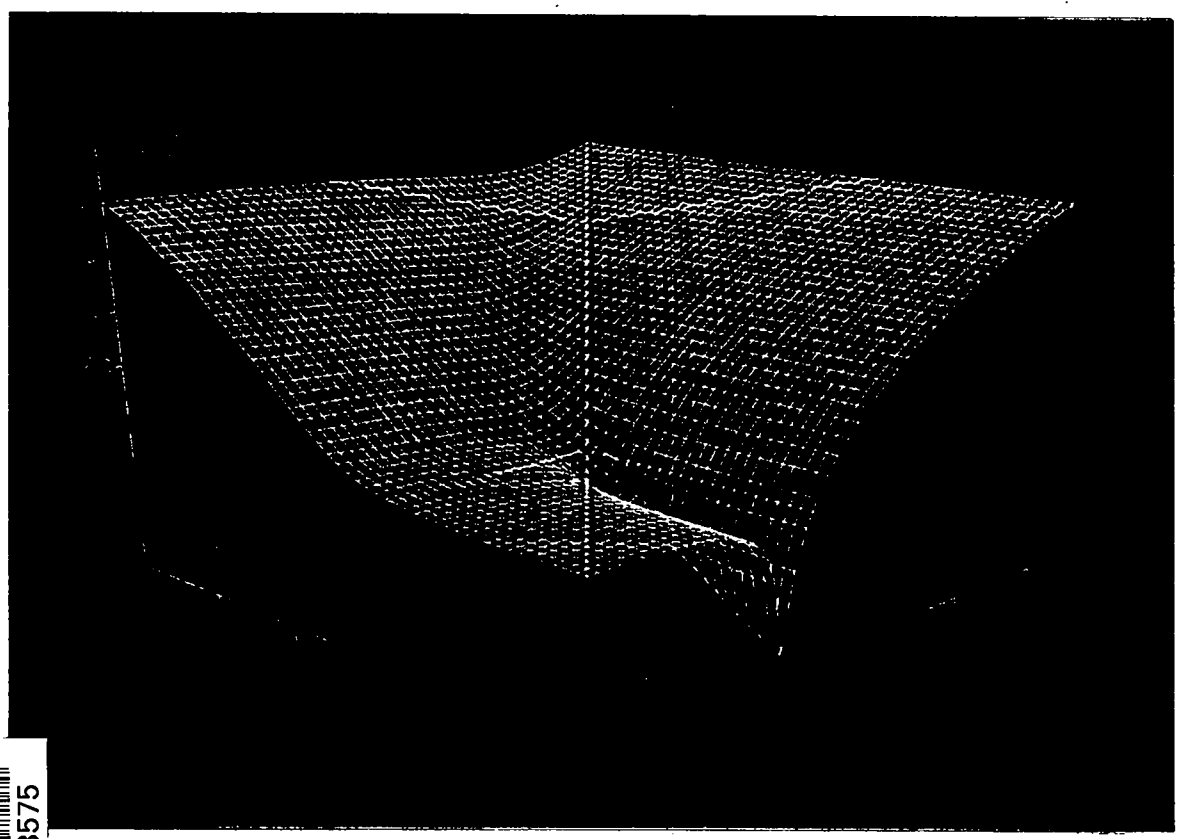
An Invitation to Participate in the LASL Equation of State Library



Jerry Kerley has available copies 5476

LOS ALAMOS
SCIENTIFIC LABORATORY

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An Invitation to Participate in the LASL Equation of State Library

This brochure is an invitation to participate in the SESAME EOS library, an effort by LASL's Equation of State and Opacity Group to create a standard computer-based data library for thermodynamic properties. This project is supported by the DOE Division of Basic Energy Sciences. The data base is available to all interested users free of charge. It is designed to be used in hydrodynamic codes for energy and defense applications. The library is still in its infancy and requires collaboration with users and other researchers to make it a useful tool for a wide spectrum of research needs. We invite you to send for the library, to use it, and to offer suggestions for improvement and expansion. The contents of this brochure will introduce you to the basic features of the library and to the research effort at LASL that goes into generating it. After reading this material, please let us know your interests and research requirements by filling out the attached comment sheet and returning it to us. We welcome your interest and participation.

Photo: Developers of the SESAME library at Los Alamos Scientific Laboratory: From left to right, Bard Bennett, Joe Abdallah, J. D. Johnson, Stan Lyon, Bob Albers, Jerry Kerley—project leader, and Jack Barnes, originator of the library.

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Executive Summary

Standardizing EOS Data

The SESAME EOS library is a computer-based library of EOS data and FORTRAN subroutines developed by LASL for internal and external use. With cooperation from outside users the developers hope to make it a standard reference for energy research analogous to the ENDF/B national nuclear data base currently used in the nuclear industry.

Basic Features of the Library

The library contains EOS tables of pressure and internal energy as functions of temperature and density for approximately 30 different materials. The tabular format has several advantages: (1) it can represent phase transitions accurately, (2) it covers a wide range of temperatures and densities, and (3) it is easily updated to incorporate new experimental or theoretical results in specific regions of temperature and density.

Accurate schemes to interpolate on the tabulated data are contained in the SESAME subroutine library as well as subroutines to preprocess the data into a compact binary file, search this file for a given material, load data into a local array, and compute thermodynamic functions by search and interpolation. 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.

The contents of the library are listed on page 13.

User Experience

The library has been used in many LASL programs, and more recently, by outside scientists involved in laser fusion research, reactor safety analysis, and defense projects. Outside users include scientists at the Air Force Weapons Laboratory, Physics International, England's Atomic Weapons Research Laboratory, Lockheed Missiles and Space, University of Rochester Laser Energetics Laboratory, Sandia Laboratories, Oak Ridge National Laboratory, Brookhaven National Laboratory, University of Wisconsin, and University of Arizona.

Materials, Methods, and Applications

Recent EOS research for the SESAME library includes

- New techniques for constructing consistent multiphase EOS tables appropriate for materials subjected to shock phenomena.
- New, more accurate EOS for laser fusion studies including EOS for deuterium, and two-temperature EOS for nonequilibrium conditions in laser pellet implosions.
- New, more accurate EOS for reactor safety studies including sodium and uranium dioxide. A new theory of liquids was developed and applied to liquid sodium, and a refined treatment of thermal electronic excitations was an important new feature of the UO_2 EOS.

How to Send for the Library

The SESAME library is available to users free of charge. A user should send two or more magnetic tapes, a list of materials required, and a specification of the tape parameters to

SESAME Library, MS-925
P. O. Box 1663
Los Alamos Scientific Laboratory
Los Alamos, NM 87545

Future Developments of the Library

Future work will focus on adding new materials appropriate to nonnuclear energy research, as well as improvement of existing tables where the need arises. Eventually the library will be expanded to include transport properties such as viscosity, diffusivity, thermal conductivity, and electrical conductivity.

Outside participation will be crucial to the establishment of the library as a standard data base. This participation should include requests for data and feedback on the usefulness of the SESAME tables and software packages, as well as more detailed evaluation of the EOS data and suggestions and contributions to the library.

You can begin this cooperative effort by returning the response form on p. 31.

Standardizing EOS Data

As national efforts in energy research continue to expand, there is an increased need to develop and maintain standard data bases. These libraries focus attention on the data needed in the research programs and develop systems of acquiring and evaluating the data. They help to coordinate related efforts and are useful in comparing research results. Equation-of-state data and related material properties are in need of such standardization. These data form the input to numerical hydrodynamics codes that are used to study a wide variety of energy and defense related problems such as reactor safety, laser fusion, studies of shock phenomena and detonations.

Depending on the specific application, these codes must model the effects of material strength, fracture, viscosity, chemical reaction, heat conduction, and radiation transport in order to make realistic predictions for the complicated hydrodynamic flows involved. Frequently, the discrepancies among independent hydrodynamic calculations occur because different equations of state and related material properties are used in each calculation. A standard data base for EOS and other material properties, along the lines of the evaluated nuclear data file (ENDF/B), would end this unnecessary confusion. The ENDF/B has been developed over the last 13 years through a coordinated effort of nuclear scientists from many institutions and is the reference data set used in almost all nuclear applications in the United States.

The SESAME EOS library, developed at LASL by the Equation of State and Opacity Group, is a first step in the establishment of such a standard data base for thermodynamic properties of materials. It is a computer-based library of tabular data along with a set of FORTRAN subroutines, which adapt the library contents to the user's local computing system, and compute thermodynamic functions for specific applications. The library has been in use for several years at LASL and more recently by scientists at outside institutions. The development of the library is supported by the DOE Division of Basic Energy Sciences.

The contents of the library are the result of a coordinated effort of many LASL scientists over several decades to develop EOS data that agree with available experimental data but extend to regions of temperature and density that are inaccessible to direct laboratory measurement. Consequently, the contents of the SESAME library are constructed largely from theory in contrast to the ENDF/B nuclear data base. Initial EOS research at LASL was devoted to the behavior of condensed matter during high compressions produced in explosively driven shock wave experiments. These experiments performed at LASL were an important tool for constructing the EOS. Recent work has been devoted to developing EOS for laser fusion and reactor safety studies in which material behavior at lower densities and higher temperatures becomes more important. In general, the SESAME EOS tables cover a very wide range of

temperatures and densities as illustrated by the SESAME EOS surface for lithia-boria glass shown in Fig. 1. The tables are particularly useful for hydrodynamics codes that model systems undergoing wide variations in these variables.

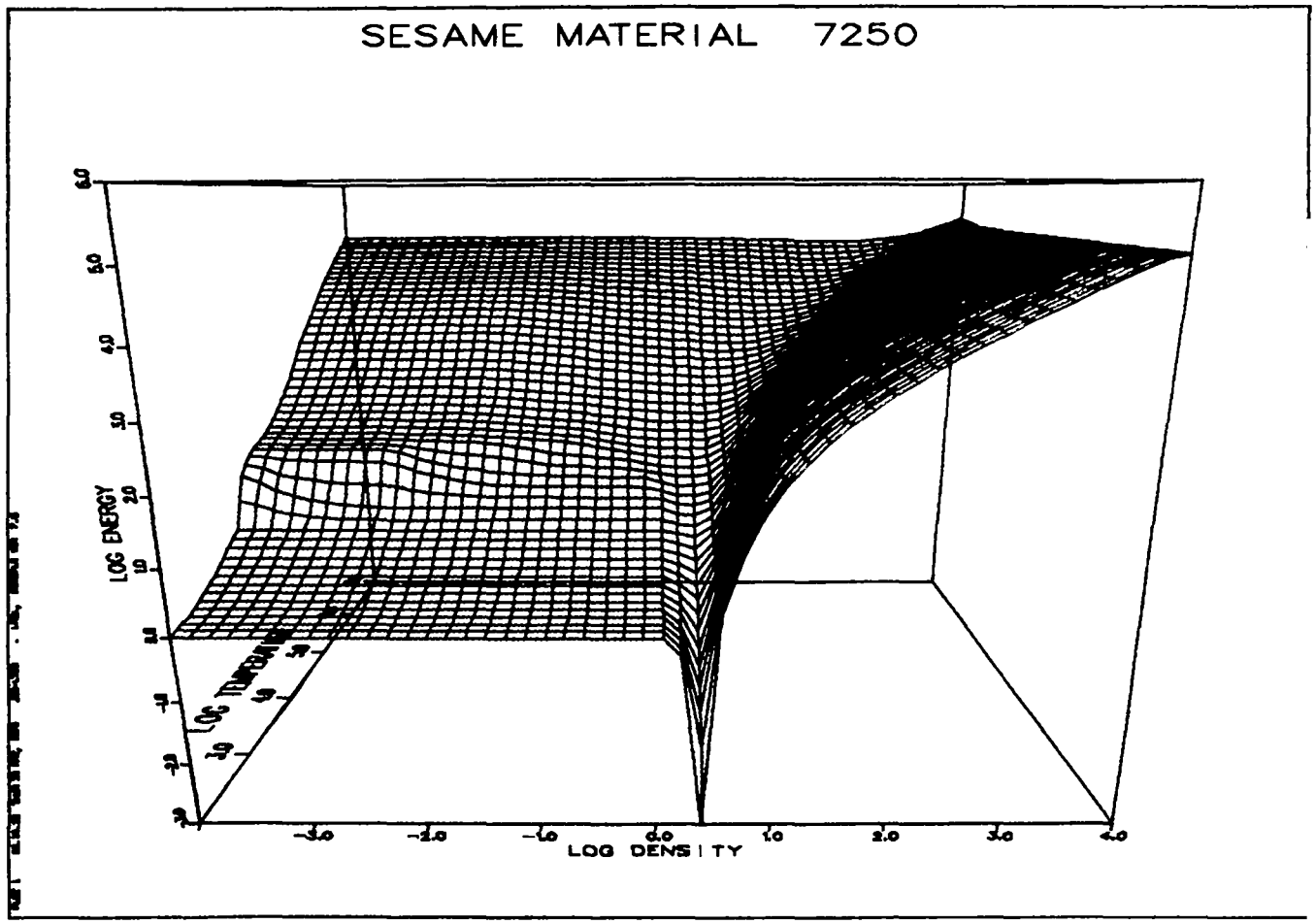


Fig. 1. EOS surface for lithia-boria glass, SESAME Material 7250, over densities 10^{-4} to 10^{4} gm/cm^3 and temperatures 10^{2}—10^{7} K.

