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Manual

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**EOSMOD:**

*Subroutine Package for Calculating  
Equations of State and Opacities*

LOS ALAMOS NATL. LAB. LIBS.



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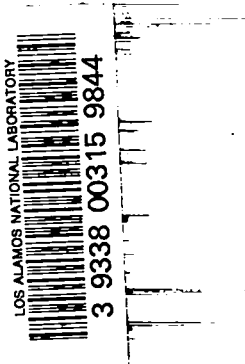
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# EOSMOD: A Subroutine Package for Calculating Equations of State and Opacities

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EOSMOD: A SUBROUTINE PACKAGE FOR  
CALCULATING EQUATIONS OF STATE AND OPACITIES

by

James M. Hyman and Morris M. Klein

ABSTRACT

The EOSMOD package includes a set of FORTRAN subroutines written to make the SESAME equation-of-state and opacity tables readily available. We have tried to make these routines as accessible as possible for casual users with routine problems and at the same time, allow sufficient flexibility for sophisticated users with complicated situations. This has caused only a slight loss in efficiency (~5%) compared to using the SESAME routines directly.

---

I. INTRODUCTION

The SESAME library is a collection of data files containing equations of state (EOS), Rosseland mean opacities, and other material properties over a wide range of temperatures, pressures, and densities. Group T-4 at Los Alamos National Laboratory developed a FORTRAN subroutine library<sup>1-3</sup> to access and analyze these data files. The EOSMOD subroutine package was developed to complement the T-4 routines and simplify the interface between these codes and the user's program. The EOSMOD routines do the bookkeeping, unit's conversion, and large core memory (LCM) initialization; reduce the number of parameters the casual user needs to be aware of; and are written in a structured modular design to allow a sophisticated user to modify and optimize the package easily for a particular problem.

To use the package, just access the SESAME data files as described in Sec. VIII and call the driver subroutine. The package then locates the requested data file, converts it to the units specified by the user, and stores it in LCM. On all subsequent calls, the package remembers the contents and location of the file and interpolates the data at the user's requested values.

If the EOS or opacity of a mixture is needed, then the directory of mixtures currently available (MIXDIR) should be checked. If the specific mixture is not in the library, then a SESAME data file may be generated using the procedure described in Refs. 4, 5, and 6.

## II. EQUATION-OF-STATE AND OPACITY ROUTINES

The first time a routine is called for each new material (LMAT), the table is converted to the kind of units (KUNIT) requested by the user and copies into LCM. The location or material table number (IMATE) is returned to indicate the location of the EOS table or to indicate whether an error was encountered in the initialization; for example, if the material was not found in the library.

The EOS tables can be loaded in two different formats. The standard SESAME format is for calculating the pressure P and internal energy E of a material as a function of the density R and temperature T. Subroutine EOSDRT loads and reads the tables in this format.

The inverted SESAME format is for calculating P and T as a function of R and E with subroutine EOSDRE. These inverted tables also can be accessed in other ways using the iterative subroutines EOSIRT and EOSIPT. Subroutine EOSIPT calculates E and R as function of P and T, and subroutine EOSIRT calculates P and E as a function of R and T. These iterative subroutines use an iterative scheme that is slow compared to the direct methods used in subroutines EOSDRT and EOSDRE. Their main use is for initial state computations and occasional diagnostics.

To speed up the execution time when using subroutine EOSDRE or EOSDRT, the user can request that the package return only T, P, or E using the computational mode flag KBR. Computer time can also be saved by using the KFN flag to indicate a bilinear interpolation of the data rather than the more accurate (but slower) rational interpolation. These interpolation procedures are described in more detail in Refs. 1 and 7.

A. Subroutine EOSDRE (input R and E, output P and T)

The calling sequence when  $\rho$  and E are independent variables (input) and  $P(\rho,E)$  and  $T(\rho,E)$  are dependent variables (output) is

CALL EOSDRE (LMAT,R,E,P,T,KEOS,IMATE).

The arguments are defined as follows.

INPUT VARIABLES

LMAT Material name in an A10 field; for example, LMAT = "HELIUM."  
The materials available are listed in Sec. VII and the file MIXDIR. (The material SESAME number can also be used to specify the material by setting LMAT to the SESAME number; for example, LMAT = "5760" for helium.)

R Density ( $\rho$ ).  
E Internal energy.

KEOS Multiple parameter flag to describe how to write and retrieve the data file. KEOS has four decimal digits: KBR, KUNIT, KREPE, and KFN (KEOS = 1000\*KBR + 100\*KUNIT + 10\*KREPE + KFN).

KBR Computational flag to indicate which quantities and their partial derivatives are to be calculated and returned by the package.

0 Compute P and T and their partial derivatives  $\partial P/\partial\rho$ ,  $\partial P/\partial E$ ,  $\partial T/\partial\rho$ , and  $\partial T/\partial E$ .  
1 Compute P and its partial derivatives  $\partial P/\partial\rho$  and  $\partial P/\partial E$ .  
2 Compute T and its partial derivatives  $\partial T/\partial\rho$  and  $\partial T/\partial E$ .

KUNIT Kind of units for writing the data file. The units are explained fully in Sec. IX.

0 SESAME EOS units.  
1 CGS units.  
2 Standard International Units (SIU).  
3 Hydrox EOS units.  
4 Hydrox opacity units.  
5 SESAME opacity units.  
6 LASNEX units.

KREPE Computational flag to indicate whether E is to be represented as energy per unit mass or energy per unit volume.

0 Energy in units of energy per unit mass (for example, ergs/g). This is the usual E.



1 Energy in units of energy per unit volume (for example, ergs/cm<sup>3</sup>). This is the energy density  $\rho E$  commonly computed in hydrodynamic computer codes.

KFN Indicates the form of the function used to interpolate the data tables.

0 Accurate rational function interpolation.  
1 Fast bilinear function interpolation.

IMATE Indicates whether to load the data file if it does not exist for LMAT or go directly to a previously loaded file.

0 Check if the data file for LMAT has been loaded. If not, search for the file, convert it to the proper units, and copy it into LCM using the inverted SESAME format.  
N>0 Equal to the LMAT table number. This number was returned by the package on a previous call to subroutine EOSDRE, EOSIPT, or EOSIRT and is distinct for each LMAT. This option is faster than IMATE = 0 because it skips searching the directory of previously loaded data files.

#### OUTPUT VARIABLES

P Array of dimension 3 containing the pressure and its partial derivatives.

P(1) Pressure.  
P(2) Density derivative of the pressure ( $\partial P/\partial \rho$ ).  
P(3) Energy derivative of the pressure ( $\partial P/\partial E$ ).

T Array of dimension 3 containing the temperature and its partial derivatives. This array must be dimensional even if the partial derivatives are not computed.

T(1) Temperature.  
T(2) Density derivative of the temperature ( $\partial T/\partial \rho$ ).  
T(3) Energy derivative of the temperature ( $\partial T/\partial E$ ).

IMATE Indicates the success or failure of locating and loading the data file for LMAT.

0 LMAT not found.  
N>0 LMAT table number (success).  
N<0 Insufficient LCM storage. The LCM memory allocation must be increased by at least  $|N|$  storage locations by the procedure described in Sec. V.

B. Subroutine EOSIPT (input P and T, output R and E)

The calling sequence when P and T are independent variables (input) and  $\rho(P,T)$  and  $E(P,T)$  are dependent variables (output) is

CALL EOSIPT (LMAT,P,T,R,E,KEOS,IMATE).

This routine reads the EOS data in the inverted SESAME format and uses an iterative method to interpolate the data. The arguments are defined as follows.

INPUT VARIABLES

LMAT Material name in an A10 field; for example, LMAT = "HELIUM."  
The materials available are listed in Sec. VII and the file MIXDIR. (The material SESAME number can also be used to specify the material by setting LMAT to the SESAME number; for example, LMAT = "5760" for helium.)

P Pressure.

T Temperature.

KEOS Multiple parameter flag to describe how to write and retrieve the data file. KEOS has three decimal digits: KUNIT, KREPE, and KFN (KEOS = 100\*KUNIT + 10\*KREPE + KFN).

KUNIT Kind of units for writing the data file. The units are explained fully in Sec. IX.

0 SESAME EOS units.

1 CGS units.

2 Standard International Units (SIU).

3 Hydrox EOS units.

4 Hydrox opacity units.

5 SESAME opacity units.

6 LASNEX units.

KREPE Computational flag to indicate whether E is to be represented as energy per unit mass or energy per unit volume.

0 Energy in units of energy per unit mass (for example, ergs/g). This is the usual E.

1 Energy in units of energy per unit volume (for example, ergs/cm<sup>3</sup>). This is the energy density  $\rho E$  commonly computed in hydrodynamic computer codes.

KFN Indicates the form of the function used to interpolate the data tables.

0 Accurate rational function interpolation.

1 Fast bilinear function interpolation.

IMATE Indicates whether to load the data file if it does not exist for LMAT or go directly to a previously loaded file.

0 Check if the data file for LMAT has been loaded. If not, search for the file, convert it to the proper units, and copy it into LCM using the inverted SESAME format.

N>0 Equal to the LMAT table number. This number was returned by the package on a previous call to subroutine EOSDRE, EOSIPT, or EOSIRT and is distinct for each LMAT. This option is faster than IMATE = 0 because it skips searching the directory of previously loaded data files.

#### OUTPUT VARIABLES

R Density.

E Internal energy.

IMATE Indicates the success or failure of locating and loading the data file for LMAT.

0 LMAT not found or the iteration failed to converge.

N>0 LMAT table number (success).

N<0 Insufficient LCM storage. The LCM memory allocation must be increased by at least |N| storage locations by the procedure described in Sec. V.

C. Subroutine EOSIRT (input R and T, output P and E)

The calling sequence when  $\rho$  and T are independent variables (input) and  $P(\rho,T)$  and  $E(\rho,T)$  are dependent variables (output) is

CALL EOSIRT (LMAT,R,T,P,E,KEOS,IMATE).

This routine reads the EOS data in the inverted SESAME format and uses an iterative method to interpolate the data. The arguments are defined as follows.

INPUT VARIABLES

LMAT      Material name in an A10 field; for example, LMAT = "HELIUM."  
The materials available are listed in Sec. VII and the file MIXDIR. (The material SESAME number can also be used to specify the material by setting LMAT to the SESAME number; for example, LMAT = "5760" for helium.)

R          Density.  
T          Temperature.

KEOS      Multiple parameter flag to describe how to write and retain the data file. KEOS has three decimal digits: KUNIT, KREPE, and KFN (KEOS = 100\*KUNIT + 10\*KREPE + KFN).

          KUNIT      Kind of units for writing the data file. The units are explained fully in Sec. IX.

                  0          SESAME EOS units.  
                  1          CGS units.  
                  2          Standard International Units (SIU).  
                  3          Hydrox EOS units.  
                  4          Hydrox opacity units.  
                  5          SESAME opacity units.  
                  6          LASNEX units.

          KREPE      Computational flag to indicate whether E is to be represented as energy per unit mass or energy per unit volume.

                  0          Energy in units of energy per unit mass (for example, ergs/g). This is the usual E.  
                  1          Energy in units of energy per unit volume (for example, ergs/cm<sup>3</sup>). This is the energy density  $\rho E$  commonly computed in hydrodynamic computer codes.

          KFN        Indicates the form of the function used to interpolate the data tables.

                  0          Accurate rational function interpolation.  
                  1          Fast bilinear function interpolation.

IMATE Indicates whether to load the data file if it does not exist for LMAT or go directly to a previously loaded file.

0 Check if the data file for LMAT has been loaded. If not, search for the file, convert it to the proper units, and copy it into LCM using the inverted SESAME format.

N>0 Equal to the LMAT table number. This number was returned by the package on a previous call to subroutine EOSDRE, EOSIPT, EOSDRT, or EOSIRT and is distinct for each LMAT. This option is faster than IMATE = 0 because it skips searching the directory of previously loaded data files.

#### OUTPUT VARIABLES

P Pressure.

E Internal energy.

IMATE Indicates the success or failure of locating and loading the data file for LMAT.

0 Material not found or iteration failed to converge.

N>0 LMAT table number (success).

N<0 Insufficient LCM storage. The LCM memory allocation must be increased by at least |N| storage locations by the procedure described in Sec. V.

D. Subroutine EOSDRT (input R and T, output P and E)

The calling sequence when  $\rho$  and T are independent variables (input) and P( $\rho$ ,T) and E( $\rho$ ,T) are dependent variables (output) is

CALL EOSDRT (LMAT,R,T,P,E,KEOS,IMATE).

The arguments are defined as follows.

INPUT VARIABLES

LMAT Material name in an A10 field; for example, LMAT = "HELIUM."  
The materials available are listed in Sec. VII and in the file MIXDIR. (The material SESAME number can also be used to specify the material by setting LMAT to the SESAME number; for example, LMAT = "5760" for helium.)