As with the ENDF/B system when it began, the contents of the SESAME library vary in accuracy. In many cases, the tables were generated for specific applications, using the best data and theory available at the time. Of course, in their present form, they are all useful for a variety of applications; however, efforts are continuing at LASL to improve the contents as new theoretical tools and models are developed. Since the library is being developed to serve the needs of modern research for energy and defense, it is important for users to make known their experience with the library, their needs with regard to more accurate or extensive treatment of specific materials, and their requests for the addition of new materials to the library. Contributions to the data base from scientists outside LASL, in the form of new experimental data or theoretical models, are also welcome and should increase the pace of library development. It is hoped that a coordinated effort among all those involved will result in improvement of the current data base and expansion of the library to include materials of interest to nonnuclear energy sources.

Basic Features of the SESAME Library

Advantages of a Tabular Library

The choice of a tabular format for the library was made after long experience of providing EOS for a wide variety of problems at LASL.

This format allows EOS data to be represented accurately over many orders of magnitude in temperature and density. The SESAME library contains tables of pressure and internal energy as functions of temperature and density. Since all thermodynamic quantities of interest in hydrodynamic calculations can be calculated from the tabulated functions and their first derivatives, internal consistency among the various quantities computed from the tables is maintained for all points on the EOS surface. The tables, when used in conjunction with the accurate interpolation scheme developed at LASL, provide a convenient, accurate, and easy-to-use standard package for hydrodynamic and other applications of EOS data. The flexible format of the library will also allow inclusion of other thermodynamic quantities (e.g., the Helmholtz free-energy and two-temperature EOS) as well as opacities and transport properties within the existing structure for data storage, acquisition, and interpolation.[1] This expansion is contemplated.

At present, analytic formulations of the pressure as a function of density and energy are often used in certain types of hydrodynamic applications. However, analytic formulas are not essential; the SESAME tables were specifically designed for use in such calculations and, in fact, work quite well. Moreover, a single analytic expression cannot accurately represent an entire EOS surface including melting, vaporization, solid-solid phase transitions, and large amounts of electronic excitation and ionization.

For example, a typical and popular analytic form is the Tillotson equation of state. It works well for many applications but does not account for phase transitions. The plot of the iron Hugoniot for low pressures (Fig. 2) compares the results from the Tillotson analytic equation of state for iron and the SESAME EOS No. 2140 with experimental data. The data show a two-wave shock structure that is known to result from a phase transition in iron at about 130 kbar. The SESAME EOS, which explicitly accounts for the phase transition, agrees well with these data, whereas the Tillotson EOS smears out the phase transition giving a single shock wave. In general, the tabular format is superior to analytic formulations in regions where the thermodynamic functions are rapidly varying, e.g., phase transitions and regions of dissociation and ionization.

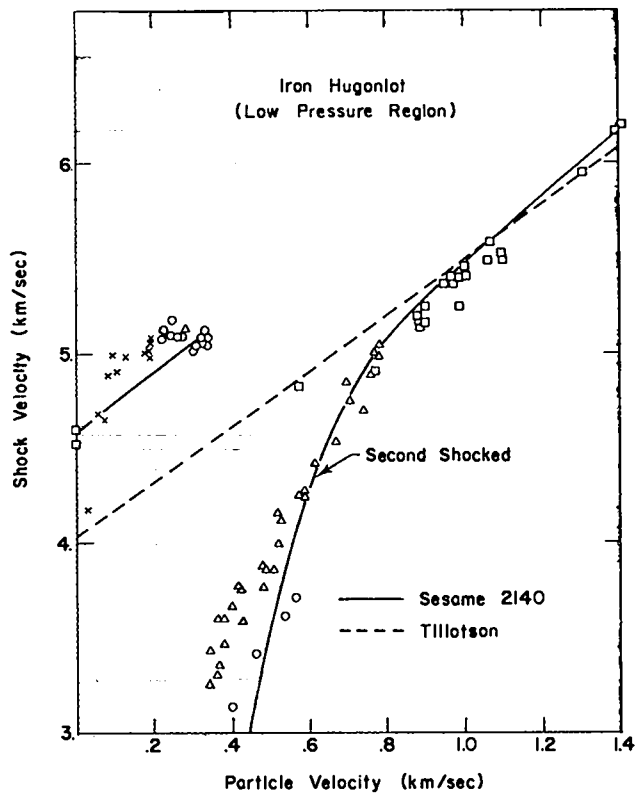


Fig. 2. Experimental data for the iron Hugoniot compared with predictions from the SESAME tables (solid line) and the Tillotson analytic EOS (dashed line).

Another advantage of tables is the relative ease with which entries can be adjusted as new experimental data become available. The adjustment in one region of thermodynamic space will not disrupt the representation of proven data in another, as often happens when analytic fits are used. For example, typical analytic fits to the experimental data for the vapor pressure of UO_2 have had the form $\ell n\ P = (A/T) + B + C\ \ell n\ T$. However, a fit of this form to the new high-temperature data for UO_2 is inaccurate when extrapolated to low temperatures. (See UO_2 vapor pressure curve on page 25.) Incorporation of the new vapor pressure data on UO_2 into the tabular format poses no such difficulties.

Finally, and most important, the developers of the SESAME library have the interest, the knowledge, and the expertise to make the necessary changes and to maintain a library that is as accurate as available knowledge allows.

Rational Function Interpolation

The feasibility of a tabular EOS library depends crucially on an accurate interpolation scheme. Since the tables cover a wide range of temperatures and densities, the mesh points are often quite coarse. Also, thermodynamic functions are not smooth in the neighborhood of phase transitions, and frequently, the user needs to determine first derivatives of these functions (sound speeds, specific heats) that are rapidly changing or discontinuous in this region. The rational function method of interpolation, developed to handle these problems, is part of the SESAME search and interpolation subroutine.[2]

For functions of one variable, the method uses a ratio of two polynomials to estimate the function and its first derivative between mesh points, plus a special prescription for computing the first derivative at the end points of the tabulated set. In Fig. 3 several standard interpolation schemes are applied to a function with a discontinuous derivative, in this case, the intersection of two straight lines tabulated at five points. This problem is a trivial one, and the rational function algorithm gives the exact answer, whereas the other methods introduce unwanted oscillations. The rational function method has been tested on many other problems as well. In general, the method is competitive with other schemes for smooth functions and is significantly better for functions that have discontinuities or rapid changes in the derivatives.

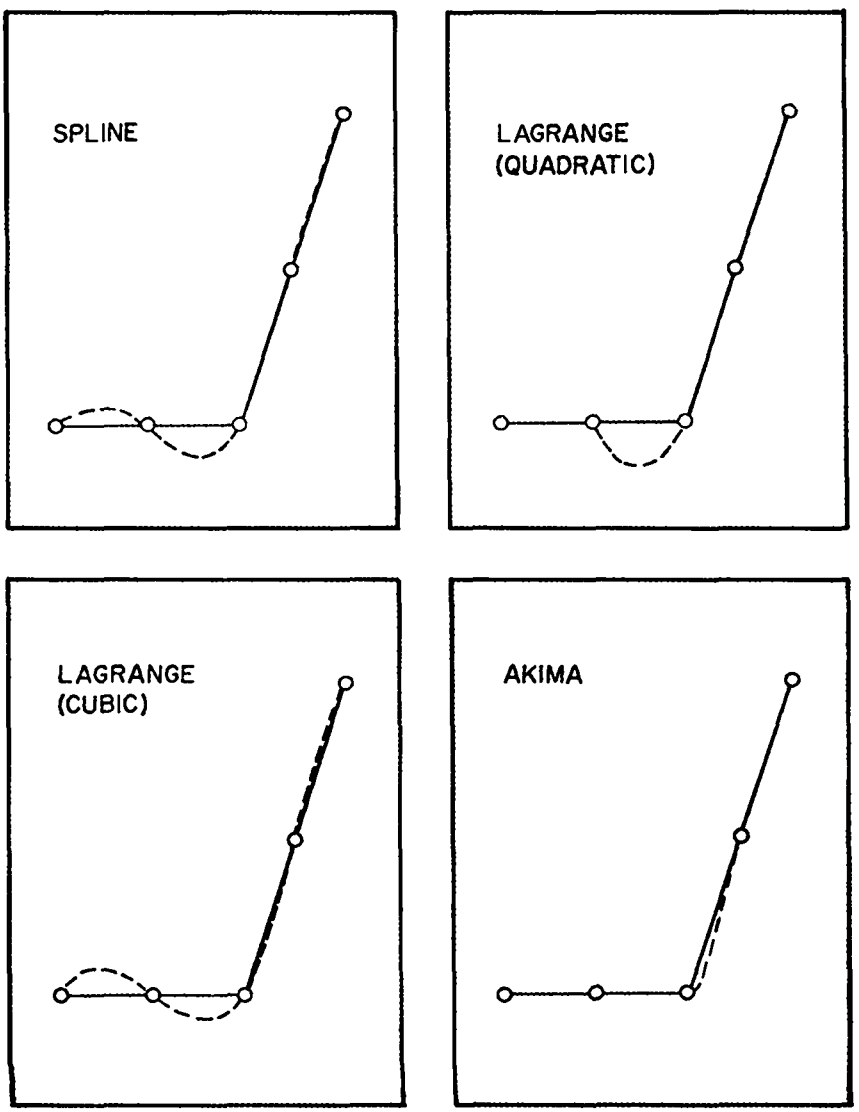


Fig. 3. Interpolation schemes applied to the intersection of two straight lines. The tabulated points are shown as circles.

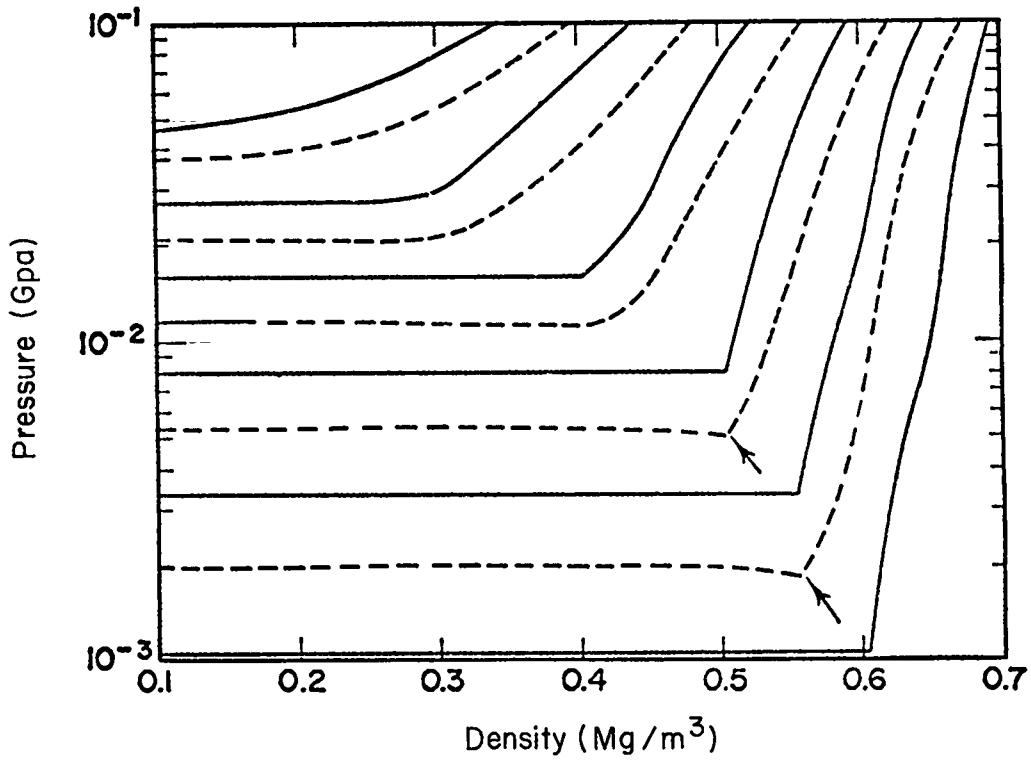


Fig. 4. Interpolated pressure-density-temperature surface.