R Density ( $\rho$ ).  
T Temperature.

KEOS Multiple parameter flag to describe how to write and retrieve the data file. KEOS has four decimal digits: KBR, KUNIT, KREPE, and KFN (KEOS = 1000\*KBR + 100\*KUNIT + 10\*KREPE + KFN).

KBR Computational flag to indicate which quantities and their partial derivatives are to be calculated and returned by the package.

0 Compute P and E and their partial derivatives  $\partial P/\partial \rho$ ,  $\partial P/\partial T$ ,  $\partial E/\partial \rho$ , and  $\partial E/\partial T$ .  
1 Compute P and its partial derivatives  $\partial P/\partial \rho$  and  $\partial P/\partial T$ .  
2 Compute T and its partial derivatives  $\partial E/\partial \rho$  and  $\partial E/\partial T$ .

KUNIT Kind of units for writing the data file. The units are explained fully in Sec. IX.

0 SESAME EOS units.  
CGS units.  
2 Standard International Units (SIU).  
3 Hydrox EOS units.  
4 Hydrox opacity units.  
5 SESAME opacity units.  
6 LASNEX units.

KREPE Computational flag to indicate whether E is to be represented as energy per unit mass or energy per unit volume.

0 Energy in units of energy per unit mass (for example, ergs/g). This is the usual E.

1 Energy in units of energy per unit volume (for example, ergs/cm<sup>3</sup>). This is the energy density  $\rho E$  commonly computed in hydrodynamic computer codes.

KFN Indicates the form of the function used to interpolate the data tables.

0 Accurate rational function interpolation.  
1 Fast bilinear function interpolation.

IMATE Indicates whether to load the data file if it does not exist for LMAT or go directly to a previously loaded file.

0 Check if the data file for LMAT has been loaded. If not, search for the file, convert it to the proper units, and copy it into LCM using the standard SESAME format.

N>0 Equal to the LMAT table number. This number was returned by the package on a previous call to subroutine EOSDRE, EOSIPT, EOSDRT, or EOSIRT and is distinct for each LMAT. This option is faster than IMATE = 0 because it skips searching the directory of previously loaded data files.

#### OUTPUT VARIABLES

P Array of dimension 3 containing the pressure and its partial derivatives.

P(1) Pressure.  
P(2) Density derivative of the pressure ( $\partial P/\partial \rho$ ).  
P(3) Temperature derivative of the pressure ( $\partial P/\partial T$ ).

E Array of dimension 3 containing the internal energy and its partial derivatives. This array must be dimensional even if the partial derivatives are not computed.

E(1) Internal energy.  
E(2) Density derivative of the internal energy ( $\partial E/\partial \rho$ ).  
E(3) Energy derivative of the internal energy ( $\partial E/\partial T$ ).

IMATE Indicates the success or failure of locating and loading the data file for LMAT.

0 LMAT not found.  
N>0 LMAT table number (success).  
N<0 Insufficient LCM storage. The LCM memory allocation must be increased by at least |N| storage locations by the procedure described in Sec. V.

E. Subroutine EOSORT (input R and T, output O)

The Rosseland mean opacity<sup>8</sup> of the material (LMAT) can be calculated by calling subroutine OPCRT. The density R and temperature T are the independent input variables, and the opacity O is the dependent output variable. When the internal energy, but not the temperature, is known, the user must first call subroutine EOSDRE to get the temperature. The (KUNIT) that the table is to be written in and the type of interpolation function (KFN) to be used must be provided by the user. The material opacity table number (IMATO) is returned by the package to indicate the location of the opacity table in LCM or if an error was encountered by the routine.

The calling sequence when  $\rho$  and T are independent variables (input) and O is the dependent variable (output) is

```
CALL EOSORT (LMAT,R,T,O,KOPC,IMATO)
```

The arguments are defined as follows.

INPUT VARIABLES

LMAT	Material name in an A10 field; for example, LMAT = "HELIUM." The materials available are listed in Sec. VII and in the file MIXDIR. (The material SESAME number can also be used to specify the material by setting LMAT to the SESAME number; LMAT = "15760".
R	Density ( $\rho$ ).
T	Temperature.
KOPC	Multiple parameter flag to describe how to write and retrieve the data file. KEOS has three decimal digits: KUNIT, KREPO, and KFN (KEOS = 100*KUNIT + 10*KREPO + KFN).
KUNIT	Computational flag to indicate the kind of units for writing the data file. The units are explained fully in Sec. IX.  0        SESAME EOS units. 1        CGS units. 2        Standard International Units (SIU). 3        Hydrox EOS units. 4        Hydrox opacity units. 5        SESAME opacity units. 6        LASNEX units.
KREPO	Computational flag to indicate which representation to use for the opacity.  0        Opacity represented as $\kappa$ in dimensional units of length <sup>2</sup> /mass. 1        Opacity represented as a mean-free path, $\Lambda = 1/(\kappa\rho)$ , in dimensional units of length.



KFN            Indicates the form of the function used to interpolate the data tables.

              0            Accurate rational function interpolation.

              1            Fast bilinear function interpolation.

IMATO         Indicates whether to load the data file if it does not exist for LMAT or go directly to a previously loaded file.

              0            Check if the data file for LMAT has been loaded. If not, search for the file, convert it to the proper units, and copy it into LCM.

              N>0          Equal to the LMAT table number. This number was returned by the package on a previous call to subroutine OPCRT and is distinct for each LMAT. This option is faster than IMATE = 0 because it skips searching the directory of previously loaded data files.

OUTPUT VARIABLES

0            Opacity.

IMATEO       Indicates the success or failure of locating and loading the data file for LMAT.

0            LMAT not found.

N>0          LMAT table number (success).

N<0          Insufficient LCM storage. The LCM memory allocation must be increased by at least |N| storage locations by the procedure described in Sec. V.

### III. SCALING THE TABLES

#### A. Density Scaling

When the atomic mass of the desired material is different from the mass of the SESAME material and the material properties are expected to be similar, then a simple density scale factor can be incorporated into the EOS and opacity tables. This is usually sufficient for isotope mixtures of a specific material.

The density scale factor (DSFAC) for the material LMAT can be incorporated into the tables through the user supplied subroutine EOSSCL(LMAT, DSFAC). This routine will be called by EOSMOD, and the routine should return DSFAC equal to the ratio of the atomic mass of the SESAME material and the desired material; that is,

$$\text{DSFAC} = \frac{\text{atomic mass of SESAME material LMAT}}{\text{atomic mass of desired material}}$$

In example B, Sec. VI, the EOS of a 60% deuterium/40% tritium mixture is approximated from the EOS of deuterium by defining

$$\text{DSFAC} = \frac{2}{0.60 \times 2 + 0.40 \times 3} = 0.833 \quad .$$

#### B. Adding New Units

When the EOS and opacity tables are copied from the SESAME data file into LCM, they are converted to the user's specified units by multiplying the data by a conversion factor. The EOS conversion factors for temperature, density, pressure, and internal energy are TFACE, RFACE, PFACE, and EFACE, respectively. The opacity conversion factors for density, temperature, and opacity are RFACO, TFACO, and OFACO, respectively.

These factors are defined in the EOSMOD subroutine EOSCON according to the user's specifications (KUNIT) and communicated to the various EOSMOD routines through the common blocks

```
COMMON /EOSCCE/ TFACE,RFACE,PFACE,EFACE  
COMMON /EOSCCO/ TFACO,RFACO,OFACO
```

If the desired units are not automatically available in the package, the user can reset the conversion factors at execution time (not in a data statement) in the user-provided routine EOSSCL (See Sec. V.A). This is done in example 5B.

The scale factor is the constant that the data in the original SESAME EOS table units (KUNIT = 0) or SESAME opacity table units (KUNIT = 5) must be multiplied by to convert the data to the desired units. The conversion factors for KUNIT = 0-6 are easily found in subroutine EOSCON listed in the Appendix A.

#### IV. USER NOTES

##### A. Information File

The file EOSINFO contains the latest user notes and information on the EOSMOD package. Users are encouraged to add notes to this file that will be helpful to others using the package.

##### B. Graphic Output

Several plotting routines exist for displaying EOS and opacity data stored in the SESAME format. The routines are maintained by Los Alamos Group T-4 and are described in the data file S2DHELP. See Ref. 9.

##### C. Increasing LCM Allocation

On the CDC 7600's at the Laboratory, the EOSMOD default LCM allocation is 12 000 words. This is enough storage to load approximately four EOS tables. The allocation can be increased to LCMX, say 20 000 words, by declaring

```
LEVEL 2, TBLS
COMMON /S2DIR/ LCMX
COMMON /SESDAT/ TBLS (20000)
LCMX=20000
```

in the main program. LCMX must be set to the dimension of TBLS at execution time not in a data statement. Example 2B in Sec. VI does this.

##### D. Reducing the EOS Data Range

Subroutine WINDOW in the Hydses package can be used to reduce the size of a standard temperature-based SESAME data table when the full density and temperature range are not needed. Because the use of this routine requires knowledge of where and how the tables are stored in LCM, we refer the interested user to the HYDSES report<sup>2,10</sup> for further information.

##### E. Error Flags and Messages

All error messages are written into a file called "OUTPUT." The name of this file is defined at compile time in the Hollerith variable LOUT in the common block

```
COMMON/EOSCZ/LOUT.
```

LOUT can be changed to another file name or unit number of the user at execution time before the first call to EOSMOD.

##### F. Creating an EOS/Opacity Table for Mixtures

The EOS/opacity tables suitable for gas mixtures can be created with the aid of the BCON controller MIXB.<sup>5</sup> These EOS mixture tables currently are prepared under the assumption that the ideal mixing of individual com-

ponent parts occurs. The pressure of the mixture is taken, as in Dalton's law, to be the weighted mole fraction of the partial pressures of the component parts. Opacity mixture tables are created by weighing the opacities of each component in frequency space according to the component's fraction of the total mass and then by integrating the resultant frequency spectrum to obtain the Rossland mean opacity for the mixture. These tables are generated in SESAME format with a simple input deck.

#### G. Listing the Available Materials

The EOS and opacity materials, and SESAME numbers are listed in the common blocks

```
COMMON/EOSC5/NMAT,LABMAT(40),IDMAT(40)
COMMON/EOSC7/NMATO,LABMO(40),IDMATO(40).
```

There are NMAT (NMATO) EOS (opacity) materials in the common blocks. The labels in LABMAT (LABMO) are in an A10 format and correspond to the SESAME material ID in IDMAT (IDMATO).

To list the EOS tables, execute the code

```
DO 10 I = 1,NMAT
10 PRINT 20, LABMAT(I),IDMAT(I)
20 FORMAT (1X,A10,I10).
```

A complete description of each material can be found using the T-4 SESAME utility LSTX. (See Sec. VIII and Ref. 11.)

### V. EXAMPLES

#### A. Simplest Example

The following program will compute the pressure of helium in microbars at a temperature of 300 K and a density of 0.01 g/cm<sup>3</sup>.

```
PROGRAM TST(OUTPUT)
DIMENSION P(3),E(3)
LMAT = "HELIUM"
R = 0.01
T = 300.0
KEOS = 110
IMATE = 0
CALL EOSDRT(LMAT,R,T,P,E,KEOS,IMATE)
PRINT 10, P(1)
10 FORMAT("PRESSURE = ", 1PE12.4," MICROBARS")
CALL EXIT
END
```

The execute line is

```
FTN (I=TEST, GLIB=EOSLIB, GO)
```

The output from this program is:

```
PRESSURE = 6.3498E+07 MICROBARS
```

### B. Advanced EOS Example

In this example we scale the density for a 60% deuterium/40% tritium mixture, add a new set of MKS units, and increase LCM so we can load four EOS tables.

```
PROGRAM TST(OUTPUT)
C
C DECLARE THE COMMON BLOCKS USED BY EOSMOD(HYDSES) TO STORE THE TABLES
LEVEL 2, TBLS
COMMON /S2DIR/ LCMX
COMMON /SESDAT/ TBLS(20000)
C
C DECLARE THE COMMON BLOCK WITH THE FILE LABELS
COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
C
C DIMENSION P(3), E(3)
C
C INCREASE THE LCM STORAGE AVAILABLE TO EOSMOD
C THE MAXIMUM LCM STORAGE IN /SESDAT/ IS LCMX WORDS
LCMX = 20000
C
C SET THE DENSITY IN KILOGRAMS
C AND THE TEMPERATURE IN DEGREES KELVIN
R = 1.E-5
T = 300.0
KEOS = 110
C
C THE TABLE FOR DEUTERIUM IS CONVERTED BY EOSMOD TO A MIXTURE BY
C SCALING THE DENSITY IN SUBROUTINE EOSLL.
LMAT = "DEUTERIUM"
IMATE = 0
CALL EOSDRT(LMAT, R, T, P, E, KEOS, IMATE)
PRINT 10, P(1)
10 FORMAT ("40% D + 60% T, PRESSURE =", 1PE12.4, "BARS")
C
C LMAT = "HELIUM"
IMATE = 0
CALL EOSDRT(LMAT, R, T, P, E, KEOS, IMATE)
PRINT 20, LMAT, P(1)
C
```

```

C   DECLARE THE NAME OF THE PRIVATE EOS DATA TABLES AND DIRECTORY
      LF44 = "MIXLIB"
      LF45 = "MIXDIR"

C
C   FIND EOS PRESSURE OF A 90% DEUTERIUM 10% NEON MIXTURE.
C   THE EOS IS CONTAINED IN THE PRIVATE TABLES MIXLIB AND MIXDIR
      LMAT = "D9ONE10"
      IMATE = 0
      CALL EOSDRT(LMAT,R,T,P,E,KEOS,IMATE)
      PRINT 20,LMAT,P(1)

C
20  FORMAT(1X,A10," PRESSURE = ",1PE12.4," "BARS")

C
      CALL EXIT
      END

      SUBROUTINE EOSSCL (LMAT,DSFAC)
      COMMON /EOSCCE/ TFACE,RFACE,PFACE,EFACE,KPE

C
C   SET UP A NEW SET OF UNITS TO BE USED BY THE CODE
C   PFACE AND EFACE ARE THE CONVERSION FACTORS FOR THE MKS SYSTEM
C   YOU ONLY NEED TO DEFINE THE CONVERSION FACTORS THAT DIFFER
C   FROM THE KEOS DECLARED UNITS (CGS SYSTEM)
C   CONVERT THE PRESSURE TO BARS
      PFACE = 1.E+6
      EFACE = 1.E+6

C
C   WE NOW RESCALE THE DENSITY FOR DEUTERIUM TO WHAT IT
C   SHOULD BE FOR A 60% DEUTERIUM AND 40% TRIDIUM MIXTURE

      IF(LMAT.EQ."DEUTERIUM") DSFAC=0.833

C
      RETURN
      END

```

The output from this program is

```

40% D + 60% T      PRESSURE = 6.1923E+04 BARS
HELIUM             PRESSURE = 5.6817E+04 BARS
D9ONE10           PRESSURE = 7.3926E+05 BARS

```

## VI. MATERIALS AVAILABLE

The following materials are currently available using EOSMOD.<sup>11</sup>

Material Name (LMAT)	EOS File Name	Opacity File Name	Temperature Maximum (K)	Density Minimum (g/cm <sup>3</sup> )	Density Minimum (g/cm <sup>3</sup> )	SESAME Material Number
ALLUVIUM (Nevada)	SESAME		4×10 <sup>8</sup>	0.018	4.7×10 <sup>4</sup>	7111
ALUMINUM	SESAME	SESAME	4×10 <sup>8</sup>	0.021	2.7×10 <sup>3</sup>	3710
AL2O3 (= Al <sub>2</sub> O <sub>3</sub> )	SESAME		4×10 <sup>8</sup>	0.031	4.0×10 <sup>8</sup>	7410
ARGON		SESAME				5170
BERYLLIUM	SESAME	SESAME	4×10 <sup>8</sup>	0.014	4.0×10 <sup>4</sup>	2020
BORON		SESAME				2330
BORON CARB(ide)	SESAME		6×10 <sup>4</sup>	0.0002	3.2	7081
BRASS	SESAME		4×10 <sup>8</sup>	0.066	1.7×10 <sup>5</sup>	4100
CALCIUM		SESAME				2030
CARBON		SESAME				2180
CH (= polystyrene)	SESAME		4×10 <sup>8</sup>	0.0082	2.1×10 <sup>4</sup>	7590
CH2 (= polyethylene)	SESAME		4×10 <sup>8</sup>	0.082	1.8×10 <sup>4</sup>	7170
CHLORINE		SESAME				5020
CHROMIUM		SESAME				3070
COPPER	SESAME		4×10 <sup>8</sup>	0.070	1.8×10 <sup>5</sup>	3330
DEUTERIUM	SESAME	SESAME	4×10 <sup>8</sup>	0.0	3.5×10 <sup>3</sup>	5263
GOLD	SESAME		4×10 <sup>8</sup>	0.15	3.9×10 <sup>5</sup>	2700
GRANITE	SESAME		4×10 <sup>8</sup>	0.021	5.3×10 <sup>4</sup>	7390
HELIUM	SESAME	SESAME	1×10 <sup>8</sup>	0.0018	4.7×10 <sup>3</sup>	5760
HE (= High Explosive)	SESAME		4×10 <sup>8</sup>	0.014	3.7×10 <sup>4</sup>	8180
IRON	SESAME	SESAME	4×10 <sup>8</sup>	0.061	1.6×10 <sup>5</sup>	2140
IRON2	SESAME		1.2×10 <sup>4</sup>	0.0	12.5	2145
LEAD	SESAME		4×10 <sup>8</sup>	0.088	2.3×10 <sup>5</sup>	3200
LITHIUM		SESAME				2290
6LID (= <sup>6</sup> LiD)	SESAME		4×10 <sup>8</sup>	0.0062	1.6×10 <sup>4</sup>	7240
6LIH (= <sup>6</sup> LiH)	SESAME		4×10 <sup>8</sup>	0.0053	1.4×10 <sup>4</sup>	7370
MAGNESIUM		SESAME				3080
MOLYBDENUM	SESAME		4×10 <sup>8</sup>	0.08	0.2×10 <sup>5</sup>	2980
NEON	SESAME		4×10 <sup>8</sup>	0.011	2.9×10 <sup>4</sup>	5410
NICKEL	SESAME		4×10 <sup>8</sup>	0.069	1.8×10 <sup>5</sup>	3100
NITROGEN		SESAME				5000
OXYGEN		SESAME				5010
PBX-9502		SESAME				8200
PHOSPHORUS		SESAME				3910
PLATINUM	SESAME		4×10 <sup>8</sup>	0.17	2.1×10 <sup>4</sup>	3730
POLYE (= polyethylene)	SESAME		4×10 <sup>8</sup>	0.0072	1.8×10 <sup>4</sup>	7170

Material Name (LMAT)	EOS File Name	Opacity File Name	Temperature Maximum (K)	Density Minimum (g/cm <sup>3</sup> )	Density Minimum (g/cm <sup>3</sup> )	SESAME Material Number
POLYS (= polystyrene)	SESAME		4×10 <sup>8</sup>	0.0082	2.1×10 <sup>4</sup>	7590
POTASSIUM		SESAME				2460
SiO2 (= SiO <sub>2</sub> )	SESAME	SESAME	4×10 <sup>8</sup>	0.017	4.4×10 <sup>4</sup>	7380
SILICON		SESAME				3810
SODIUM	SESAME	SESAME	1×10 <sup>4</sup>	0.0	1.3	2448
SS (Steel)	SESAME	SESAME	4×10 <sup>8</sup>	0.062	1.6×10 <sup>5</sup>	4270
STAINLESS (Steel)	SESAME		4×10 <sup>8</sup>	0.062	1.6×10 <sup>5</sup>	4270
STEAM	SESAME		1300	0.0	0.9	7151
SULPHUR		SESAME				4010
TITANIUM		SESAME				2960
TITANIUM N (Nitride)		SESAME				6000
UO2 (= UO <sub>2</sub> )	SESAME		3×10 <sup>4</sup>	0.0	14.3	7432
URANIUM	SESAME		4×10 <sup>8</sup>	0.15	4.0×10 <sup>5</sup>	1540
URETHANE	SESAME		4×10 <sup>9</sup>	0.0099	2.5×10 <sup>4</sup>	7560
VERMICULIT	SESAME		4×10 <sup>8</sup>	0.021	5.4×10 <sup>4</sup>	7520
WATER	SESAME	SESAME	1.8×10 <sup>8</sup>	2.0×10 <sup>-6</sup>	4.0×10 <sup>2</sup>	7150

On the CRAY-1 use only the first eight characters in the above material names.

## VII. LOCATION OF COMPUTER FILES AT LOS ALAMOS

The files needed to execute any of the EOSMOD subroutines are available on the CDC 7600 computers at Los Alamos. For most users, it will be sufficient to attach the EOSMOD library,

MASS GET/EOSMOD/EOSLIB

and load the binary source with their program, that is,

FTN (I = program, GLIB = EOSLIB, ...)

For more advanced users, we list the location of most of the SESAME files which may be useful in complicated situations

File Name	Description	CFS File Location
EOSFTN	FORTTRAN source of EOSMOD	/EOSMOD/EOSFTN
EOSINFO	User information	/EOSMOD/EOSINFO
EOSLIB	Compiled FTN Library file of EOSMOD	/EOSMOD/EOSLIB



<u>File Name</u>	<u>Description</u>	<u>CFS File Location</u>
MIXDATA	T-7 mixture EOS and opacity data file	/EOSMOD/MIXLIB
MIXDIR	directory of MIXLIB	/EOSMOD/MIXDIR
EOSTST	Test program	/EOSMOD/EOSTST
MIXB	T-4 procedure to generate mixture	
HYDSES	Subroutine package for using SESAME in hydrodynamic codes	
SAC		/088077/SES/SAC
SAX	change files in a library	/088077/SES/SAX
SESAME	unclassified EOS data file	public
SESAMEA	classified EOS data file	secret
SESAME	unclassified opacity data file	public
S2MV2	create, modify, and print EOS data	/SESAME/SEM2
S2DV3	plots SESAME data	/SESAME/S2DV3
S2DHELP	help package for SES2D	/SESAME/S2DHELP
DSPLX	computes Hugoniot, isentropes and isobars <sup>12</sup>	/SESAME/DSPLX
S3D	3-D graphics for EOS data	/SESAME/S3D
LSTX	list of current SESAME materials	/SESAME/LSTX

#### VIII. RELATIONSHIPS BETWEEN UNITS

The KUNIT parameter indicates the kind of units the table is to be written in for R, T, P, E, and O. This parameter can have the following integer values and corresponding meanings

KUNIT	0	SESAME EOS Units
		R - grams/cm <sup>3</sup>
		E - megajoules/kilogram (= 10 <sup>10</sup> ergs/gram)
		P - gigapascals (= 10 <sup>10</sup> dyne/cm <sup>2</sup> )
		T - degrees Kelvin
		O - cm <sup>2</sup> /gram <sup>1</sup>
	1	CGS Units
		R - grams/cm <sup>3</sup>
		E - ergs/gram
		P - microbars (= 1 dyne/cm <sup>2</sup> )
		T - degrees Kelvin
		O - cm <sup>2</sup> /gram
	2	Standard International Units (SIU)
		R - kilograms/meter <sup>3</sup>
		E - joules/kilogram (= 10 ergs/gram)
		P - pascals (= 10 dyne/cm <sup>2</sup> )

T - degrees Kelvin  
O - meter<sup>2</sup>/kilogram<sup>2</sup>

3 Hydrox EOS Units

R - grams/cm<sup>3</sup>  
E - megabar cm<sup>3</sup>/gram (= 10<sup>12</sup> ergs/gram)  
P - megabar (= 10<sup>12</sup> dyn/cm<sup>2</sup>)  
T - degrees Kelvin  
O - gram/cm<sup>2</sup>

4 Hydrox Opacity Units

R - grams/cm<sup>3</sup>  
E - megabar cm<sup>2</sup>/gram (= 10<sup>12</sup> ergs/gram)  
P - megabars (= 10<sup>12</sup> dyne/cm<sup>2</sup>)  
T - electron volts  
O - gram/cm<sup>2</sup>

5 SESAME Opacity Units

R - grams/cm<sup>3</sup>  
E - megajoules/kilogram (= 10<sup>10</sup> ergs/gram)  
P - gigapascals (= 10<sup>10</sup> dyne/cm<sup>2</sup>)  
T - electron volts  
O - cm<sup>2</sup>/gram<sup>1</sup>

6 LASNEX Units

R - grams/cm<sup>3</sup>  
E - jerks (= 1 erg/gram)  
P - jerks/cm<sup>3</sup> (= 1 dyne/cm<sup>2</sup>)  
T - keV  
O - cm<sup>2</sup>/gram

The EOS and opacity tables are scaled according to the numerical value of KUNIT when the tables are copied into LCM. The scaling factors used to convert the tables are defined in subroutine EOSCON listed in the Appendixes. This subroutine can be changed easily by the user to write the tables in units other than those provided automatically by the package.