The rational function algorithm has also been generalized to functions of two variables. This latter scheme is satisfactory for a wide range of applications. For some, however, spurious oscillations are introduced as shown in the interpolated pressure-density-temperature surface in Fig. 4. The isotherms interpolated along the tabulated points (solid lines) have the correct behavior, but the interpolated isotherms at intermediate temperatures (dashed lines) have negative slopes in a small region indicated by arrows. The pressure should be a monotonically increasing function of density to satisfy thermodynamic stability. Additional work needs to be done, but the problem can be minimized by a good choice of mesh. In general, the mesh must always be tailored to the problem.

The rational function interpolation scheme can be used with confidence for most applications. This scheme does use somewhat more computing time than some simple analytical formulations for the EOS, but as a percentage of problem running time the increase is small. Recently, modifications in the subroutines have been made that greatly increase the speed of the interpolation subroutine when applied to numerical hydrodynamic calculations. In addition, a very fast linear interpolation option is available as part of the SESAME interpolation subroutine for those problems not requiring greater accuracy.

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. For specific applications, 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. These routines provide for computations involving several SESAME tables, for the use of the tables along with other EOS options, and for the specification of the same table in more than one region. All the necessary bookkeeping is internal to the routines. SESAME tables can be used with both LaGrangian and Eulerian codes in problems that involve elastic-plastic flow, spall, foams, non-equilibrium phase transitions, and radiation flow.

A brief description of some of the subroutines in the library is given below. Details concerning their use are given in the instructions provided with the tapes and in comment cards at the beginning of each routine.

To preprocess the data tapes, a user calls a single subroutine named UPDATE. This routine will create a binary file or add new data to an old file. The user must write a simple driver program to call UPDATE and perform certain system-dependent functions such as creating and opening files. This driver can also call a routine named CKLIB, to test the binary file for internal consistency, and a routine named TPRB1, to run a test problem. Once established, the binary file should be saved on a disk file, tape, or other mass storage device where it can be used again and again.

Routines S2GET and S2EOS are used to compute pressure and internal energy as functions of density and temperature.

$$P = F_1(\rho,T), \qquad E = F_2(\rho,T) .$$

These routines require a local array for storage of the tables and a COMMON block for a directory to this array. Routine S2GET is called to load data from the binary library and set up the directory for each material specified by the user. Storage for the data can be allocated dynamically if desired. Once the data have been loaded, routine S2EOS can be called over and over to compute the EOS. This routine computes not only pressure and energy but also the density and temperature derivatives as well.

For many applications, it is desirable to compute an "inverted" EOS, in which internal energy is the independent variable.

$$P = G_1(\rho,E), \qquad T = G_2(\rho,E) .$$

These calculations are carried out using subroutines S2GETI and S2EOSI. When loading the data, routine S2GETI reformats the EOS tables into a structure that is more efficient for energy-based computation. Usage of these two routines is similar to those discussed above.

The subroutine library also contains routines for calculating Hugonlots and isentropes, vapor-liquid coexistence curves, and other speclalized functlons.

The routines described above have proven to be particularly useful for hydrodynamic code calculations. In working with local users of the SESAME tables, LASL scientists have learned several techniques for reducing storage requirements and computing time by significant amounts in hydro codes. These newest methods will be made available in packaged form and will be discussed in future reports.

Display Codes

Two codes have been written for performing certain computations and displaying data from the SESAME library. Both are interactive and contain system-dependent features. Although documentation of these programs is limited at present, they may be of interest to some users.

DSPLX is a program that computes Hugoniots, isentropes, isobars, and other information. When running this code, the user enters commands and receives output listings at a computer terminal. DSPLX is useful for examining a small region of the EOS surface, for making idealized shock wave and isentropic flow calculations, and for comparing results with experimental data. Although system-dependent, it has a modular structure and could be converted to another interactive computing system without a major effort. Output from this code is shown in Fig. 5.

SHOCK HUGONIOT FOR SESAME MATERIAL NUMBER 3710

R	P	E	T	US	UP
GM/CC	GPA	MJ/KG	KELVIN	KM/SEC	KM/SEC
2.835E+00	4.122E+00	3.635E-02	3.532E+00	5.662E+00	2.696E-01
2.977E+00	9.155E+00	1.576E-01	3.227E+01	6.039E+00	5.615E-01
3.126E+00	1.529E+01	3.855E-01	1.192E+02	6.449E+00	8.781E-01
3.282E+00	2.276E+01	7.473E-01	2.927E+02	6.895E+00	1.223E+00
3.446E+00	3.186E+01	1.277E+00	4.915E+02	7.383E+00	1.598E+00
3.618E+00	4.294E+01	2.018E+00	7.881E+02	7.916E+00	2.009E+00
3.799E+00	5.645E+01	3.025E+00	1.237E+03	8.501E+00	2.460E+00
3.989E+00	7.298E+01	4.367E+00	1.902E+03	9.145E+00	2.955E+00
4.189E+00	9.342E+01	6.148E+00	2.871E+03	9.867E+00	3.507E+00
4.398E+00	1.187E+02	8.490E+00	4.240E+03	1.067E+01	4.121E+00

ISENTROPE FOR SESAME MATERIAL NUMBER 3710

R	P	E	T	C	UP
GM/CC	GPA	MJ/KG	KELVIN	KM/SEC	KM/SEC
3.500E+00	3.516E+01	1.488E+00	5.719E+02	7.550E+00	1.725E+00
3.413E+00	3.031E+01	1.249E+00	5.533E+02	7.333E+00	1.914E+00
3.327E+00	2.585E+01	1.038E+00	5.349E+02	7.118E+00	2.096E+00
3.244E+00	2.176E+01	8.547E-01	5.169E+02	6.906E+00	2.274E+00
3.163E+00	1.802E+01	6.978E-01	4.993E+02	6.691E+00	2.446E+00
3.084E+00	1.459E+01	5.659E-01	4.821E+02	6.480E+00	2.613E+00
3.007E+00	1.145E+01	4.579E-01	4.652E+02	6.268E+00	2.774E+00
2.932E+00	8.597E+00	3.726E-01	4.485E+02	6.057E+00	2.930E+00
2.858E+00	5.999E+00	3.090E-01	4.321E+02	5.848E+00	3.081E+00
2.787E+00	3.643E+00	2.660E-01	4.160E+02	5.637E+00	3.226E+00
2.717E+00	1.510E+00	2.425E-01	3.999E+02	5.425E+00	3.366E+00
2.649E+00	-4.290E-01	2.376E-01	3.826E+02	5.251E+00	3.502E+00

Fig. 5. DSPLX output for aluminum shock Hugoniot and isentrope.

SES2D is a sophisticated graphics code that produces plots of EOS data on a variety of output devices. The heart of this code is a plotting module that can produce graphs using three different methods 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 SES2D are generated by another module that uses the same interpolation routines as those in the subroutine library. 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 with each curve labeled for identification.

Figure 6 is an example of a graph produced by the code SES2D.

The three-dimensional plots of EOS surfaces on the cover and in Fig. 1 were generated from the SESAME Library with a third code, called SES3D. This code is still under development.

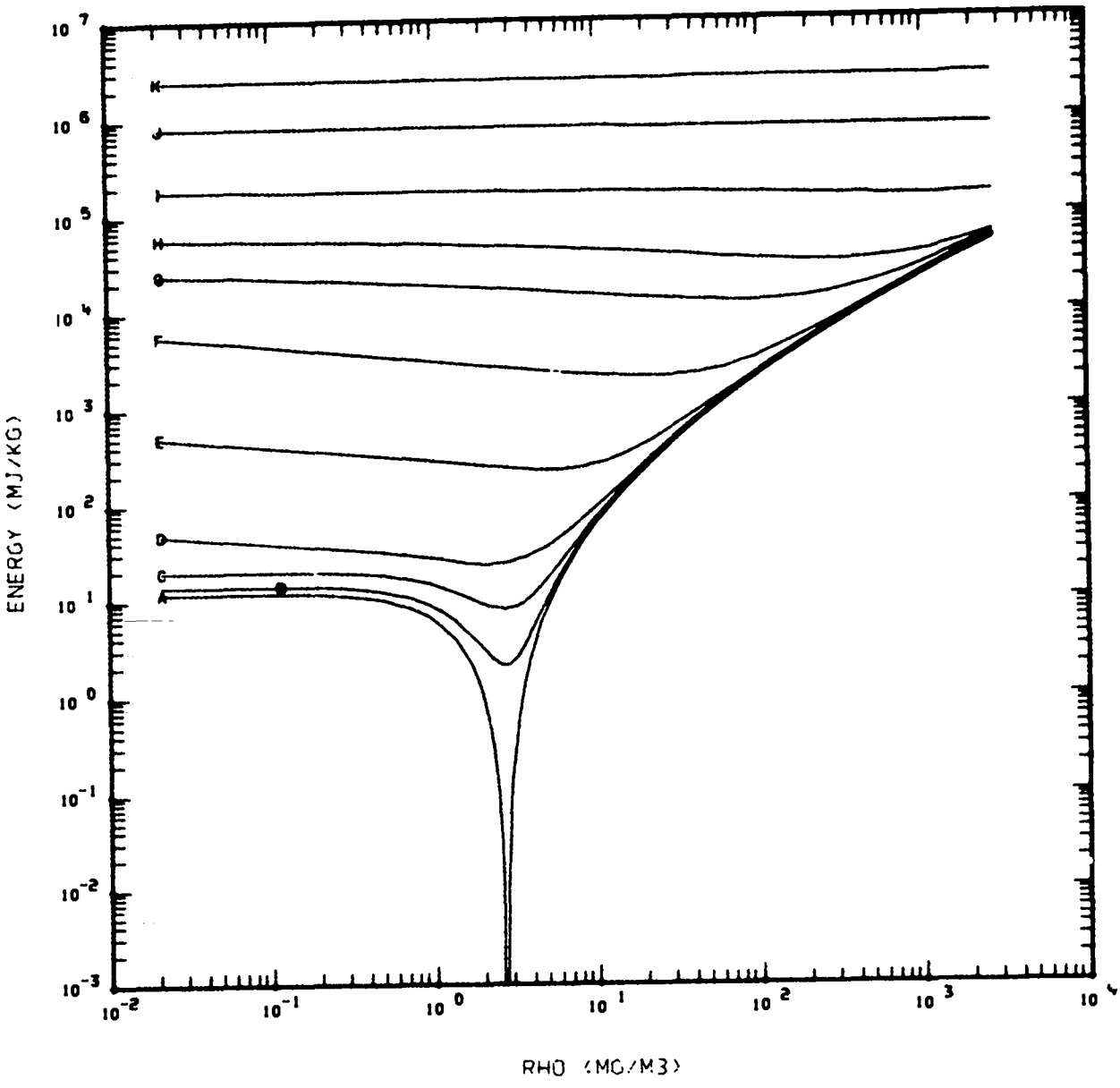


Fig. 6. Graph of aluminum energy-density-isotherms produced by the SES2D code.