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APPENDIX A

SUBROUTINE LISTING

User Callable Routines

EOSDRE (input R and E, output P and T) . . . . .	24
EOSDRT (input R and T, output P and E) . . . . .	28
EOSIPT (input P and T, output R and E) . . . . .	32
EOSIRT (input R and T, output P and E) . . . . .	35
EOSORT (input R and T, output O) . . . . .	38

```

1      SUBROUTINE EOSDRE (LMAT,R,E,P,T,KEOS,IMATE)
2 C
3 C
4 C      *****
5 C      *
6 C      * PURPOSE-
7 C      * GIVEN THE DENSITY (R) AND ENERGY (E) OF A MATERIAL (LMAT)
8 C      * THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
9 C      * TEMPERATURE (T) USING THE LASL T-4 SESAME EOS ROUTINES
10 C
11 C      * INPUT VARIABLES-
12 C      *
13 C      * LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
14 C      * THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
15 C      * THE MATERIAL BY SETTING LMAT TO THE SESAME
16 C      * NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
17 C
18 C      * R = DENSITY (RHO)
19 C
20 C      * E = INTERNAL ENERGY
21 C
22 C      * KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
23 C      * AND RETRIEVE THE DATA FILE. KEOS HAS FOUR DECIMAL DIGITS.
24 C
25 C      * KEOS = 1000*KBR + 100*KUNIT + 10*KREPE + KFN WHERE
26 C
27 C      * KBR = COMPUTATIONAL MODE FLAG TO INDICATE WHICH
28 C      * QUANTITIES AND THEIR PARTIAL DERIVATIVES ARE TO
29 C      * BE CALCULATED AND RETURNED BY THE PACKAGE.
30 C      * = 0 COMPUTE PRESSURE AND TEMPERATURE
31 C      * = 1 COMPUTE PRESSURE ONLY
32 C      * = 2 COMPUTE TEMPERATURE ONLY
33 C
34 C      * KUNIT= KIND OF UNITS
35 C      * 0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
36 C      * 1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
37 C      * 2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
38 C      * 3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/G,O-CM**2/G
39 C      * 4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
40 C      * 5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
41 C      * 6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
42 C
43 C      * LEGEND-
44 C      * R = DENSITY
45 C      * T = TEMPERATURE
46 C      * O = OPACITY
47 C      * P = PRESSURE
48 C      * E = INTERNAL ENERGY
49 C
50 C      * CC = CUBIC CENTIMETER
51 C      * CM = CENTIMETER
52 C      * DEG. K = DEGREES KELVIN
53 C      * EV = ELECTRON VOLT
54 C      * G = GRAM
55 C      * GPA = GIGA PASCALS
56 C      * J = JOULES
57 C      * JRKS = JERKS
58 C      * KEV = KILO ELECTRON VOLTS
59 C      * KG = KILOGRAM
60 C      * M = METER
61 C      * MBR = MEGABAR
62 C      * MUBR = MICROBAR
63 C      * PA = PASCAL

```

```

63 C      *
64 C      *
65 C      *   KREPE = COMPUTATION FLAG TO INDICATE WHETHER E IS
66 C      *           IS TO BE REPRESENTED AS ENERGY PER UNIT MASS OR ENERGY
67 C      *           PER UNIT VOLUME
68 C      *           0 ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-
69 C      *           UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
70 C      *           1 ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
71 C      *           UNITS OF ERGS/CM**3 WHEN KUNIT = 1. THIS IS THE ENERGY
72 C      *           DENSITY RHO*E COMMONLY COMPUTED IN HYDRODYNAMIC
73 C      *           COMPUTER CODES.
74 C      *
75 C      *   KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES
76 C      *           = 0 RATIONAL APPROXIMATIONS (ACCURATE)
77 C      *           = 1 BILINEAR APPROXIMATIONS (FAST)
78 C      *
79 C      *   IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
80 C      *           IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
81 C      *           PREVIOUSLY LOADED FILE.
82 C      *           =0 CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
83 C      *           IF NOT, SEARCH FOR THE FILE, COMVERT IT TO THE PROPER UNITS
84 C      *           AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
85 C      *           >0 EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
86 C      *           BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSDRE,
87 C      *           EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMATE = 0
88 C      *           BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
89 C      *
90 C      *   OUTPUT VARIABLES-
91 C      *
92 C      *   P = ARRAY OF DIMENSION 3 CONTAINING THE PRESSURE AND
93 C      *           ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
94 C      *           EVEN IF THE PARTIAL DERIVATIVES ARE NOT COMPUTED.
95 C      *
96 C      *   P(1) = PRESSURE
97 C      *   P(2) = DENSITY DERIVATIVE OF THE PRESSURE (DP/DR)
98 C      *   P(3) = TEMPERATURE DERIVATIVE OF THE PRESSURE (DP/DE)
99 C      *
100 C      *   T = ARRAY OF DIMENSION 3 CONTAINING THE TEMPERATURE AND
101 C      *           ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
102 C      *           EVEN IF THE PARTIAL DERIVATIVES ARE NOT COMPUTED
103 C      *
104 C      *   T(1) = INTERNAL TEMPERATURE
105 C      *   T(2) = DENSITY DERIVATIVE OF THE TEMPERATURE (DT/DR)
106 C      *   T(3) = ENERGY DERIVATIVE OF THE TEMPERATURE (DT/DE)
107 C      *
108 C      *   IMATE = INDICATES THE SUCCESS OR FAILURE OF
109 C      *           LOCATING AND LOADING THE DATA FILE FOR LMAT.
110 C      *
111 C      *           = N>0 MATERIAL TABLE NUMBER (SUCCESS)
112 C      *           0 MATERIAL (LMAT) NOT IN LIBRARY
113 C      *           -N (N>1) INSUFFICIENT STORAGE
114 C      *           THE LCM STORAGE MUST BE INCREASED BY AT LEAST
115 C      *           N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
116 C      *
117 C      *   REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
118 C      *
119 C      *   SAMPLE DRIVER PROGRAM-
120 C      *
121 C      *   PROGRAM TST(OUTPUT)
122 C      *   DIMENSION P(3),E(3)
123 C      *   LMAT = "HELIUM"
124 C      *   R = 0.001
125 C      *   E = 1.0

```

```

125 C      *      KEOS = 110
126 C      *      IMATE = 0
127 C      *      CALL EOSDRE(LMAT,R,E,P,T,KEOS,IMATE)
128 C      *      PRINT 10,P(1)
129 C      *      10 FORMAT(" PRESSURE = ",E10.2," MICROBARS")
130 C      *      CALL EXIT
131 C      *      END
132 C      *
133 C      * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
134 C      *
135 C      * REFERENCE- J. M. HYMAN, M. M. KLEIN
136 C      *      EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
137 C      *      EQUATIONS-OF-STATE AND OPACITIES
138 C      *      LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
139 C      *
140 C      * DATE- MARCH 6, 1980
141 C      *
142 C      * *****
143 C
144 C      COMMON BLOCKS FOR THE SESAME EOS ROUTINES
145 C      LEVEL 2, TBLS
146 C      COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
147 C      COMMON /SESDATX/ TBLS(11000)
148 C      COMMON /INTORDX/ KFN
149 C      COMMON /SESINX/ IRC, IDT, RHO, ENERGY, KBR, IFL
150 C      COMMON /SESOUTX/ PRES(3), TEMP(3)
151 C
152 C      COMMON BLOCKS FOR THE EOSMOD ROUTINES
153 C      COMMON /EOSCZ/ LOUT
154 C      COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
155 C      COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
156 C
157 C      DIMENSION T(3), P(3)
158 C      DATA KEOSS /-99/,KBR5/O/,KFNS/O/,LMATS/1H /
159 C
160 C      * *****
161 C
162 C      IDT=1 LOCATOR OF DATA TYPE FOR IR,GETINX(.. IDT,...)
163 C      FOR THE INVERTED SESAME FORMAT
164 C      IDT=1
165 C
166 C      CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
167 C      IF(KEOSS.NE.KEOS.OR.LMAT.NE.LMATS) GO TO 5
168 C      LMATS=LMAT
169 C      KBR=KBR5
170 C      KFN=KFNS
171 C      GO TO 10
172 C      5 CONTINUE
173 C
174 C      CHECK THE VALIDITY OF THE INPUT PARAMETERS
175 C      CALL EOSKUT(KEOS,KBR,KUNIT,KREPE,KFN,KEOSS,KBR5,KFNS,IMATE,IDT
176 C      1 ,IERR)
177 C      IF(IERR.LT.0) GO TO 80
178 C      10 CONTINUE
179 C
180 C      FIND THE MATERIAL
181 C      IF (IMATE.GT.0) GO TO 60
182 C      CALL EOSGET(LMAT,KUNIT,KREPE,IMATE,IDT,IERR)
183 C      IF(IMATE.LE.0.OR.IERR.LT.0) GO TO 80
184 C      60 CONTINUE
185 C
186 C      TRANSFER INPUT CALL PARAMETERS TO COMMON BLOCK

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187 ENERGY=E
188 RHO=R
189 IRC=IR(IMATE,1)
190 C
191 C CALCULATE THE EQUATION OF STATE
192 CALL T4DATIX
193 C + T4DATIX DOES NOT RETURN AN ERROR FLAG FOR DATA OUT OF RANGE
194 C
195 C RESTORE OUTPUT VARIABLES FOR RETURN
196 75 CONTINUE
197 P(1)=PRES(1)
198 P(2)=PRES(2)
199 P(3)=PRES(3)
200 T(1)=TEMP(1)
201 T(2)=TEMP(2)
202 T(3)=TEMP(3)
203 C
204 80 CONTINUE
205 IFLP=IERR
206 RETURN
207 END
```



```

1      SUBROUTINE EOSDRT (LMAT,R,T,P,E,KEOS,IMATE)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      * GIVEN THE DENSITY (R) AND TEMPERATURE (T) OF A MATERIAL (LMAT)
7 C      * THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
8 C      * ENERGY (E) USING THE LASL T-4 SESAME EOS ROUTINES
9 C      *
10 C     *
11 C     * INPUT VARIABLES-
12 C     *
13 C     * LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
14 C     * THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
15 C     * THE MATERIAL BY SETTING LMAT TO THE SESAME
16 C     * NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
17 C     *
18 C     * R = DENSITY (RHO)
19 C     *
20 C     * T = TEMPERATURE
21 C     *
22 C     * KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
23 C     * AND RETRIEVE THE DATA FILE. KEOS HAS FOUR DECIMAL DIGITS.
24 C     *
25 C     * KEOS = 1000*KBR + 100*KUNIT + 10*KREPE + KFN WHERE
26 C     *
27 C     * KBR = COMPUTATIONAL MODE FLAG TO INDICATE WHICH
28 C     * QUANTITIES AND THEIR PARTIAL DERIVATIVES ARE TO
29 C     * BE CALCULATED AND RETURNED BY THE PACKAGE.
30 C     * = 0 COMPUTE PRESSURE AND TEMPERATURE
31 C     * = 1 COMPUTE PRESSURE ONLY
32 C     * = 2 COMPUTE TEMPERATURE ONLY
33 C     *
34 C     * KUNIT= KIND OF UNITS
35 C     * 0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
36 C     * 1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
37 C     * 2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
38 C     * 3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/GM,O-CM**2/G
39 C     * 4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
40 C     * 5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
41 C     * 6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
42 C     *
43 C     * LEGEND-
44 C     * R = DENSITY
45 C     * T = TEMPERATURE
46 C     * O = OPACITY
47 C     * P = PRESSURE
48 C     * E = INTERNAL ENERGY
49 C     *
50 C     * CC = CUBIC CENTIMETER
51 C     * CM = CENTIMETER
52 C     * DEG. K = DEGREES KELVIN
53 C     * EV = ELECTRON VOLT
54 C     * G = GRAM
55 C     * GPA = GIGA PASCALS
56 C     * J = JOULES
57 C     * JRKS = JERKS
58 C     * KEV = KILO ELECTRON VOLTS
59 C     * KG = KILOGRAM
60 C     * M = METER
61 C     * MBR = MEGABAR
62 C     * MUBR = MICROBAR

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63 C      *           PA = PASCAL
64 C      *
65 C      *   KREPE = COMPUTATION FLAG TO INDICATE WHETHER E IS
66 C      *           IS TO BE REPRESENTED AS ENERGY PER UNIT MASS OR ENERGY
67 C      *           PER UNIT VOLUME
68 C      *           0 ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-
69 C      *           UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
70 C      *           1 ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
71 C      *           UNITS OF ERGS/CM**3 WHEN KUNIT = 1. THIS IS THE ENERGY
72 C      *           DENSITY RHO*E COMMONLY COMPUTED IN HYDRODYNAMIC
73 C      *           COMPUTER CODES.
74 C      *
75 C      *   KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES
76 C      *           = 0 RATIONAL APPROXIMATIONS (ACCURATE)
77 C      *           = 1 BILINEAR APPROXIMATIONS (FAST)
78 C      *
79 C      *   IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
80 C      *           IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
81 C      *           PREVIOUSLY LOADED FILE.
82 C      *           =0 CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
83 C      *           IF NOT, SEARCH FOR THE FILE, CONVERT IT TO THE PROPER UNITS
84 C      *           AND COPY IT INTO LCM USING THE STANDARD SESAME FORMAT.
85 C      *           >0 EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
86 C      *           BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSORE,
87 C      *           EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMATE = 0
88 C      *           BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
89 C      *
90 C      *   OUTPUT VARIABLES-
91 C      *
92 C      *   P = ARRAY OF DIMENSION 3 CONTAINING THE PRESSURE AND
93 C      *           ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
94 C      *           EVEN IF THE PARTIAL DERIVATIVES ARE NOT COMPUTED.
95 C      *
96 C      *   P(1) = PRESSURE
97 C      *   P(2) = DENSITY DERIVATIVE OF THE PRESSURE (DP/DR)
98 C      *   P(3) = TEMPERATURE DERIVATIVE OF THE PRESSURE (DP/DT)
99 C      *
100 C      *   E = ARRAY OF DIMENSION 3 CONTAINING THE ENERGY AND
101 C      *           ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
102 C      *           EVEN IF THE PARTIAL DERIVATIVES ARE NOT COMPUTED
103 C      *
104 C      *   E(1) = INTERNAL ENERGY
105 C      *   E(2) = DENSITY DERIVATIVE OF THE ENERGY (DE/DR)
106 C      *   E(3) = TEMPERATURE DERIVATIVE OF THE ENERGY (DE/DT)
107 C      *
108 C      *   IMATE = INDICATES THE SUCCESS OR FAILURE OF
109 C      *           LOCATING AND LOADING THE DATA FILE FOR LMAT.
110 C      *
111 C      *           = N>0 MATERIAL TABLE NUMBER (SUCCESS)
112 C      *           0 MATERIAL (LMAT) NOT IN LIBRARY
113 C      *           -N (N>1) INSUFFICIENT STORAGE
114 C      *           THE LCM STORAGE MUST BE INCREASED BY AT LEAST
115 C      *           N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
116 C      *
117 C      *   REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
118 C      *
119 C      *   SAMPLE DRIVER PROGRAM-
120 C      *
121 C      *           PROGRAM TST(OUTPUT)
122 C      *           DIMENSION P(3),E(3)
123 C      *           LMAT = "HELIUM"
124 C      *           R = 0.001

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125 C      *      T = 300.0
126 C      *      KEOS = 110
127 C      *      IMATE = 0
128 C      *      CALL EOSDRT(LMAT,R,T,P,E,KEOS,IMATE)
129 C      *      PRINT 10,P(1)
130 C      *      10 FORMAT(" PRESSURE = ".E10.2," MICROBARS")
131 C      *      CALL EXIT
132 C      *      END
133 C      *
134 C      * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
135 C      *
136 C      * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
137 C      *
138 C      * REFERENCE- J. M. HYMAN, M. M. KLEIN
139 C      *      EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
140 C      *      EQUATIONS-OF-STATE AND OPACITIES
141 C      *      LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
142 C      *
143 C      * DATE- MARCH 6, 1980
144 C      *
145 C      *****
146 C
147 C      COMMON BLOCKS FOR THE SESAME EOS ROUTINES
148 C      LEVEL 2, TBLS
149 C      COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
150 C      COMMON /SESDATX/ TBLS(11000)
151 C      COMMON /INTORDX/ KFN
152 C      COMMON /SESINX/ IRC, IDT, RHO, TEMP, KBR, IFL
153 C      COMMON /SESOUTX/ PRES(3), ENERGY(3)
154 C
155 C      COMMON BLOCKS FOR THE EOSMOD ROUTINES
156 C      COMMON /EOSCZ/ LOUT
157 C      COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
158 C      COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
159 C      COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
160 C      COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
161 C
162 C      DIMENSION E(3), P(3)
163 C      DATA KEOSS /-99/,KBR5/O/,KFNS/O/,LMATS/1H /
164 C
165 C      *****
166 C
167 C      IDT=3 LOCATOR OF DATA TYPE FOR IR,GETEOSX(.., IDT,...)
168 C      FOR THE STANDARD SESAME FORMAT
169 C      IDT=3
170 C
171 C      CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
172 C      IF(KEOSS.NE.KEOS.OR.LMAT.NE.LMATS) GO TO 5
173 C      LMATS=LMAT
174 C      KBR=KBR5
175 C      KFN=KFNS
176 C      GO TO 10
177 C      5 CONTINUE
178 C
179 C      CHECK THE VALIDITY OF THE INPUT PARAMETERS
180 C      CALL EOSKUT(KEOS,KBR,KUNIT,KREPE,KFN,KEOSS,KBR5,KFNS,IMATE,IDT
181 C      1 ,IERR)
182 C      IF(IERR.LT.0) GO TO 80
183 C      10 CONTINUE
184 C
185 C      FIND THE MATERIAL
186 C      IF (IMATE.GT.0) GO TO 60

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187     CALL EOSGET(LMAT,KUNIT,KREPE,IMATE,IDT,IERR)
188     IF(IMATE.LE.0.OR.IERR.LT.0) GO TO 80
189     60 CONTINUE
190 C
191 C     TRANSFER INPUT CALL PARAMETERS TO COMMON BLOCK
192     TEMP=T
193     RHO=R
194     IRC=IR(IMATE,3)
195 C
196 C     CALCULATE THE EQUATION OF STATE
197     CALL T4DATX
198 C     * T4DATX DOES NOT RETURN AN EROR FLAG FOR DATA OUT OF RANGE
199 C
200     75 CONTINUE
201 C     RESTORE OUTPUT VARIABLES FOR RETURN TO CALL
202     P(1)=PRES(1)
203     P(2)=PRES(2)
204     P(3)=PRES(3)
205     E(1)=ENERGY(1)
206     E(2)=ENERGY(2)
207     E(3)=ENERGY(3)
208 C
209     80 CONTINUE
210     IFLP=IERR
211     RETURN
212     END

```

```

1      SUBROUTINE EOSIPT (LMAT,P,T,R,E,KEOS,IMATE)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      * GIVEN THE PRESSURE (P) AND TEMPERATURE (T) OF A MATERIAL (LMAT)
7 C      * THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
8 C      * ENERGY (E) USING THE LASL T-4 SESAME EQUATION OF STATE ROUTINES
9 C      *
10 C     * AN ITERATIVE METHOD IS USED TO INTERPOLATE THE TABLES
11 C     *
12 C     * INPUT VARIABLES-
13 C     *
14 C     * LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
15 C     * THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
16 C     * THE MATERIAL BY SETTING LMAT TO THE SESAME
17 C     * NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
18 C     *
19 C     * P = PRESSURE
20 C     *
21 C     * T = TEMPERATURE
22 C     *
23 C     * KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
24 C     * AND RETRIEVE THE DATA FILE. KEOS HAS FOUR DECIMAL DIGITS.
25 C     *
26 C     * KEOS = 100*KUNIT + 10*KREPE WHERE
27 C     *
28 C     * KUNIT= KIND OF UNITS
29 C     * 0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
30 C     * 1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
31 C     * 2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
32 C     * 3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/GM,O-CM**2/G
33 C     * 4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
34 C     * 5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
35 C     * 6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
36 C     *
37 C     * LEGEND-
38 C     * R = DENSITY
39 C     * T = TEMPERATURE
40 C     * O = OPACITY
41 C     * P = PRESSURE
42 C     * E = INTERNAL ENERGY
43 C     *
44 C     * CC = CUBIC CENTIMETER
45 C     * CM = CENTIMETER
46 C     * DEG. K = DEGREES KELVIN
47 C     * EV = ELECTRON VOLT
48 C     * G = GRAM
49 C     * GPA = GIGA PASCALS
50 C     * J = JOULES
51 C     * JRKS = JERKS
52 C     * KEV = KILO ELECTRON VOLTS
53 C     * KG = KILOGRAM
54 C     * M = METER
55 C     * MBR = MEGABAR
56 C     * MUBR = MICROBAR
57 C     * PA = PASCAL
58 C     *
59 C     * KREPE = COMPUTATION FLAG TO INDICATE WHETHER E IS
60 C     * IS TO BE REPRESENTED AS ENERGY PER UNIT MASS OR ENERGY
61 C     * PER UNIT VOLUME
62 C     * O ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-

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63 C *          UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
64 C *          1 ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
65 C *          UNITS OF ERGS/CM**3 WHEN KUNIT = 1. THIS IS THE ENERGY
66 C *          DENSITY RHO*E COMMONLY COMPUTED IN HYDRODYNAMIC
67 C *          COMPUTER CODES.
68 C *
69 C * IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
70 C *          IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
71 C *          PREVIOUSLY LOADED FILE.
72 C *          =0 CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
73 C *          IF NOT, SEARCH FOR THE FILE, CONVERT IT TO THE PROPER UNITS
74 C *          AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
75 C *          >0 EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
76 C *          BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSDRE,
77 C *          EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMATE = 0
78 C *          BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
79 C *
80 C * OUTPUT VARIABLES-
81 C *
82 C * R = DENSITY
83 C *
84 C * E = INTERNAL ENERGY
85 C *
86 C * IMATE = INDICATES THE SUCCESS OR FAILURE OF
87 C *          LOCATING AND LOADING THE DATA FILE FOR LMAT.
88 C *
89 C *          = N>0 MATERIAL TABLE NUMBER (SUCCESS)
90 C *          0 MATERIAL (LMAT) NOT IN LIBRARY
91 C *          -N (N>1) INSUFFICIENT STORAGE
92 C *          THE LCM STORAGE MUST BE INCREASED BY AT LEAST
93 C *          N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
94 C *
95 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
96 C *
97 C * SAMPLE DRIVER PROGRAM-
98 C *
99 C *          PROGRAM TST(OUTPUT)
100 C *          DIMENSION P(3),E(3)
101 C *          LMAT = "HELIUM"
102 C *          R = 0.001
103 C *          T = 300.0
104 C *          KEOS = 110
105 C *          IMATE = 0
106 C *          CALL EOSIPT(LMAT,P,T,R,E,KEOS,IMATE)
107 C *          PRINT 10,P(1)
108 C *          10 FORMAT(" DENSITY = ".E10.2." MICROBARS")
109 C *          CALL EXIT
110 C *          END
111 C *
112 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
113 C *
114 C * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
115 C *
116 C * REFERENCE- J. M. HYMAN, M. M. KLEIN
117 C *          EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
118 C *          EQUATIONS-OF-STATE AND OPACITIES
119 C *          LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
120 C *
121 C * DATE- MARCH 6, 1980
122 C *
123 C * *****
124 C

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```

125 C    COMMON BLOCKS FOR THE SESAME EOS ROUTINES
126      LEVEL 2, TBLS
127      COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
128      COMMON /SESDATX/ TBLS(11000)
129      COMMON /SESINX/ DUM(4), KBR, DUM1
130      COMMON /INTOROX/ KFN
131 C
132 C    COMMON BLOCKS FOR THE EOSMOD ROUTINES
133      COMMON /EOSCZ/ LOUT
134      COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
135      COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
136 C
137      DIMENSION R(3), E(3)
138      DATA KEOSS /-99/,KBR5/O/,KFNS/O/,LMATS/1H /
139 C
140 C    *****
141 C
142 C    IDT=1 LOCATOR OF DATA TYPE FOR IR,GETINX(., IDT,...)
143 C    FOR THE INVERTED SESAME FORMAT
144      IDT=1
145 C
146 C    CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
147      IF(KEOSS.NE.KEOS.OR.LMAT.NE.LMATS) GO TO 5
148      LMATS=LMAT
149      KBR=KBR5
150      KFN=KFNS
151      GO TO 10
152      5 CONTINUE
153 C
154 C    CHECK THE VALIDITY OF THE INPUT PARAMETERS
155      CALL EOSKUT(KEOS,KBR,KUNIT,KREPE,KFN,KEOSS,KBR5,KFNS,IMATE,IDT
156      1 ,IERR)
157      IF(IERR.LT.0) GO TO 75
158      10 CONTINUE
159 C
160 C    FIND THE MATERIAL
161      IF (IMATE.GT.0) GO TO 60
162      CALL EOSGET(LMAT,KUNIT,KREPE,IMATE,IDT,IERR)
163      IF(IMATE.LE.0.OR.IERR.LT.0) GO TO 75
164      60 CONTINUE
165 C
166 C    CALCULATE THE EQUATION OF STATE
167      CALL T4PTREX (IR(IMATE,1),1,TBLS,P,T,R,E,IERR)
168 C
169 C    PRINT AN ERROR MESSAGE IF T4PTREX FAILS TO CONVERGE
170      IF (IERR.EQ.0) WRITE(LOUT,80) LMAT,P,T
171      IF (IERR.EQ.0) IMATE=0
172 C
173      75 CONTINUE
174      IFLP=IERR
175      RETURN
176 C
177      80 FORMAT(" FAILED TO CONVERGE WHEN ITERATING ON THE INVERTED",
178      1 /," EOS TABLES IN SUBROUTINE T4PTREX CALLED BY EOSIPT"/,
179      2 " THE REQUESTED VALUES FOR RHO, PRESSURE, TEMPERATURE AND ENERGY"
180      2 ./," MAY BE OUT OF RANGE OR NEAR THE EDGE OF THE TABLE"/,
181      3 " CHECK THE EOSMOD WRITEUP FOR THE DATA RANGE"/,
182      1 " LMAT =",A10,
183      4 " PRESSURE =",1PE12.4," TEMPERATURE =",1PE12.4)
184      END

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```

1      SUBROUTINE EOSIRT (LMAT,R,T,P,E,KEOS,IMATE)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      * GIVEN THE DENSITY (R) AND TEMPERATURE (T) OF A MATERIAL )
7 C      * (LMAT), THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
8 C      * ENERGY (T) USING THE LASL E-4 SESAME EQUATION OF STATE ROUTINES
9 C      *
10 C     * AN ITERATIVE METHOD IS USED TO INTERPOLATE THE TABLES
11 C     * SUBROUTINE EOSDRT USES A FASTER DIRECT METHOD
12 C     *
13 C     * INPUT VARIABLES-
14 C     *
15 C     * LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
16 C     * THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
17 C     * THE MATERIAL BY SETTING LMAT TO THE SESAME
18 C     * NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
19 C     *
20 C     * R = DENSITY (RHO)
21 C     *
22 C     * T = TEMPERATURE
23 C     *
24 C     * KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
25 C     * AND RETRIEVE THE DATA FILE. KEOS HAS FOUR DECIMAL DIGITS,
26 C     *
27 C     * KEOS = 100*KUNIT + 10*KREPE WHERE
28 C     *
29 C     * KUNIT= KIND OF UNITS
30 C     * 0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
31 C     * 1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
32 C     * 2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
33 C     * 3 (HYDROXE) R-G/CC,T-DEG.K,P=MBR,E-MBR*CC/GM,O-CM**2/G
34 C     * 4 (HYDROXD) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
35 C     * 5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
36 C     * 6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
37 C     *
38 C     * LEGEND-
39 C     * R = DENSITY
40 C     * T = TEMPERATURE
41 C     * O = OPACITY
42 C     * P = PRESSURE
43 C     * E = INTERNAL ENERGY
44 C     *
45 C     * CC = CUBIC CENTIMETER
46 C     * CM = CENTIMETER
47 C     * DEG. K = DEGREES KELVIN
48 C     * EV = ELECTRON VOLT
49 C     * G = GRAM
50 C     * GPA = GIGA PASCALS
51 C     * J = JOULES
52 C     * JRKS = JERKS
53 C     * KEV = KILO ELECTRON VOLTS
54 C     * KG = KILOGRAM
55 C     * M = METER
56 C     * MBR = MEGABAR
57 C     * MUBR = MICROBAR
58 C     * PA = PASCAL
59 C     *
60 C     * KREPE = COMPUTATION FLAG TO INDICATE WHETHER T IS
61 C     * IS TO BE REPRESENTED AS ENERGY PER UNIT MASS OR ENERGY
62 C     * PER UNIT VOLUME

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63 C *      O ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-
64 C *      UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL T.
65 C *      ! ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
66 C *      UNITS OF ERGS/CM**3 WHEN KUNIT = 1. THIS IS THE ENERGY
67 C *      DENSITY RHO*T COMMONLY COMPUTED IN HYDRODYNAMIC
68 C *      COMPUTER CODES.
69 C *
70 C * IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
71 C *      IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
72 C *      PREVIOUSLY LOADED FILE.
73 C *      =O CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
74 C *      IF NOT, SEARCH FOR THE FILE, CONVERT IT TO THE PROPER UNITS
75 C *      AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
76 C *      >O EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
77 C *      BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSORE,
78 C *      EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMATE = O
79 C *      BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
80 C *