Contents of the SESAME Library

The SESAME library contains unclassified EOS for about 30 materials. In the table following, these materials are listed along with comments on the range of applicability. There is no universal method for calculating EOS that is valid for all temperatures, pressures, and chemical compositions. The EOS in the library at present were generated in response to user requests and are based on models and experimental data available at the time of request. All tables have been used in specific applications and have been found satisfactory for those situations. Improvements are possible in many, and are being made as the need arises.

Number	Name	ρ_0(gm/cc)	Density Range	Temperature Range	Comments
1540	Uranium	18.983	$.15 \le \rho \le 4\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
2020	Beryllium	1.845	$1.4\times10^{-2} \le \rho \le 4\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
2140	Iron	7.85	$6.1\times10^{-2} \le \rho \le 1.6\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
2145	Iron	7.91	$0 \le \rho \le 12.5$	$0 \le T \le 1.2\times10^{4}$K	Reactor Safety (Temporary)
2448	Sodium	1.011	$0 \le \rho \le 1.3$	$0 \le T \le 10^{4}$K	Reactor Safety (Temporary)
2700	Gold	19.3	$.15 \le \rho \le 3.9\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
2980	Molybdenum	10.2	$8\times10^{-2} \le \rho \le 2\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
3100	Nickel	8.882	$6.9\times10^{-2} \le \rho \le 1.8\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
3200	Lead	11.34	$8.8\times10^{-2} \le \rho \le 2.3\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
3330	Copper	8.93	$7\times10^{-2} \le \rho \le 1.8\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
3710	Aluminum	2.7	$2.1\times10^{-2} \le \rho \le 2.7\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
3730	Platinum	21.419	$.17 \le \rho \le 2.1\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
4100	Brass	8.45	$6.6\times10^{-2} \le \rho \le 1.7\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
4270	Stainless Steel	7.896	$6.2\times10^{-2} \le \rho \le 1.6\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
5268	Deuterium	1.766	$0 \le \rho \le 3.5\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
5410	Neon	1.44	$1.1\times10^{-2} \le \rho \le 2.9\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
5760	Helium	.23372	$1.8\times10^{-6} \le \rho \le 4.7\times10^{5}$	$0 \le T \le 1\times10^{8}$K	General Purpose
7081	Boron Carbide	2.45	$2\times10^{-4} \rho 3.2$	$0 \le T \le 6\times10^{4}$K	Reactor Safety
7111	Nev. Alluvium	2.35	$1.8\times10^{-2} \le \rho \le 4.7\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7150	Water	.9982	$2\times10^{-6} \le \rho \le 4\times10^{2}$	$290. \le T \le 1.8\times10^{8}$K	General Purpose
7151	Steam	.9982	$0 \le \rho \le .9$	$290. \le T \le 1300$K	Steam Tables—Limited ρ,T Range
7170	Polyethylene	.917	$7.2\times10^{-6} \le \rho \le 1.8\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7240	^{6}LiD	.8	$6.2\times10^{-6} \le \rho \le 1.6\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7250	Li/B Glass	2.215	$10^{-10} \le \rho \le 4\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7370	^{6}LiH	.684	$5.3\times10^{-6} \le \rho \le 1.4\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7380	SiO_2	2.204	$1.7\times10^{-2} \le \rho \le 4.4\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7390	Granite	2.627	$2.1\times10^{-2} \le \rho \le 5.3\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7410	Al_2O_3	3.97	$3.1\times10^{-2} \le \rho \le 4\times10^{5}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7432	UO_2	11.00	$0 \le \rho \le 14.3$	$0 \le T \le 3\times10^{4}$K	Reactor Safety (Temporary)
7520	Vermiculite	2.7	$2.1\times10^{-2} \le \rho \le 5.4\times10^{+4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7560	Urethane	1.265	$9.9\times10^{-6} \le \rho \le 2.5\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
7590	Polystyrene	1.044	$8.2\times10^{-3} \le \rho \le 2.1\times10^{4}$	$0 \le T \le 4\times10^{8}$K	General Purpose
8180	High Explosive	1.84	$1.4\times10^{-2} \le \rho \le 3.7\times10^{4}$	$0 \le T \le 4\times10^{8}$K	EOS for Detonation Products

General remarks

- In all cases, the temperature grid is too coarse to reproduce detailed structure below room temperature. Not intended for cryogenic studies.
- In many cases, the lower limit on ρ needs to be extended. Improved grids for going to very low densities have been constructed for materials 2145, 2448, 5263, 7150, 7151, 7432.
- Tables marked "Reactor Safety" cover the region below normal density. They are intended for problems in which only slight compressions occur.
- Tables marked "Temporary" are of very preliminary nature and will be replaced in the near future.
- Tables marked "General Purpose" are suitable for shock wave calculations, high temperature and high density applications as in laser fusion, and problems in which expansions are encountered, at either high or low temperature. However, see the above comment on the low density limit.

User Experience

The library has been in use for several years at LASL and more recently has been exported to users at outside institutions with considerable success. According to outside users, the incorporation of SESAME data into hydrodynamics codes has been a relatively easy and painless task. The convenience is multiplied many times for cases in which many materials (sometimes as many as 10) are involved in a given problem. Applications of the SESAME library have included defense problems, reactor safety analysis, and inertial confinement fusion studies at LASL and elsewhere. In some instances, special packages were developed to meet individual user requests. In all cases, users are encouraged to consult with LASL developers of the SESAME library. Jerry Kerley, coordinator of the library development, is shown offering suggestions to Charles Cranfill, a member of LASL's laser fusion research effort (Fig. 7).

For defense applications, users include scientists at the Air Force Weapons Laboratory, Physics International, England's Atomic Weapons Research Establishment (AWRE), Lockheed Missiles and Space, and the University of Rochester, as well as Staff Members at LASL involved in weapons effects, new measurements of EOS, and experimental shock wave studies of material behavior.

SESAME tables are also useful for analysis of hypothetical accident sequences in fast breeder reactors in which the behavior of UO_2, Na, and steel over wide ranges of temperature and density must be considered. Temporary EOS data for these materials have been developed and incorporated into the SESAME library for use in the SIMMER code, a fast-reactor accident analysis code under development at LASL. (Development of more accurate EOS for these materials is progressing rapidly as discussed below.) The SIMMER code solves coupled sets of hydrodynamic equations for the solid, liquid, and a vapor mixture of varying chemical composition. A special SESAME EOS package written for this problem includes an algorithm 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 included in the SESAME subroutine library, but they can be made available to interested users.

SESAME EOS tables have also been requested by the European reactor safety effort at AWRE and by scientists at Sandia Laboratories performing EOS experiments for reactor safety applications. Scientists at LASL are also in contact with the effort at Oak Ridge National Laboratory to develop the SACRD Data Base for reactor safety analysis. Recent work at LASL on the UO_2 EOS (described below) should be of considerable interest to those involved in development of SACRD.

Applications of the SESAME Library in inertial confinement fusion studies are many and include studies recently reported in Physical Review Letters[3] and Nuclear Fusion.[4]

Fig. 7. Chuck Cranfill (left), a member of LASL's laser fusion effort, and Jerry Kerley (right), project leader of the SESAME library confer on the two-temperature EOS that was designed for studying laser-pellet implosions.

Physical Review Letters reported observation of a group of energetic ions produced as long laser pulses ablate the surface of planar targets. This ablation structure was observed for targets ranging from aluminum to uranium. The SESAME EOS tables for the target materials were used in two-temperature numerical simulations of the ablation process. These calculations reproduced the formation and the velocity structure measured for the fast-ion group. Models were also developed to estimate from the SESAME tables the average ionization stage for a given velocity; calculated results were in good qualitative agreement with measured values.

In Nuclear Fusion, LASL scientists reported use of the SESAME tables to compute the rapid implosion of compressible metal liners for plasma heating and fusion-energy production. Copper, nickel, and gold liners were investigated. The interactive effects of liner compressibility and cylindrical convergence were emphasized in the analysis. Realistic EOS were needed to model the increase in sound speed with increasing pressure. In the several-megabar range of interest, the "cold pressure" due to repulsive forces between atoms dominates by far the thermal (lattice vibrational pressure) and electronic thermal pressure, and is primarily responsible for the increase in isentropic bulk modulus with pressure for a number of metals. The compressibility behavior was calculated from the SESAME tables and the tables were accessed by the numerical hydrodynamic code to calculate the instantaneous compression profile of the liner.

Other users of SESAME tables for laser fusion studies include Sandia Laboratories, University of Rochester, Brookhaven National Laboratories, University of Wisconsin, Physics International, and University of Arizona, as well as members of the appropriate Divisions at LASL. Researchers at Rochester, representing one of the Nation's largest efforts in laser fusion, are not only using the SESAME library to model laser-target interactions, but their experiments using lasers to measure EOS will have an impact on the further development of the SESAME library for laser and other applications.

Materials, Methods, and Applications

In order to convey some understanding of the theoretical work that goes into constructing the SESAME tables, a number of materials being studied are discussed below. These materials are grouped according to the type of application for which they are being developed—namely, shock wave studies, laser fusion, and reactor safety. The need for more accurate EOS in these areas has led to new developments in the theory of liquids, the phenomenological treatment of phase transitions, the construction of two-temperature EOS, and more refined treatments of thermal electronic excitations. These theoretical developments are discussed in the context of specific materials.

EOS for Shock Wave Studies

Shock wave studies at LASL are the experimental basis for generating many of the SESAME EOS. These EOS, in turn, can be applied to the prediction of new shock wave experiments. Densities from solid density at room temperature to 10 times solid density, and temperatures from 10^2 - 10^5 K are relevant to these experiments.

The data from shock wave measurements yield the locus of states that can be reached in a single shock process from a given initial state. This locus is called the Hugoniot and is frequently plotted in terms of shock velocity (u_s) vs particle velocity (u_p). These data are combined with thermodynamic relationships and empirical models to generate the EOS.

Lithia-Boria Glass

A new SESAME table for lithia-boria glass has been developed recently based on shock data obtained by the Dynamic Testing Group at LASL. The construction of the EOS for this material illustrates some of the techniques employed for many materials in the regions of temperature and density achieved in shock wave work.

The experimental Hugoniot data for lithia-boria glass are plotted in Fig. 8. The data have a region of roughly constant shock velocity ($u_s \sim 6.0$ km/s) over a pressure range from ~90-260 kbar. The data indicate that the glass undergoes a phase transition at ~90 kbar. The region of constant shock velocity corresponds to the arrival of the first of two shock waves present in the 90- to 260-kbar range. Above 260 kbar, a single shock is stable and corresponds to the high-density phase of lithia-boria glass.

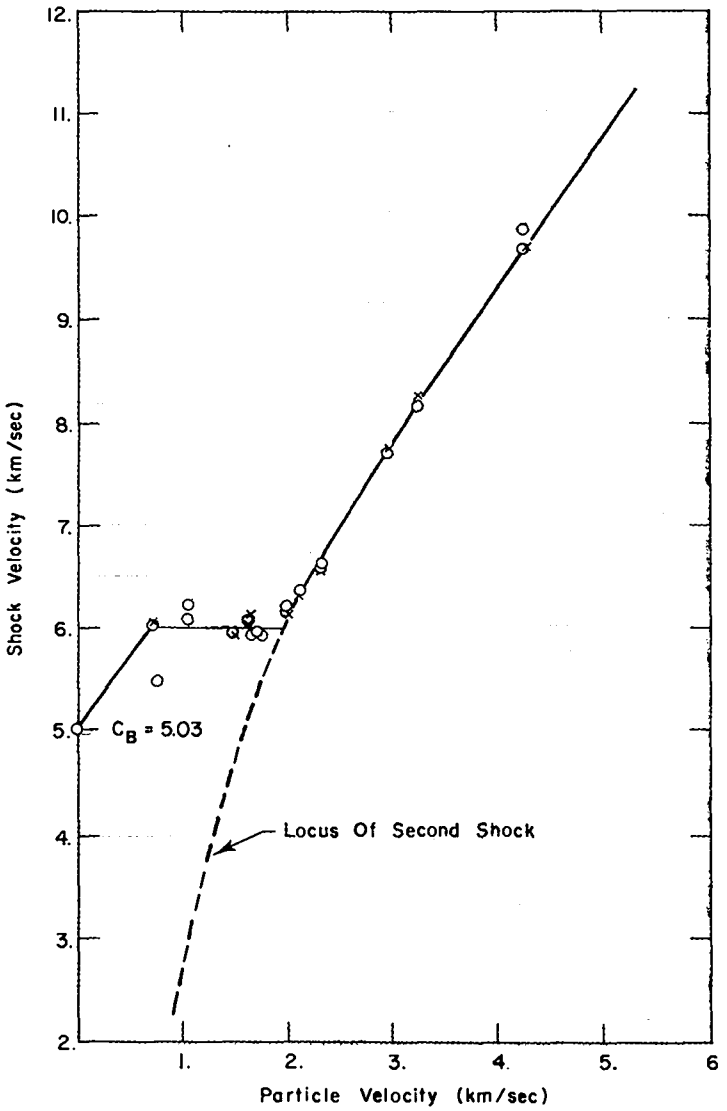


Fig. 8. Experimental Hugoniot data for lithia-boria glass compared with predictions of the SESAME EOS (solid and dashed curves). For particle velocities below .8 km/sec there is no phase transition and a single shock wave is stable. For particle velocities greater than 2 km/sec, the substance transforms to the high density phase and a single shock wave is stable. For intermediate velocities, calculations predict two shock waves. The leading wave corresponds to the low density phase and has U_p = .8 km/sec, U_s = 6 km/sec. The calculated locus of the second shock is shown by a dashed line; this wave has not been studied experimentally.

A new technique based upon the free energy was used to take the phase transition into account. To model the EOS including the Helmholtz free energy for each phase, a form for the Grüneisen parameter was assumed, and the cold curve was computed from the shock data using the Mie-Grüneisen EOS. For the contribution from nuclear vibrations, the Debye model was used, but modified to go to an ideal gas at high temperatures and low densities. The Thomas-Fermi-Dirac (TFD) statistical model of the atom was used for electronic excitations.

The separate EOS tables for each phase were input to a code that computes the phase boundaries and constructs a multiphase EOS table by minimizing the Gibbs free energy at constant pressure. This method ensures thermodynamic consistency.

The shock Hugoniot calculated from the multiphase tables is compared with experimental data in the figure and agreement is good, showing that the analysis is internally consistent. The multiphase EOS table gives a realistic

description of the shock behavior in the region where two distinct shocks are generated. The locus of the second shock calculated with the DSPLX code (described under "Display Codes") is shown in Fig. 8. This prediction must be checked by new experiments.

The details of the lithia-boria glass EOS in the region of phase transition are shown in Fig. 9.

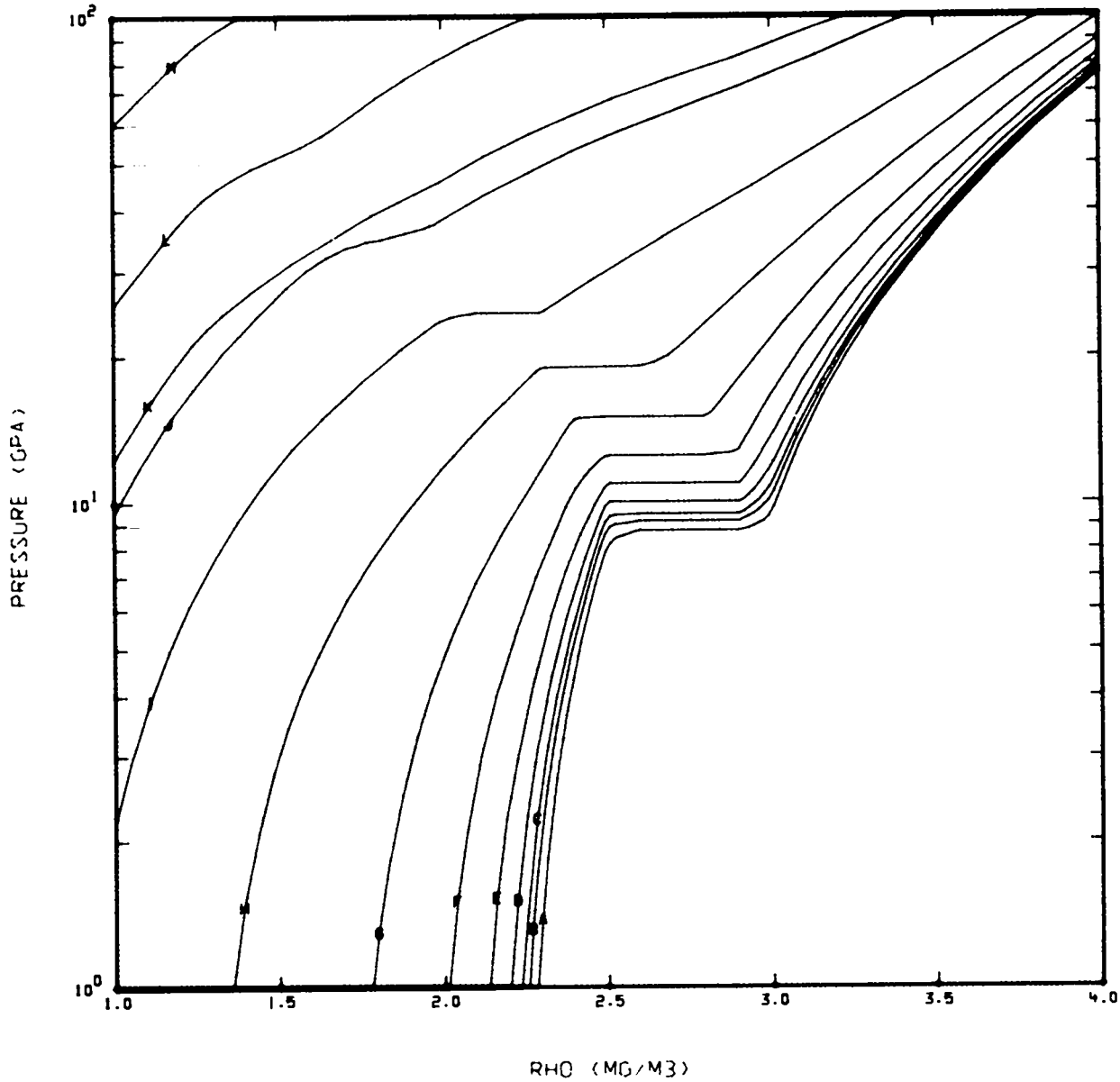


Fig. 9. Pressure-density isotherms for LiB glass in the region of phase transition.

EOS for Laser Fusion

EOS for laser fusion and other applications in which materials are subjected to radiation-induced shock waves must cover density ranges from 0.5 times normal density to 10 or 100 times normal density and temperatures up to 10^4-10^7 K. At these high temperatures, the materials are partially ionized. The problem is complicated by the fact that equilibrium between the electrons and the ions cannot be assumed in some cases.

The deuterium EOS and the two-temperature EOS for SiO_2 described below are of particular interest to laser fusion studies and illustrate some of the complex physical phenomena that are being tackled theoretically in modern EOS research.

Deuterium

The thermodynamic properties of deuterium[5] have been calculated for densities ranging from 10^{-3} to 10^3 g/cm^3 and for temperatures from 2×10^2 to 10^6 K. This information is needed for the design and analysis of thermonuclear energy applications. The theory developed is also applicable to tritium and hydrogen and therefore useful in studying the planets Jupiter and Saturn, which contain large concentrations of dense hydrogen.

Although it might seem to be a simple substance, deuterium poses nearly all the difficulties that arise in EOS theory including fluid and solid theory, molecular and metallic binding, phase transitions, molecular vibration and rotation, and chemical reactions (dissociation and ionization). The EOS calculated for deuterium includes two solid phases—a molecular solid calculated to be stable at pressures below 2 Mbar and a metallic solid stable at high pressures—as well as a liquid phase (see phase diagrams in Fig. 10).

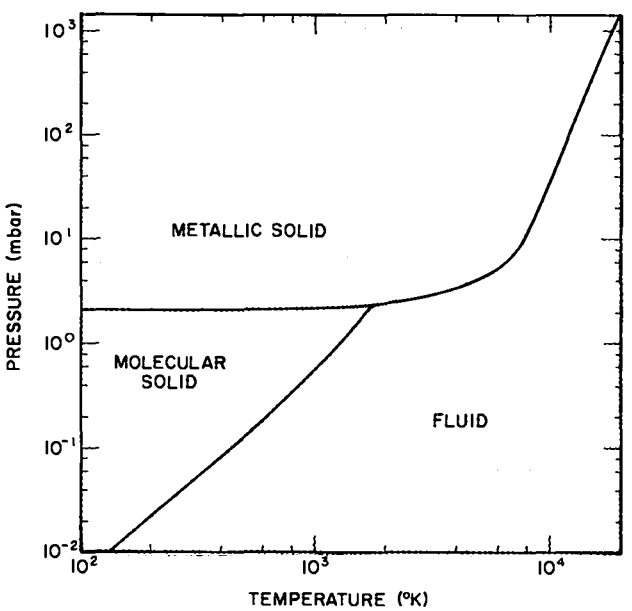


Fig. 10a. Phase diagram for deuterium (from Ref. 5).

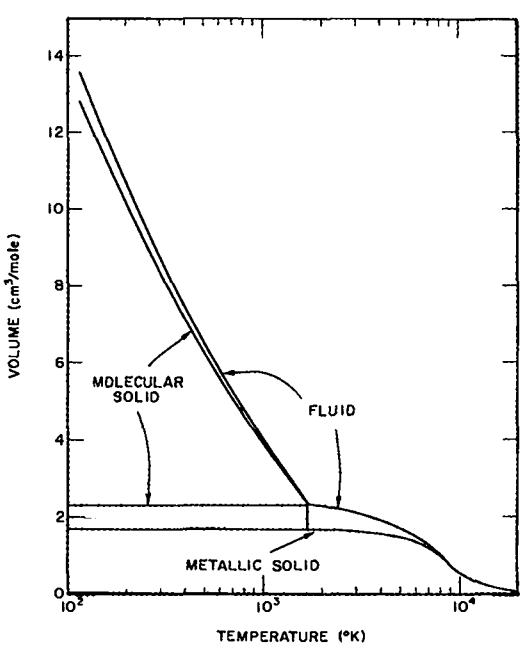


Fig. 10b. Specific volumes on the phase lines of deuterium (from Ref. 5).

In the October 1978 Issue of Physical Review Letters,[6] a group at Lawrence Livermore Laboratory claims to have seen the transition to a metallic solid in hydrogen at 2 ± 1 Mbar and a density of 1.06 ± 0.18 g/cm³ for the metallic phase. This transition for H_2 may be calculated from the SESAME deuterium EOS and is found to be at P = 2.8 Mbar and ρ = 1.26 g/cm³, satisfactory agreement with the Livermore results.

The treatment of the liquid phase of deuterium has received special attention. The CRIS model developed at LASL was the basis for calculating the thermodynamic properties of the atomic and the molecular fluids for deuterium. This model is a thermodynamic perturbation expansion about a hard sphere fluid in which the energy of a fluid molecule is determined from the zero-temperature isotherm of the solid. (This new model for fluids is described in more detail in the section on liquid sodium.) The effects of molecular dissociation, vibration-rotation and thermal electronic excitations, and the transition to the metallic state were also included in the EOS for the liquid phase of deuterium. Recent measurements by Mills et al.[7] of pressures and sound speeds in liquid H_2 and D_2 up to 20 kbar agree very well with the SESAME EOS for the liquid phase (see Figs. 11 and 12).

A detailed presentation of the theoretical methods used to construct the EOS for deuterium can be found in Ref. 5.