81 C * OUTPUT VARIABLES-
82 C *
83 C * P = PRESSURE
84 C *
85 C * E = INTERNAL ENERGY
86 C *
87 C * IMATE = INDICATES THE SUCCESS OR FAILURE OF
88 C *      LOCATING AND LOADING THE DATA FILE FOR LMAT.
89 C *
90 C *      = N>O MATERIAL TABLE NUMBER (SUCCESS)
91 C *      O MATERIAL (LMAT) NOT IN LIBRARY
92 C *      -N (N>1) INSUFFICIENT STORAGE
93 C *      THE LCM STORAGE MUST BE INCREASED BY AT LEAST
94 C *      N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
95 C *
96 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
97 C *
98 C * SAMPLE DRIVER PROGRAM-
99 C *
100 C *      PROGRAM TST(OUTPUT)
101 C *      DIMENSION P(3),T(3)
102 C *      LMAT = "HELIUM"
103 C *      R = 0.001
104 C *      T = 300.0
105 C *      KEOS = 110
106 C *      IMATE = 0
107 C *      CALL EOSIRT(LMAT,R,T,P,E,KEOS,IMATE)
108 C *      PRINT 10,P(1)
109 C *      10 FORMAT(" PRESSURE = ",E10.2," MICROBARS")
110 C *      CALL EXIT
111 C *      END
112 C *
113 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
114 C *
115 C * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
116 C *
117 C * REFERENCE- J. M. HYMAN, M. M. KLEIN
118 C *      EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
119 C *      EQUATIONS-OF-STATE AND OPACITIES
120 C *      LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
121 C *
122 C * DATE- MARCH 6, 1980
123 C *
124 C *****

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125 C
126 C   COMMON BLOCKS FOR THE SESAME EOS ROUTINES
127   LEVEL 2, TBLS
128   COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
129   COMMON /SESATX/ TBLS(11000)
130   COMMON /SESINX/ DUM(4), KBR, DUM1
131   COMMON /INTORDX/ KFN
132 C
133 C   COMMON BLOCKS FOR THE EOSMOD ROUTINES
134   COMMON /EOSCZ/ LOUT
135   COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
136   COMMON /EOSC4/ NTABLE, NTABLO, *IFLP, LCNT
137 C
138   DIMENSION P(3), E(3)
139   DATA KEOSS /-99/,KBR5/O/,KFNS/O/,LMATS/1H /
140 C
141 C   *****
142 C
143 C   IDT=1 LOCATOR OF DATA TYPE FOR IR.GETINX(.. IDT....)
144 C   FOR THE INVERTED SESAME FORMAT
145   IDT=1
146 C
147 C   CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
148   IF(KEOSS.NE.KEOS.OR.LMAT,NE.LMATS) GO TO 5
149   LMATS=LMAT
150   KBR=KBR5
151   KFN=KFNS
152   GO TO 10
153   5 CONTINUE
154 C
155 C   CHECK THE VALIDITY OF THE INPUT PARAMETERS
156   CALL EOSKUT(KEOS,KBR,KUNIT,KREPE,KFN,KEOSS,KBR5,KFNS,IMATE,IDT
157   1 ,IERR)
158   IF(IERR.LT.0) GO TO 75
159   10 CONTINUE
160 C
161 C   FIND THE MATERIAL
162   IF (IMATE.GT.0) GO TO 60
163   CALL EOSGET(LMAT,KUNIT,KREPE,IMATE,IDT,IERR)
164   IF(IMATE.LE.0.OR.IERR.LT.0) GO TO 75
165   60 CONTINUE
166 C
167 C   CALCULATE THE EQUATION OF STATE
168   CALL T4RTPEX (IR(IMATE,1),1,TBLS,R,T,P,E,IERR)
169 C
170 C   PRINT AN ERROR MESSAGE IF T4RTPEX FAILED TO CONVERGE
171   IF (IERR.EQ.0) WRITE(LOUT,80) LMAT,R,T
172   IF (IERR.EQ.0) IMATE=0
173 C
174   75 CONTINUE
175   . IFLP=IERR
176   RETURN
177 C
178   80 FORMAT(" FAILED TO CONVERGE WHEN ITERATING ON THE INVERTED",
179   1 /," EOS TABLES IN SUBROUTINE T4PTREX CALLED BY EOSIRT",/,
180   2 " THE REQUESTED VALUES FOR RHO, PRESSURE, TEMPERATURE AND ENERGY"
181   2 ,/," MAY BE OUT OF RANGE OR NEAR THE EDGE OF THE TABLE",/,
182   3 " CHECK THE EOSMOD WRITEUP FOR THE DATA RANGE",/,
183   1 " LMAT =",A10,
184   4 " DENSITY =",1PE12.4," TEMPERATURE =",1PE12.4)
185   END

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1      SUBROUTINE EOSORT (LMAT,R,T,O,KOPC,IMATO)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      * GIVEN THE DENSITY (R) AND TEMPERATURE(T) OF A MATERIAL (LMAT)
7 C      * THIS ROUTINE RETURNS THE OPACITY (O) USING THE LASL
8 C      * HYDOSES (T-4) ROUTINES
9 C      *
10 C     * INPUT VARIABLES-
11 C     *
12 C     * LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
13 C     * THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
14 C     * THE MATERIAL BY SETTING LMAT TO THE SESAME
15 C     * NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
16 C     *
17 C     * R = DENSITY (RHO)
18 C     *
19 C     * T = TEMPERATURE
20 C     *
21 C     * KOPC = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
22 C     * AND RETRIEVE THE DATA FILE. KOPC HAS FOUR DECIMAL DIGITS.
23 C     *
24 C     * KOPC = 100*KUNIT + 10*KREPE + KFN WHERE
25 C     *
26 C     * KUNIT= KIND OF UNITS
27 C     * 0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
28 C     * 1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
29 C     * 2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
30 C     * 3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/GM,O-CM**2/G
31 C     * 4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
32 C     * 5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
33 C     * 6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
34 C     *
35 C     * LEGEND-
36 C     * R = DENSITY
37 C     * T = TEMPERATURE
38 C     * O = OPACITY
39 C     * P = PRESSURE
40 C     * E = INTERNAL ENERGY
41 C     *
42 C     * CC = CUBIC CENTIMETER
43 C     * CM = CENTIMETER
44 C     * DEG. K = DEGREES KELVIN
45 C     * EV = ELECTRON VOLT
46 C     * G = GRAM
47 C     * GPA = GIGA PASCALS
48 C     * J = JOULES
49 C     * JRKS = JERKS
50 C     * KEV = KILO ELECTRON VOLTS
51 C     * KG = KILOGRAM
52 C     * M = METER
53 C     * MBR = MEGABAR
54 C     * MUBR = MICROBAR
55 C     * PA = PASCAL
56 C     *
57 C     * KREPO = COMPUTATIONAL FLAG TO INDICATE WHICH REPRESENTATION
58 C     * TO USE FOR THE OPACITY VARIABLE.
59 C     * 0 OPACITY REPRESENTED AS KAPPA IN DIMENSIONAL
60 C     * UNITS OF LENGTH**2/MASS
61 C     * 1 OPACITY REPRESENTED AS A MEAN-FREE PATH,
62 C     * LAMBDA = 1/(KAPPA*RHO), IN DIMENSIONAL

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63 C      *           UNITS OF LENGTH.
64 C      *
65 C      *   KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES
66 C      *   = 0 RATIONAL APPROXIMATIONS (ACCURATE)
67 C      *   = 1 BILINEAR APPROXIMATIONS (FAST)
68 C      *
69 C      *   IMATO = INDICATES WHETHER TO LOAD THE DATA FILE IF
70 C      *   IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
71 C      *   PREVIOUSLY LOADED FILE.
72 C      *   =0 CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
73 C      *   IF NOT, SEARCH FOR THE FILE, CONVERT IT TO THE PROPER UNITS
74 C      *   AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
75 C      *   >0 EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
76 C      *   BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSORT.
77 C      *   THIS OPTION IS FASTER THAN IMATO = 0
78 C      *   BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
79 C      *
80 C      * OUTPUT VARIABLES-
81 C      *
82 C      *   O = OPACITY
83 C      *
84 C      *   IMATO = INDICATES THE SUCCESS OR FAILURE OF
85 C      *   LOCATING AND LOADING THE DATA FILE FOR LMAT.
86 C      *
87 C      *   = N>0 MATERIAL TABLE NUMBER (SUCCESS)
88 C      *   O MATERIAL (LMAT) NOT IN LIBRARY
89 C      *   -N (N>1) INSUFFICIENT STORAGE
90 C      *   THE LCM STORAGE MUST BE INCREASED BY AT LEAST
91 C      *   N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
92 C      *
93 C      * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
94 C      *
95 C      * SAMPLE DRIVER PROGRAM-
96 C      *
97 C      *   PROGRAM TST(OUTPUT)
98 C      *   DIMENSION P(3),E(3)
99 C      *   LMAT = "HELIUM"
100 C     *   R = 0.001
101 C     *   T = 300.0
102 C     *   KOPC = 500
103 C     *   IMATO = 0
104 C     *   CALL EOSORT(LMAT,R,T,O,KOPC,IMATO)
105 C     *   PRINT 10,P(1)
106 C     *   10 FORMAT(" OPACITY = ",E10.2)
107 C     *   CALL EXIT
108 C     *   END
109 C     *
110 C     * EXTERNALS AND COMMON BLOCKS-
111 C     *   QLOG10 = QUICK VERSION OF ALOG10
112 C     *
113 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
114 C     *
115 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7 LASL
116 C     *
117 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
118 C     *   EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
119 C     *   EQUATIONS-OF-STATE AND OPACITIES
120 C     *   LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
121 C     *
122 C     * DATE- MARCH 6, 1979
123 C     *
124 C     * *****

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125 C
126 C   COMMON BLOCKS FOR THE SESAME EOS ROUTINES
127 C   DIMS TBLS,LCMX,NLBUF,LCFW(,),ZZ()
128   LEVEL 2, TBLS
129   COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
130   COMMON /SESDATX/ TBLS(11000)
131   COMMON /INTORDX/ KFN
132   COMMON /SESINX/ IRC, IDT, RHO, TEMP, KBR, IFL
133   COMMON /SESOUTX/ OPACITY(3), PLANKO(3)
134 C
135 C   COMMON BLOCKS FOR THE EOSMOD ROUTINES
136   COMMON /EDSCZ/ LOUT
137   COMMON /EDSCCO/ TFACO, RFACO, OFACO, KREPO
138   COMMON /EDSC1/ LU41, LU42, LU43, LU44, LU45
139   COMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
140   COMMON /EDSC4/ NTABLE, NTABLO, IFLP, LCNT
141 C
142   DATA KOPCS /-99/, KFNS/O/,LMATS/1H /
143 C
144 C   *****
145 C
146 C   CHECK POSITIVITY OF INPUT PARAMETERS
147   IF((T.GT.O.O).AND.(R.GT.O.O)) GO TO 4
148   IMATO=-1
149 C
150   WRITE(LOUT,20)R,T
151 20 FORMAT(" THE DENSITY =",1E12.4," OR THE TEMPERATURE ="
152 1 .E12.4," IS NONPOSITIVE")
153 C
154   GO TO 75
155 4 CONTINUE
156 C
157 C   SET INITIAL VARIABLES FOR OPACITY TABLES
158 C   IDT=2 LOCATOR OF DATA TYPE FOR IR AND SUB. GETPRX(.,IDT,....)
159   IDT=2
160 C
161 C   CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
162   IF(KOPCS.NE.KOPC.OR.LMAT.NE.LMATS) GO TO 5
163   KFN=KFNS
164   LMATS=LMAT
165   KOPCS=KOPC
166   GO TO 10
167 5 CONTINUE
168 C
169 C   UNSCRAMBLE MULTIPLE FLAG KOPC
170   CALL EOSKUT(KOPC,KDUMMY,KUNIT,KREPO,KFN,KOPCS,KBRS,KFNS,IMATO,IDT
171 1 ,IERR)
172   IF(IERR.LT.O) GO TO 75
173 10 CONTINUE
174 C
175 C   FIND THE MATERIAL
176   IF (IMATO.GT.O) GO TO 60
177   CALL EOSGET(LMAT,KUNIT,KREPO,IMATO,IDT,IERR)
178   IF(IMATO.LE.O.OR.IERR.LT.O) GO TO 75
179 C
180 60 CONTINUE
181 C
182 C   TRANSFER INPUT CALL PARAMETERS TO COMMON BLOCK
183   TEMP=QLOG10(T)
184   RHO=QLOG10(R)
185   KBR=1
186   IRC=IR(IMATO,2)

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187 C
188 C   CALCULATE THE EQUATION OF STATE
189 C   CALL T4DATX
190 C   T4DATX DOES NOT RETURN AN ERROR FLAG
191 C   FOR DATA OUT OF BOUNDS
192 C
193 C   RESTORE OUTPUT VARIABLES FOR RETURN TO CALL
194 C   IFLP=IERR
195 C   O=10.**OPACITY(1)
196 75 CONTINUE
197 C   RETURN
198 C   END
```