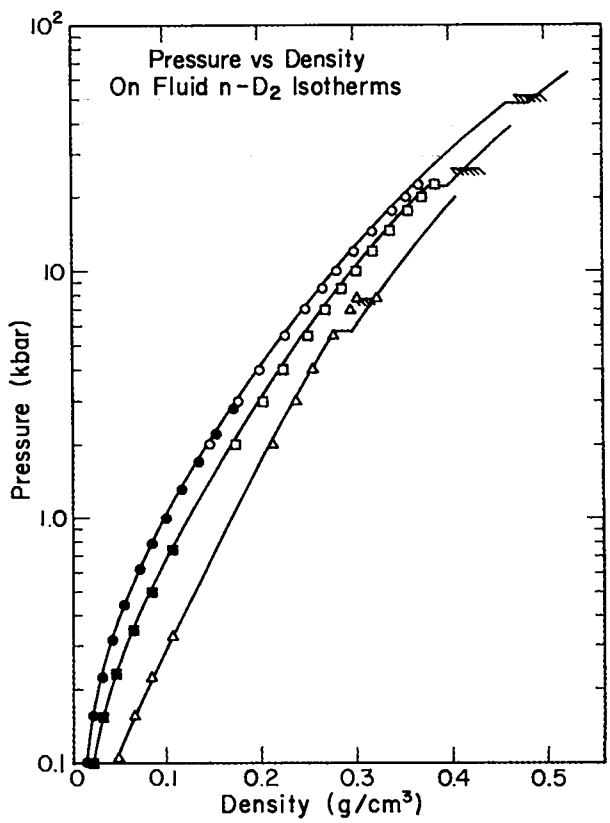


Fig. 11. Deuterium fluid isotherms. Experimental data[7] are compared with theoretical prediction (solid curves) for pressure vs. density.

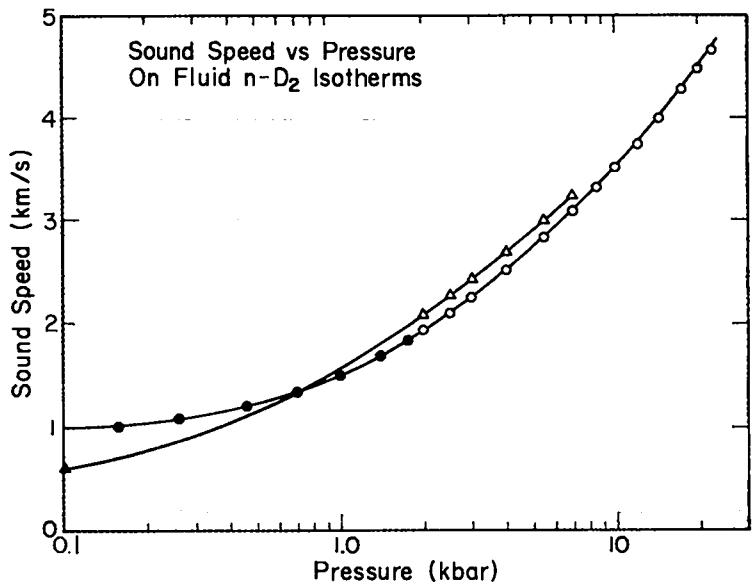


Fig. 12. Deuterium sound speed vs. pressure. Experimental data[7] are compared with theoretical prediction (solid curves).

Silicon Dioxide and the Two-Temperature EOS

Glass microspheres filled with deuterium and tritium gas are the typical targets used in laser fusion studies. The lasers deposit their energy preferentially in electronic excitations. Since the time scales for implosion of the microsphere are too fast to achieve local thermodynamic equilibrium between the electrons and ions, the system is usually modeled as a quasi-independent system of electrons at some temperature T_e and a second quasi-independent system of ions at some lower temperature T_i. This concept is called the two-temperature approximation. EOS suitable for use in two-temperature hydrodynamic calculations consequently require separate EOS for the ions and the electrons. A new EOS for SiO_2 was generated in order to allow a consistent separation into electronic and nuclear (ionic) parts.

As with many EOS, the SiO_2 EOS was constructed from three distinct contributions, (1) a cold curve due to electronic forces at T = 0 K, (2) thermal electronic excitations, and (3) thermal nuclear excitations. A TFD model was used to generate the thermal electronic part, and an analytic model of R. D. Cowan, which interpolates between an ideal gas at low densities and a Debye model at high densities, was used for the nuclear or ion part. The total pressure, for example, can then be written as:

$$P(\rho,T) = P_{cold}(\rho) + P_e^{THERMAL}(\rho,T) + P_i^{THERMAL}(\rho,T)$$

$$= P_{cold}(\rho) + P_e^{TFD}(\rho,T) + P_i^{COWAN}(\rho,T) .$$

This EOS for SiO_2 was fitted as accurately as possible to all available experimental data and includes some phase transitions.

The pressure in the simplest two-temperature approximation for the EOS is then defined to be

$$P_e(\rho,T_e) = P_{cold}(\rho) + P_e^{TH}(\rho,T_e)$$

$$= P^{TOTAL}(\rho,T_e) - P_i^{COWAN}(\rho,T_e)$$

$$P_i(\rho,T_i) = P_i^{COWAN}(\rho,T_i) ,$$

where T_i and T_e are not necessarily equal and the ion contribution is independent of electron temperature and vice versa. Isotherms for separate electronic and ionic contributions to the SiO_2 EOS are shown in Figs. 13a and 13b.

Two-temperature EOS for other elements may be generated from the SESAME library in a similar manner. However, since most SESAME tables were constructed before interest in two-temperature EOS and did not use the Cowan model, separate ion contributions to the tables are not readily available. Consequently, the use of the Cowan model to separate the electronic and ionic parts may not be consistent, although it may be good enough for some studies. In the future, when new tables are constructed or old tables redone, separate nuclear tables will be stored along with the usual EOS tabulation. In many cases tables are needed rather than the analytic Cowan model to represent accurately the nuclear contribution to the EOS.

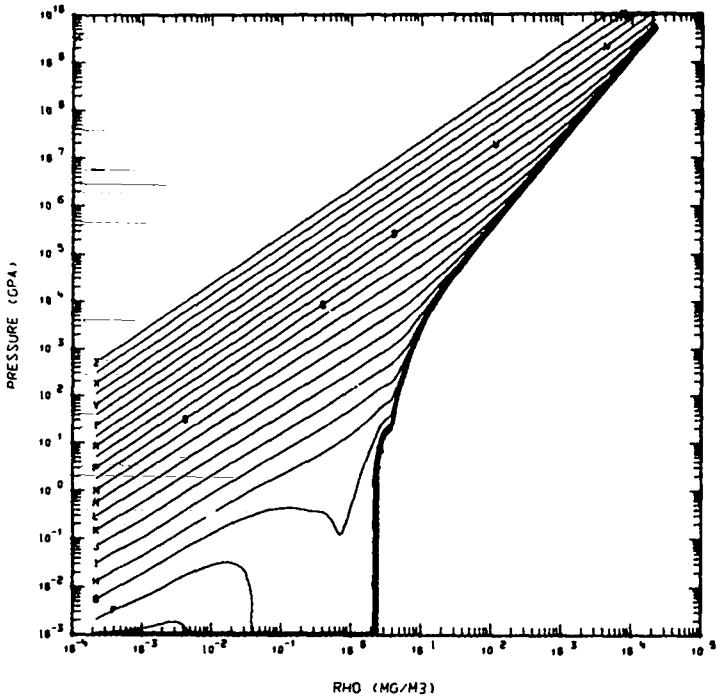


Fig. 13a. Ionic contribution to pressure-density isotherms of silicon dioxide over the temperature range 0.0-5.4 × 10^6 K.

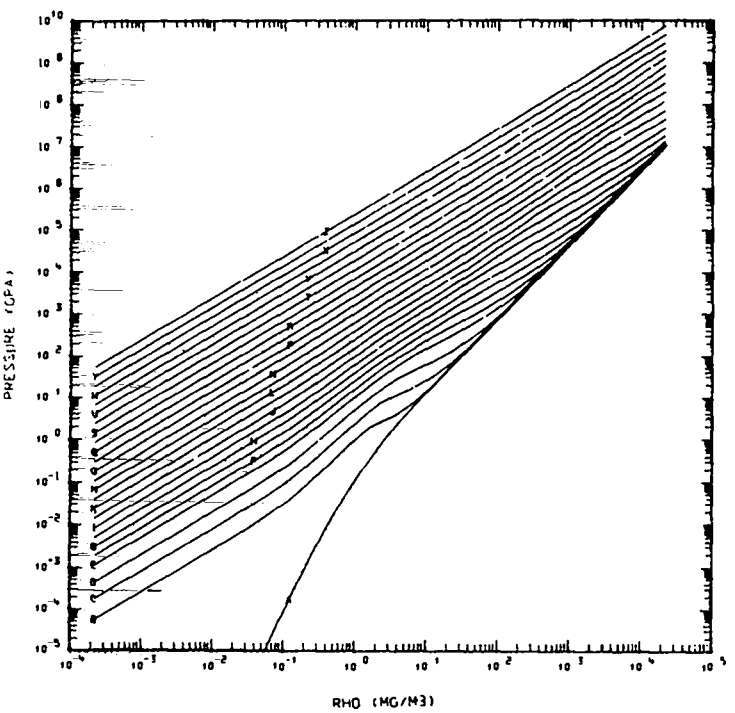


Fig. 13b. Ionic contribution to pressure-density isotherms of silicon dioxide over the temperature range 0.0-5.4 × 10^6 K.

The TFD model for thermal electronic excitations used in the SiO_2 EOS, and other EOS as well, neglects the effects of discrete electronic energy levels. However, these effects may be important at low densities in laser fusion studies. In recent work, an ionization equilibrium (Saha-type) model which takes into account the level structure has been used to construct the electronic EOS for SiO_2 at low densities and results are being compared to the TFD model. Eventually, we hope to merge the Saha-type model at low densities with the TFD model at high densities in a thermodynamically consistent fashion. Electronic models that agree well with Saha-type theories will then be consistent with the opacity tables that are generated by LASL's Equation of State and Opacity Group and used in laser fusion and other applications in conjunction with EOS data.

EOS for Reactor Safety

The "temporary" SESAME EOS tables for UO_2, Na, and iron are available for reactor safety research, but will soon be replaced by more accurate treatments. Recent progress on the UO_2 and Na EOS is described below.

Uranium Dioxide and Electronic Contributions to the Gas EOS

A variety of methods, with varying degrees of phenomenology, are being used to create the EOS for UO_2. For the condensed matter region (densities greater than the critical density), the known data and reasonable extrapolations of the known data are being fit with the analytic form of the corresponding states theory as formulated by Hirschfelder et al.[8] This procedure will yield (1) exact fits, as functions of temperature, of the experimental enthalpy and density on the coexistence curve both in the liquid and solid, and (2) very reasonable extrapolations off the coexistence curve including the region of melting.

In the gas region, the EOS is constructed from theoretical models with a few phenomenological parameters. The models are the van der Waals model for the translational degrees of freedom, and simple rotational and vibrational models.

The most important new physics is a new model for electronic excitations in the gas. Analysis of the experimental vapor pressures and condensed enthalpies suggests that electronic excitations make a significant contribution to the gas EOS, in particular, to the internal energy and specific heat. For example, the specific heat, C_p, of liquid UO_2 at ~3200 K is approximately 134 J/mol·K.[9]. At best, 75 J/mol·K can be explained by the translational, vibrational, and rotational modes of the molecule. The remaining 59 J/mol·K must come from electronic contributions.

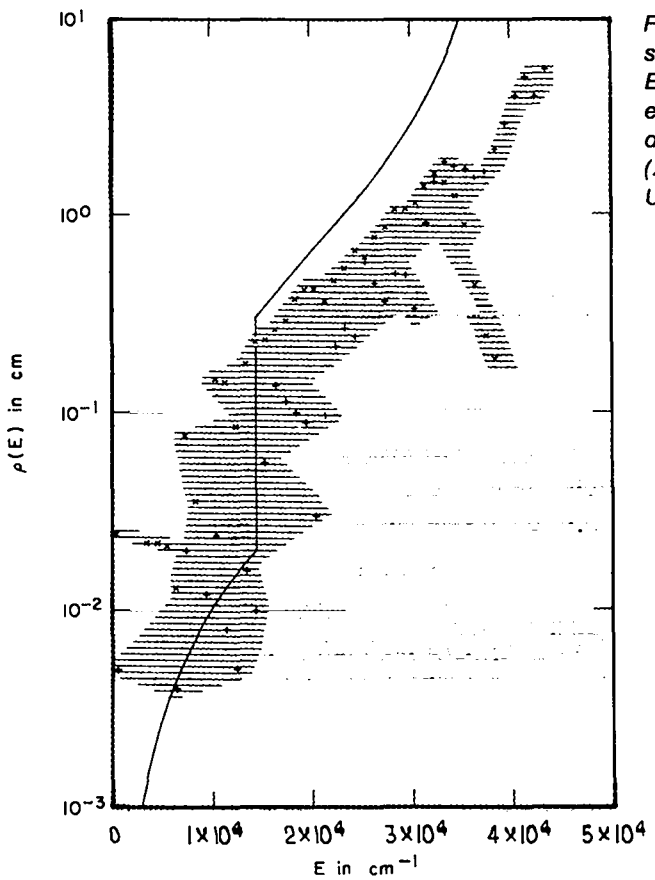


Fig. 14. UO_2 electronic density of states used in LASL EOS studies (solid curve), experimentally determined density of states for uranium (X), and RSCF calculation for UO_2 (+).

The new electronic model is essentially a Saha (ionization equilibrium) model. Along the coexistence curve for $T \leq 5000$ K, where ionization can be neglected, the electronic partition function is a product of single neutral molecule partition functions Q. Since the levels in UO_2 are very dense, the sum over electronic states can be replaced by an integral to obtain

$$Q = \int_0^{E_c} \rho(E) e^{-\beta E} dE ,$$

where $\rho(E)$ is the density of electronic states for the molecule and E_c is a cutoff.

The density of states that we use is shown by the solid curve in Fig. 14. Plotted on the same graph are the experimentally determined density of states for uranium[10] and a theoretical density of states for UO_2 obtained from a relativistic self-consistent field (RSCF) calculation at LASL. We expect the solid curve to be a more accurate representation of $\rho(E)$ than the RSCF calculations for energies above 15 000 cm^{-1} since the RSCF results neglect some levels and use the ground-state potential for all energy levels. Below 15 000 cm^{-1}, the area under our curve approximately equals the number of states found by the RSCF calculation.

The gaseous model of UO_2 for $T \leq 5000$ K is completed by adding in the other degrees of freedom, translational, vibrational, and rotational modes of the molecule. Using the ideal gas approximation, the enthalpy is

$$H = (7/2)\, NkT + H_e + H_{vib} ,$$

where $H_e = (-kT^2)\, (\partial \ell nQ/\partial T)$. H_e is the electronic enthalpy and H_{vib} is the enthalpy of the vibrational modes. The resulting enthalpy for gaseous UO_2 calculated along the coexistence curve is shown by the solid curve in Fig. 15. The result for no electronic excitations (dashed line) is significantly lower.

This increase in enthalpy due to electronic excitations tends to raise the high temperature P_v, thus producing better agreement with the data than has been obtained in the past.[11] The vapor pressure was obtained by integrating an approximate form of the Clausius-Clapeyron equation that neglects the condensed phase volume relative to the volume of the gas and uses the ideal gas approximation.

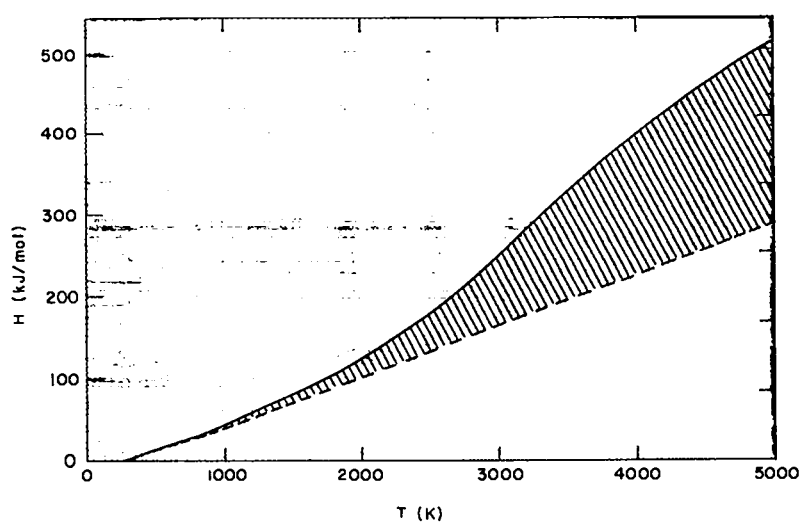


Fig. 15. UO_2 enthalpy (H) vs. temperature along liquid-vapor coexistence curve calculated with electronic excitations (solid curve) and without (dashed curve).

The resulting P_v is shown as a solid curve in Figs. 16a and 16b. The dashed curve is the IAEA standard.[11] Our curve definitely gives a better fit to the data and, in fact, differs from a least squares fit for P_v by, at most, 5% over the temperature range $1500 \leq T \leq 5000$ K.

All the various pieces of the UO_2 EOS are now being composed into a thermodynamically consistent EOS for reactor safety.

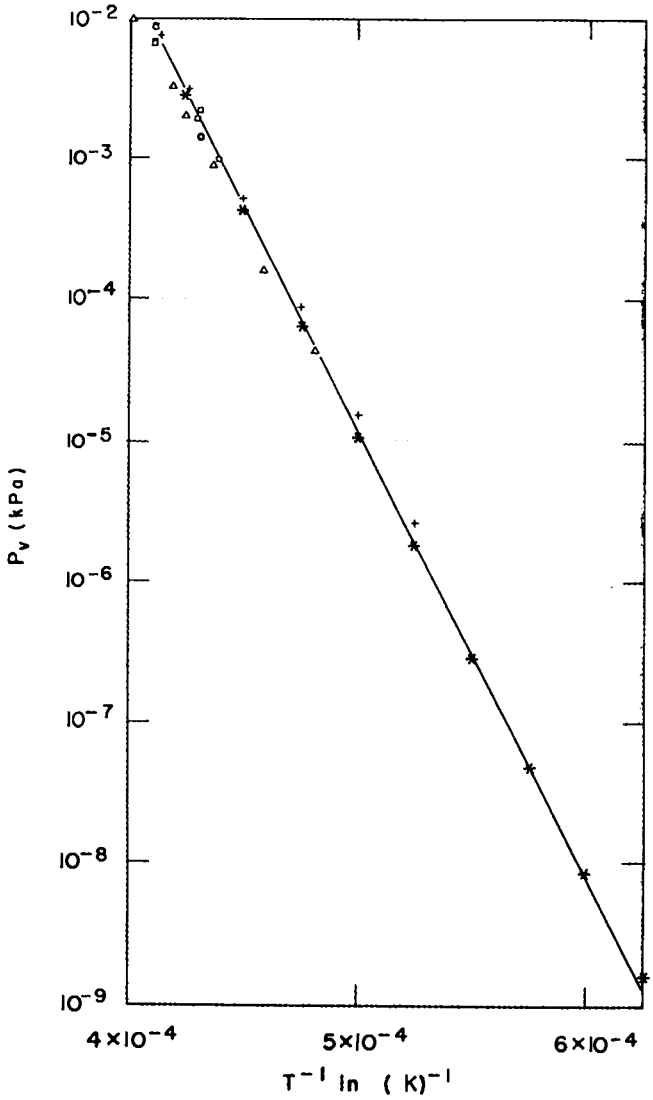


Fig. 16a. UO_2 vapor pressure for low temperatures. Calculated values (solid curve) are compared with experimental data points.

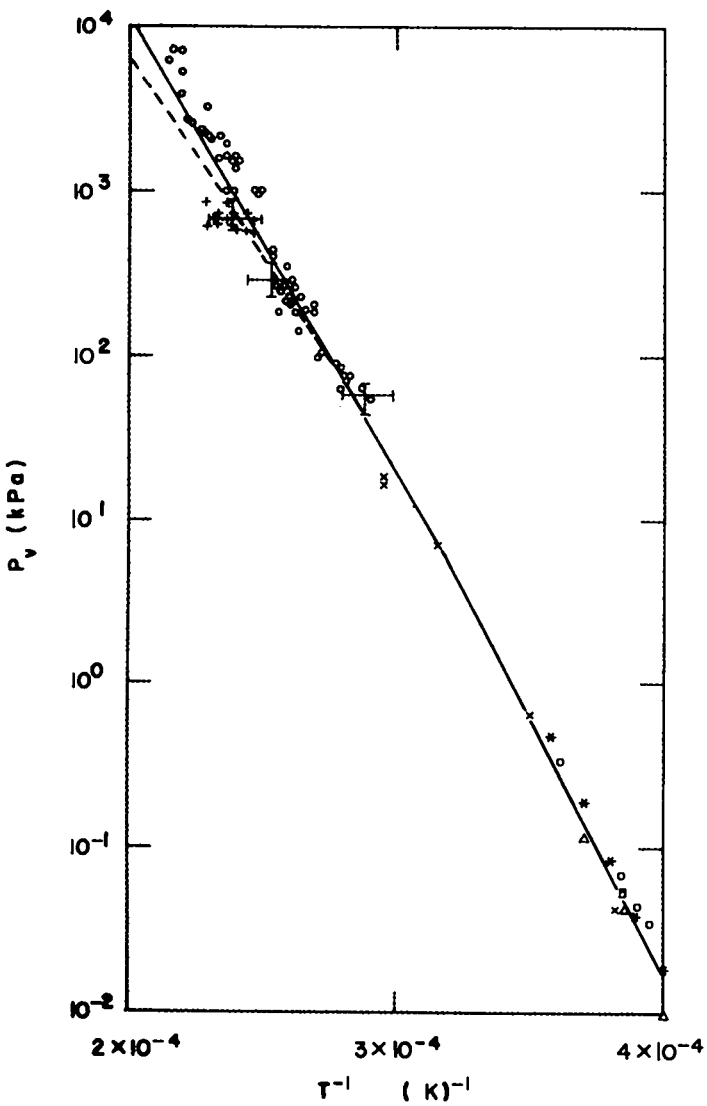


Fig. 16b. UO_2 vapor pressure for high temperatures. Calculated values (solid curve) are compared with experimental data points and IAEA standard (dashed curve).

Liquid Sodium and the CRIS Model of Fluids

The properties of liquid sodium are needed for the analysis of hypothetical accidents in sodium-cooled fast breeder reactors. Padilla has made a very good compilation of sodium data in the region of the vapor-liquid coexistence curve.[12] For detailed safety calculations, a complete EOS surface, including the supercritical and metastable regions, is needed. Although several good EOS models have been proposed, none has given satisfactory agreement with Padilla's tables.

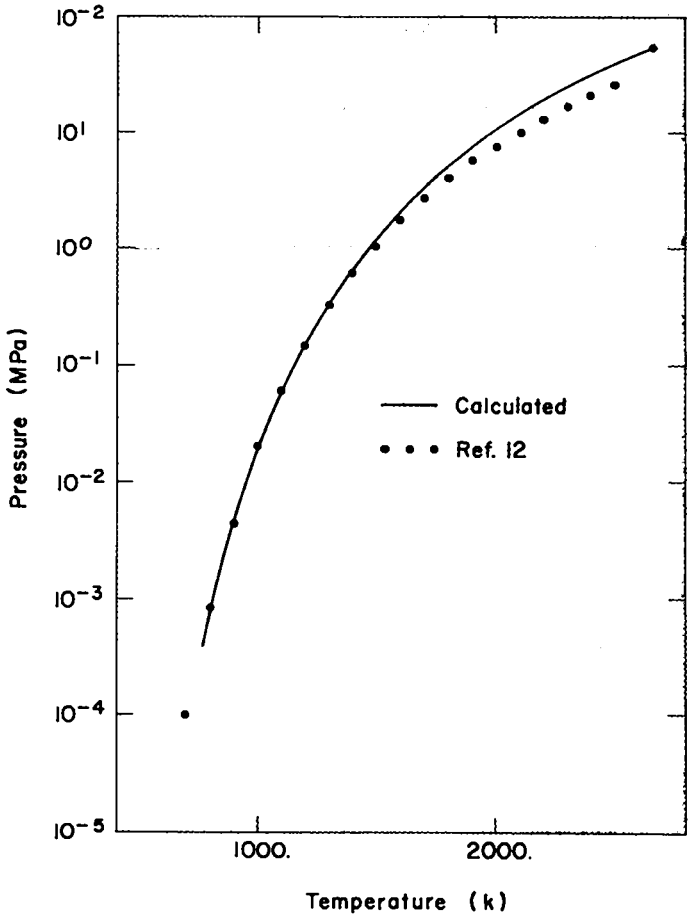
The CRIS model of fluids, which is based on thermodynamic perturbation theory, was used to compute an EOS for sodium. The effects of dimerization in the vapor phase were also included. The calculated coexistence properties compare well with Padilla's data and in addition, our results agree with PVT measurements and other experiments.