## INTERNAL SUBROUTINES

EOSBEG (initializes all the common block variables) . . . .	43
EOSCON (defines the table conversion factors) . . . . .	46
EOSDSL (allows the user to scale the density) . . . . .	49
EOSEFD (finds the EOS table) . . . . .	51
EOSFAS (assigns the input files) . . . . .	54
EOSGET (loads the Sesame EOS data files) . . . . .	56
EOSKUT (checks the validity of KPARM) . . . . .	59
EOSOFD (finds the opacity table) . . . . .	61

```

1      SUBROUTINE EOSBEG
2 C
3 C
4 C      *****
5 C      *
6 C      * PURPOSE-
7 C      *   TO INITIALIZE ALL COMMON BLOCKS IN ONE PLACE OF CODE
8 C      *
9 C      * INPUT VARIABLES-
10 C     * NONE
11 C     *
12 C     * OUTPUT VARIABLES-
13 C     * ALL OUTPUT IS AT COMPILE TIME IN THE COMMON BLOCKS.
14 C     * THIS ALLOWS THE USER AN EASY WAY TO CHANGE THE VARIABLES
15 C     * BY SETTING THEM TO ANY OTHER VALUE AT EXECUTION
16 C     * TIME IN THEIR MAIN PROGRAM
17 C     *
18 C     * -----
19 C     * LOCALLY DEFINED SESAME VARIABLES-
20 C     * TBL5 = ARRAY FOR STORAGE OF THE EOS TABLES
21 C     * LCMX = LENGTH OF THE TBL5 ARRAY
22 C     * NRS = UPPER BOUND ON THE NUMBER OF MAT REGIONS LCFW(NRS,)
23 C     * LCFW = ARRAY USED AS A DIRECTORY BY THE SESAME ROUTINES
24 C     * IR = MATERIAL REGION NUMBER
25 C     * IRC = IR (DEFINED TO PERMIT SUBROUTINE CALL
26 C     * IDS2 = SESAME MATERIAL NUMBER
27 C     * TBL5 = NAME OF AN ARRAY DESIGNATED FOR THE STORAGE OF TABLES
28 C     * LCNT = CRRRENT WORD IN THE ARRAY TBL5
29 C     * LU41 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SES2CL
30 C     * LU42 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SESAME
31 C     * LU43 = UNIT NUMBER ASSIGNED TO SESAME/8 FILES
32 C     * LU44 = UNIT NUMBER ASSIGNED TO MIXLIB (MIXTURES)
33 C     * LU45 = UNIT NUMBER ASSIGNED TO MIXLIB DIRECTORY.
34 C     * KFN = 0 RATIONAL APPROXIMATIONS (ACCURATE)
35 C     * KFN = 1 BILINEAR APPROXIMATIONS (FAST)
36 C     * ZB (OUTPUT FROM GETINX) AT. CHARGE,AT. CHG**2,MASS
37 C     * IDT = DATA TYPE INDICATOR
38 C     * MID (ID) MATERIAL ID =1 INVERSE TABLES =2 OPACITY
39 C     *
40 C     * EXTERNAL FILES TO HANDLE EOS, OPACITIES AND MIXTURES
41 C     * SES2CL - CLASSIFIED SESAME LIBRARY
42 C     * SESAME - CUCLASSIFIED SESAME LIBRARY
43 C     * SESAME - OPACITY TABLE FROM T4
44 C     * MIXLIB - PRIVATE (EOS,OPC) TABLES CREATED BY MIXB(OR MIXER)
45 C     * MIXDIR - DIRECTORY OF MIXTURES ON MIXLIB ( NAME,NO (A10,I3))
46 C     *
47 C     * EXTERNALS AND COMMON BLOCKS-
48 C     * SESAME ROUTINES- S2GET,S2EOS
49 C     * SESAME ROUTINES MATCHKX,TABRANX,INBUFRX,DPACKX,ISRCHKX,
50 C     * T4INTPX,GETINX,RATFN1X,T4DATIX,INV301X,T4RTPEX
51 C     * SESAME COMMON BLOCKS-S2DIRX,RTBLK2X,SESATX,SESINX,SESOUTX,INTORDX
52 C     * EOSMOD COMMON BLOCKS- EOSC1,-7
53 C     * EOSMOD COMMON (ALSO INSERTED INTO GETINX) EOSCCE, EOSCCO
54 C     *
55 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
56 C     *
57 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
58 C     *
59 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
60 C     * EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
61 C     * EQUATIONS-OF-STATE AND OPACITIES
62 C     * LOS ALAMOS SCIENTIFIC LABORATORY RPT..LA-8502-M,1980

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63 C      *
64 C      * DATE- MARCH 6, 1980
65 C      *
66 C      *
67 C
68 C      COMMON BLOCKS FOR THE SESAME EOS ROUTINES
69 C      DIMS TBLS,LCMX,NLBUF,LCFW(,),ZZ()
70 C      MUST BE WATCHED IF CHANGING DIMENSIONS
71 C      APPEAR IN RTBLK2X,SESDATX,S2DIRX,DATA LCMX...
72 C      LEVEL 2, TBLS
73 C      COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
74 C      COMMON /SESDATX/ TBLS(11000)
75 C      COMMON /SESINX/ DUM(4), KBR, DUM1
76 C      COMMON /INTORDX/ KFN
77 C
78 C      COMMON BLOCKS FOR THE EOSMOD ROUTINES
79 C      COMMON /EOSCZ/ LOUT
80 C      COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
81 C      COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
82 C      COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
83 C      COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
84 C      COMMON /EOSC5/ NMAT, LABMAT(60), IDMAT(60), IMATEL
85 C      COMMON /EOSC6/ NMCL, LABMCL(60), IDMCL(60)
86 C      COMMON /EOSC7/ NMATO, LABMO(60), IDMATO(60), IMATOL
87 C
88 C      EOSMOD COMMON BLOCKS USED BY THE MODIFIED SESAME ROUTINES
89 C      COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
90 C      COMMON /EOSCCO/ TFACO, RFACO, OFACO, KREPO
91 C
92 C      DESIGNATE THE OUTPUT FILE FOR THE ERROR MESSAGES
93 C      DATA LOUT/"OUTPUT"/
94 C
95 C      DATA LCMX /11000/, NRS /10/, LCNT /1/, LCFW /30*0/,
96 C      1 IR/180*0/,NTABLE/1/,NTABLO/0/,INIT/0/,IRDIM/60/,KUP/180*(-1)/
97 C
98 C      DATA LU41 /41/, LU42 /42/, LU43 /42/, LU44 /44/, LU45 /45/
99 C      DATA LF41/6HSES2CL/,LF42/6HSESAME/,LF43/6HSESAME/,LF44/6HMIXLIB/
100 C      1 ,LF45/6HMIXDIR/
101 C
102 C      INITIALIZE THE CONTENTS OF THE EOS TABLE SESAME
103 C      DATA NMAT /32/
104 C      DATA LABMAT/
105 C      1 "ALLUVIUM", "ALUMINUM", "AL2O3", "BERYLLIUM", "BORON C",
106 C      1 "BRASS", "COPPER", "DEUTERIUM", "GOLD", "GRANITE",
107 C      2 "HELIUM", "HE", "IRON", "IRON2", "LEAD", "GLID", "GLIH",
108 C      3 "MOLY", "NEON", "NICKEL", "PLATINUM", "POLYE", "POLYS", "SIO2",
109 C      4 "SODIUM", "SS", "STEAM", "UO2", "URANIUM", "URETHANE", "VERMICULIT",
110 C      6 "WATER"/
111 C      DATA IDMAT/7111,3710,7410,2020,7081,
112 C      1 4100,3330,5263,2700,7390,
113 C      2 5760,8180,2140,2145,3200,7240,7370,
114 C      3 2980,5410,3100,3730,7170,7590,
115 C      4 7380,2448,4270,7151,7432,1540,7560,7520,
116 C      5 7150/
117 C
118 C      INITIALIZE THE CONTENTS OF THE CLASSIFIED EOS TABLE SES2CL
119 C      DATA NMCL/O/
120 C      DATA LABMCL/40*(1H )/
121 C      DATA IDMCL/40*O/
122 C
123 C      INITIALIZE THE CONTENTS OF THE OPACITY TABLE SESAME
124 C      DATA NMATO /27/

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```
125     DATA LABMO/"ALUMINUM", "ARGON", "BERYLLIUM", "BORON", "CALCIUM"
126     1 , "CARBON", "CHLORINE", "CHROMIUM", "DEUTERIUM", "HELIUM"
127     2 , "IRON", "LITHIUM", "MAGNESIUM", "NITROGEN"
128     3 , "OXYGEN", "PBX-9502", "PHOSPHORUS", "POTASSIUM", "SiO2"
129     4 , "SILICON", "SODIUM", "SS", "STAINLESS", "SULPHUR"
130     5 , "TITANIUM", "TITANIUM N", "WATER"/
131 C
132     DATA IDMATO/13710, 15170, 12020, 12330, 12030
133     1 , 12180, 15020, 13070, 15263, 15760
134     2 , 12140, 12290, 13080, 15000
135     3 , 15010, 18200, 13910, 12460, 17380
136     4 , 13810, 12448, 14270, 14270, 14010
137     5 , 12960, 16000, 17150/
138 C
139     IMATEL=NMAT
140     IMATOL=NMATO
141 C
142     INIT=1
143     RETURN
144     END
```

```

1      SUBROUTINE EOSCON(KUNIT,KREP,LMAT)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      *   .TO PROVIDE THE APPROPRIATE EOS SCALE FACTORS FOR THE
7 C      *   SYSTEM OF UNITS CHOSEN BY KUNIT (SEE BELOW)
8 C      *
9 C      * INPUT VARIABLES-
10 C     *   KUNIT = KIND OF UNITS
11 C     *   0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
12 C     *   1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
13 C     *   2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
14 C     *   3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/GM,O-CM**2/G
15 C     *   4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
16 C     *   5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
17 C     *   6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
18 C     *
19 C     *   LEGEND-
20 C     *       R = DENSITY
21 C     *       T = TEMPERATURE
22 C     *       O = OPACITY
23 C     *       P = PRESSURE
24 C     *       E = INTERNAL ENERGY
25 C     *
26 C     *       CC = CUBIC CENTIMETER
27 C     *       CM = CENTIMETER
28 C     *       DEG. K = DEGREES KELVIN
29 C     *       EV = ELECTRON VOLT
30 C     *       G = GRAM
31 C     *       GPA = GIGA PASCALS
32 C     *       J = JOULES
33 C     *       JRKS = JERKS
34 C     *       KEV = KILO ELECTRON VOLTS
35 C     *       KG = KILOGRAM
36 C     *       M = METER
37 C     *       MBR = MEGABAR
38 C     *       MUBR = MICROBAR
39 C     *       PA = PASCAL
40 C     *
41 C     *
42 C     * OUTPUT VARIABLES- IN THE COMMON BLOCKS EOSCCE AND EOSCCO