Recent work has shown that the structure of liquids is determined by repulsive forces, and that the hard-sphere fluid provides a good model for this structure. In first-order perturbation theory, the entropy of the liquid is estimated by assuming the molecules to be hard spheres, and the internal energy is determined by averaging the intermolecular forces over the hard-sphere distribution. The hard-sphere diameter can be estimated by minimizing the Helmholtz free energy. In the CRIS model, it is assumed that each liquid molecule is surrounded by a spherical shell of nearest neighbors and that the coordination number and nearest-neighbor distance vary from molecule to molecule. In this approximation, the dependence of the energy of a molecule on nearest-neighbor distance can be determined from the zero-temperature isotherm of the solid.

The first-order theory gave very good results when it was applied to the EOS of argon and deuterium.[5,13] In calculations for liquid sodium and other metals, however, terms beyond first-order must be included in order to give satisfactory results for the vapor-liquid coexistence curve. The model has been extended to include these corrections and the improved theory gives very accurate results when compared with computer simulations on model liquids.[14] In fact, this method can be used to calculate the radial distribution function (distribution of neighboring molecules as a function of distance) and structure factor of a liquid as well as the thermodynamic properties.

In Fig. 17, the calculated vapor pressure is compared with experimental data, and Fig. 18 shows the liquid and vapor densities on the coexistence curve. The calculation shows discrepancy with experiment, particularly near the critical point, but the agreement is very good for a theoretical model. Since even better results may be needed for practical applications of the EOS, agreement with experiment may be forced by making relatively small adjustments to the parameters used in creating the EOS. We plan to study this problem further. The final EOS table will be included in the SESAME library.

We have also made some exploratory calculations of transport properties of liquid metals, using the hard-sphere approximation.[15] In Fig. 19 we show calculated and experimental viscosity curves for liquid sodium as a function of temperature.[16] The agreement is fairly good. We believe that even better results can be obtained if corrections to the hard-sphere model are included as we have done in the EOS theory.



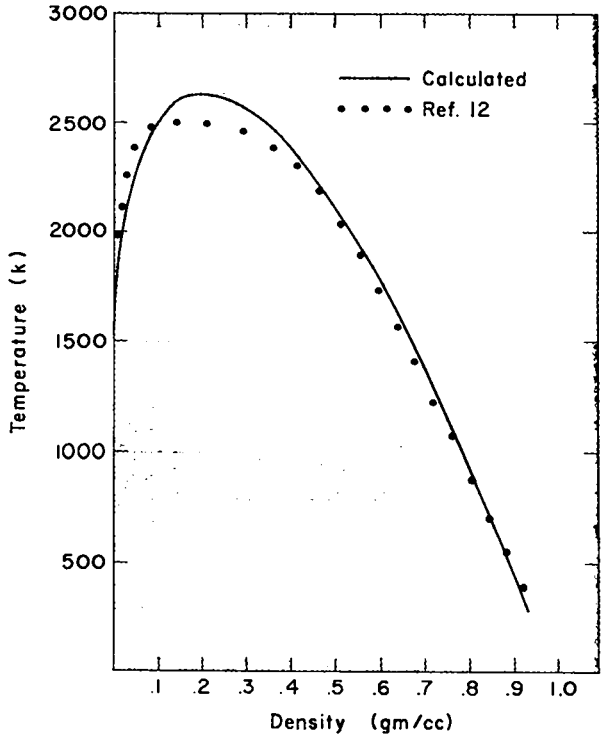
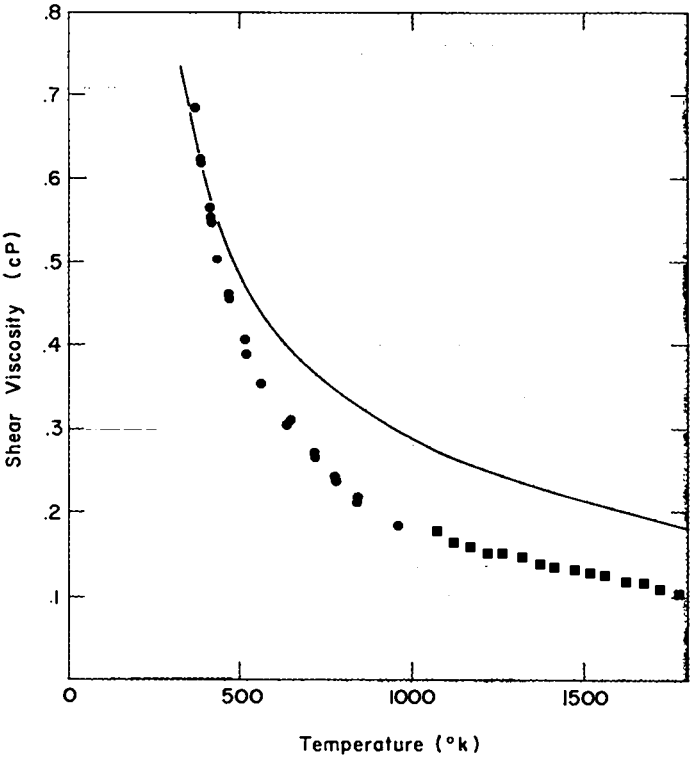


Fig. 17. (upper left) Vapor pressure of liquid sodium. Calculated results (solid curve) are compared with experimental data points.
Fig. 18. (above) Density of sodium on the liquid-vapor coexistence curve. Calculated results (solid curve) are compared with experimental data points.
Fig. 19. (below left) Viscosity of liquid sodium. Calculated values (solid curve) are compared with experimental results.[16]



How To Send for the SESAME Library

To obtain SESAME EOS data and the subroutine library, a user should send two or more magnetic tapes, a list of the materials requlred, and a specificatlon of the tape parameters to the following address.

Sesame Library, MS-925
P. O. Box 1663
Los Alamos Scientific Laboratory
Los Alamos, New Mexico 87545

The subroutine library will be copied onto one tape and tabular data will be written on the others. A set of instructions will be included when the tapes are returned. These instructions explain how to preprocess the data tapes and how to use the library routines. Users may send additional tapes for new data at any time.

The tapes will be written in an 80-character card image format that is compatible with the user's computing facilities. Standard options include the BCD character set for 7-track tapes and the EBCDIC character set for 9-track tapes. The tapes are usually written unblocked, with either 800 or 1600 BPI. The user should specify either 7-track or 9-track tapes, the character set, density, and any other parameters that are appropriate.

The number of data tapes needed depends upon the tape format, the number of materials requested, and the size of the tables. As a rough guide, allow

one 7-track tape, 800 BPI, for each 20-25 materials,
one 9-track tape, 800 BPI, for each 25-30 materials,
one 7-track tape, 1600 BPI, for each 40-50 materials,
one 9-track tape, 1600 BPI, for each 50-60 materials.

Consulting services are available to answer questions about the library and to asslst users with any problems.

Future Developments of the SESAME Library

Future work to expand the SESAME library will emphasize the needs of nonnuclear energy research. EOS for new materials will be required to model combustion and detonation processes and to study the safety of coal gasification and liquification reactors. More accurate theoretical models for the liquids and the liquid-vapor coexistence region will be needed, as well as accurate descriptions of thermal conductivities and gas mixtures. We are hopeful that the CRIS model of liquids described earlier can be applied to many materials to calculate melting properties and liquid-vapor coexistence curves more accurately. The liquid structure factor calculated from this thermodynamic perturbation expansion about a hard-sphere fluid can be used to calculate various transport properties including viscosity, diffusivity, thermal conductivity, and electrical conductivity. These transport properties will eventually be included in the SESAME library.

A problem in immediate need of EOS research is the vapor explosion. Under certain conditions, a cold liquid can become superheated and vaporize explosively when it comes in contact with a warm liquid. This phenomenon is important to the liquid natural gas (LNG) and metal casting industries and is also important in safety studies of fission reactors.

The study of methane is already in progress and work on heavier hydrocarbons, hydrocarbon mixtures and liquids that exhibit vapor explosions are planned. In preliminary studies, the CRIS model of liquids developed at LASL was tested for the metastable (superheated) region by comparing calculated and experimental values for the superheat limiting temperature (SLT) of the refrigerant R-12 (dichlorodifluoromethane). The SLT is the highest temperature to which a liquid can be heated before it spontaneously explodes. The results plotted in Fig. 20 indicate that the calculations are promising.

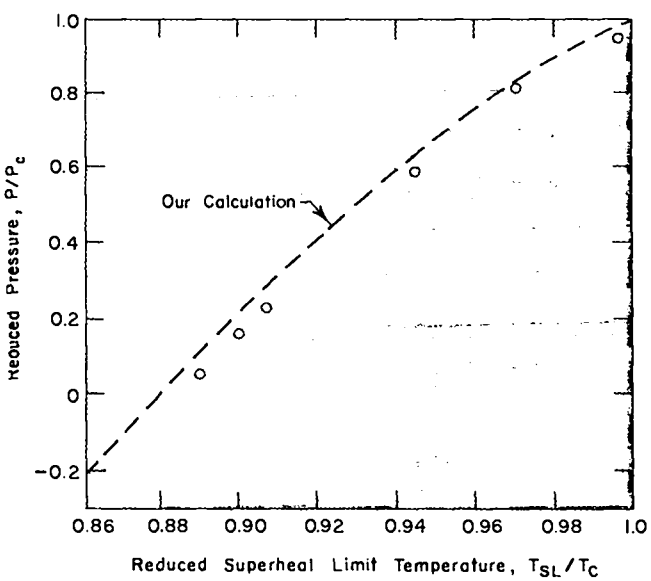


Fig. 20. Estimated limit of superheat temperatures from equation of state for dichlorodifluoromethane (R-12). Experimental values (circles) are reported by G. R. Moore, "Vaporization of Superheated Drops in Liquids," Ph.D. thesis, U. of Wisc., Madison 1956; AICh E. J. **5**, *458 (1959).*

In addition to new materials, improvements are required in the exlsting SESAME tables, especially in the low-density, high-temperature regions. Research is in progress to model the effects of shell structure and ionization that become important in this region. As mentioned earlier, the revised EOS tables will be tabulated in the SESAME library, along with separate tabulations of the ionic or nuclear contribution so that consistent two-temperature EOS can be generated conveniently.

The SESAME library can become a recognized standard only when the contents of the library represent the best EOS possible, based on existlng theory and experimental data. Moreover, objective evaluations must judge what "best" means at any given time. Therefore the establishment and malntenance of the SESAME library as a standard requires the involvement of users and scientists other than the LASL developers of the library to evaluate its contents and recommend improvements both in the data base itself and in the software packages. The incorporation of experimental and theoretical results generated outside LASL will be an important part of the evaluation procedure. A system of objective evaluation is now under discussion and users are urged to offer suggestions.

In general, the future of the library will be determined by user needs and interests. Please let us know your present interests by filling out the form on the following page and returning it to us.

We would appreciate your response.
Please tear out this form and mail to:

SESAME Library, MS-925
P.O. Box 1663
Los Alamos Scientific Laboratory
Los Alamos, New Mexico 87545

User Response Form

Name _____

Address _____

_____

_____

1. I am interested in using the SESAME library. Yes _____

No _____

Reasons: _____

_____

_____

2. I am interested in the following materials and properties.

Materials and properties of interest	Temp range	Density range

Applications of EOS data. (Type of code etc.) _____

_____

_____

_____

Present source of data. _____

_____

_____

Computing facilities used. _____

_____

_____

3. I have already used the SESAME tables. Yes _____

No _____

Comment on advantages. _____

_____

Comment on disadvantages. _____

_____

4. I am involved in EOS research. Yes _____

No _____

Describe. _____

_____

_____

5. Are you interested in becoming a member of a SESAME library advisory board to provide objective evaluation of library data and software? Yes _____

No _____

Do you have suggestions concerning the working procedures of such an advisory board?

_____

_____

_____

_____

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