43 C     *   TFACE = TEMPERATURE EOS SCALING FACTOR
44 C     *   RFACE = DENSITY EOS SCALING FACTOR
45 C     *   PFACE = PRESSURE EOS SCALING FACTOR
46 C     *   EFACE = ENERGY EOS SCALING FACTOR
47 C     *
48 C     *   TFACO = TEMPERATURE OPACITY SCALING FACTOR
49 C     *   RFACO = DENSITY OPACITY SCALING FACTOR
50 C     *   OFACO = OPACITY SCALING FACTOR
51 C     *
52 C     * LOCAL VARIABLES-
53 C     *   NONE
54 C     *
55 C     * EXTERNALS AND COMMON BLOCKS-
56 C     *   EOSMOD COMMON BLOCKS- EOSCCE,EOSCCO
57 C     *
58 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
59 C     *
60 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
61 C     *
62 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN

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63 C      *           EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
64 C      *           EQUATIONS-OF-STATE AND OPACITIES
65 C      *           LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
66 C      *
67 C      * DATE- MARCH 6, 1980
68 C      *
69 C      *****
70 C
71      COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
72      COMMON /EOSCCO/ TFACO, RFACO, DFACO, KREPO
73 C
74      KREPE=KREP
75      KREPO=KREP
76 C
77 C      DEFINE THE DEFAULE SESAME VALUES
78 C      THESE ARE THE UNITS THAT THE SESAME DATA FILES ARE WRITTEN IN
79      TFACE=1.
80      RFACE=1.
81      PFACE=1.
82      EFACE=1.
83 C
84      TFACO=4.0646423
85      RFACO=0.
86      DFACO=0.
87 C
88 C      RESET THE SCALE FACTORS THAT ARE DIFFERENT FROM THE DEFAULT
89      KP1=KUNIT+1
90      GO TO (45,40,30,20,15,10,25), KP1
91 C
92 C      LASNEX UNITS
93      25 PFACE=1.E-6
94      EFACE=1.E-6
95      TFACE=8.617346719E-8
96      TFACO=-3.
97      GO TO 50
98 C
99 C      SESAME OPACITY UNITS
100      10 TFACE=8.61703E-5
101      TFACO=0.0
102      GO TO 50
103 C
104 C      HYDROX OPACITY UNITS
105      15 PFACE=.01
106      EFACE=.01
107      TFACE=8.61703E-8
108      TFACO=-3.
109      GO TO 50
110 C
111 C      HYDROX EOS UNITS
112      20 PFACE=.01
113      EFACE=.01
114      GO TO 50
115 C
116 C      STANDARD INTERNATIONAL UNITS (SIU)
117      30 RFACE=1.E+3
118      PFACE=1.E+9
119      EFACE=1.E+6
120      RFACO=3.0
121      DFACO=-1.0
122      GO TO 50
123 C
124 C      CGS UNITS

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```
125 40 PFACE=1.E+10
126 EFACE=1.E+10
127 GO TO 50
128 C
129 C SESAME EOS UNITS
130 45 OFACO=2.0
131 50 CONTINUE
132 C
133 C RESCALE THE TABLES IN THE USER PRESCRIBED SCALE FACTORS
134 DSFAC=1.0
135 CALL EOSDSL(LMAT,DSFAC)
136 EFACE=EFACE*DSFAC
137 RFACE=RFACE/DSFAC
138 RFACO=RFACO/DSFAC
139 C
140 RETURN
141 END
```

```

1      SUBROUTINE EOSDSL(LMAT,DSFAC)
2 C
3 C
4 C      *****
5 C      *
6 C      * PURPOSE-
7 C      * TO ALLOW A USER TO RESCALE THE MASS DENSITY IN
8 C      * THE EOS TABLES. THIS IS A USEFUL ROUTINE TO APPROXIMATE THE
9 C      * EOS AND OPACITIES OF DIFFERENT ISOTOPES AND ISOTOPIC MIXTURES
10 C     * OF THE MATERIALS IN THE SESAME LIBRARY
11 C     *
12 C     * AN ALTERNATE PURPOSE IS TO ALLOW A USER TO DEFINE NEW
13 C     * SCALE FACTORS FOR THE UNITS THE TABLE IS TO BE WRITTEN IN
14 C     *
15 C     * INPUT VARIABLE-
16 C     *   LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
17 C     *           THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
18 C     *           THE MATERIAL BY SETTING LMAT TO THE SESAME
19 C     *           NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
20 C     *
21 C     * OUTPUT VARIABLE-
22 C     *   DSFAC = DENSITY SCALE FACTOR EQUAL TO THE RATIO OF THE
23 C     *           ATOMIC MASSES OF THE MATERIALS. THAT IS,
24 C     *           DSFAC=ATOMIC MASS DENSITY OF THE SESAME MATERIAL)/
25 C     *           (ATOMIC MASS DENSITY OF THE DESIRED MATERIAL)
26 C     *
27 C     * FOR EXAMPLE- THE EOS OF A 60-40 MIXTURE OF DEUTERIUM-TRIDIUM
28 C     * CAN BE APPROXIMATED BY DEFINING DSFAC=2/(0.6*2+0.4*3)=0.833
29 C     * AND CALLING EOSMOD WITH LMAT="DEUTERIUM"
30 C     *
31 C     * INPUT-OUTPUT VARIABLES IN THE COMMON BLOCKS EOSCC2 AND EOSCCO
32 C     *   TFACE = TEMPERATURE EOS SCALING FACTOR
33 C     *   RFACE = DENSITY EOS SCALING FACTOR
34 C     *   PFACE = PRESSURE EOS SCALING FACTOR
35 C     *   EFACE = ENERGY EOS SCALING FACTOR
36 C     *
37 C     *   TFACO = TEMPERATURE OPACITY SCALING FACTOR
38 C     *   RFACO = DENSITY OPACITY SCALING FACTOR
39 C     *   OFACO = OPACITY SCALING FACTOR
40 C     *
41 C     * FOR FURTHER INFORMATION ON THESE FACTORS SEE SUBROUTINE EOSCON
42 C     *
43 C     * EXTERNALS AND COMMON BLOCKS-
44 C     *   EOSMOD COMMON BLOCKS- EOSCCE, EOSCCO
45 C     *
46 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
47 C     *
48 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
49 C     *
50 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
51 C     *           EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
52 C     *           EQUATIONS-OF-STATE AND OPACITIES
53 C     *           LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M, 1980
54 C     *
55 C     * DATE- MARCH 6, 1980
56 C     *
57 C     *****
58 C     COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
59 C     COMMON /EOSCCO/ TFACO, RFACO, OFACO, KREPO
60 C
61 C     DUMMY SUBROUTINE FOR THE PACKAGE.
62 C     IF A USER SUPPLIES THIS ROUTINE THEN THE FACTORS CAN BE

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63 C BE RESET AS DESCRIBED IN THE MANUAL WHEN THE TABLES ARE  
64 C WRITTEN, OR A DENSITY SCALE FACTOR CAN BE INCLUDED  
65 C TO CHANGE THE DENSITY TABLES BY A CONSTANT FACTOR.  
66 C  
67 C FOR EXAMPLE, FOR A 60-40 MIXTURE OF DEUTERIUM-TRITIUM  
68 C THE CODE COULD BE WRITTEN AS-  
69 C IF(LMAT.EQ."DEUTERIUM") DSFAC=0.833  
70 C  
71 C RETURN  
72 C END

```

1      SUBROUTINE EOSEFD (LMAT, ID, IMATE)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      *   TO LOCATE EOS MATERIAL DEFINED BY HOLLERITH NAME
7 C      *   IN APPROPRIATE FILE AND ASSIGN IT A SESAME (OR
8 C      *   PRIVATE ID) EOS NUMBERNUMBER
9 C      *
10 C     * INPUT VARIABLES-
11 C     *   LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
12 C     *   THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
13 C     *   THE MATERIAL BY SETTING LMAT TO THE SESAME
14 C     *   NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
15 C     *
16 C     * OUTPUT VARIABLES-
17 C     *   ID = SESAME OR PRIVATE ID NUMBER AS STORED IN LIBRARY
18 C     *   SESAME ( EOS LIBRARY)
19 C     *   IMATE = LOCATION OF MATERIAL IN ARRAY LABMAT+ MIXDIR
20 C     *   PROVIDED MATERIAL HAS BEEN LOCATED
21 C     *   = 0 IF MATERIAL HAS NOT BEEN LOCATED BY ROUTINE
22 C     *   UPPER BOUND ON IMATE IS 60 (DIM IR(.))
23 C     *
24 C     * LOCAL VARIABLES-
25 C     *   ICFASE = 1 IF THE PUBLIC EOS FILES HAVE BEEN ASSIGNED
26 C     *   ICFASCL = 1 IF THE CLASSIFIED EOS FILES HAVE BEEN ASSIGNED
27 C     *   ICFASP = 1 IF THE PRIVATE EOS FILES HAVE BEEN ASSIGNED
28 C     *
29 C     * EXTERNALS AND COMMON BLOCKS-
30 C     *   EOSMOD COMMON BLOCKS- EOSC1,2,3,5,6
31 C     *   FTN ROUTINES- ENCODE, EOF
32 C     *   LASL T-4 HYDSES ROUTINE- EOSFAS
33 C     *
34 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
35 C     *
36 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
37 C     *
38 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
39 C     *   EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
40 C     *   EQUATIONS-OF-STATE AND OPACITIES
41 C     *   LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
42 C     *
43 C     * DATE- MARCH 6, 1980
44 C     *
45 C     *****
46 C
47     COMMON /EOSCZ/ LOUT
48     COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
49     COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
50     COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
51     COMMON /EOSC5/ NMAT, LABMAT(60), IDMAT(60), IMATEL
52     COMMON /EOSC6/ NMCL, LABMCL(60), IDMCL(60)
53 C
54     DATA ICFASE/O/, ICFASCL/O/, ICFASP/O/, IDCNT/1/
55 C
56 C     CHECK IF THE MATERIAL IS IN THE STANDARD SESAME LIST
57     DO 10 IMATE=1, IMATEL
58     IF (LMAT.EQ.LABMAT(IMATE)) GO TO 40
59 10 CONTINUE
60 C
61 C     CHECK IF THE MATERIAL IS IN THE CLASSIFIED EOS SESAME LIST
62     DO 12 IMATE=1, NMCL

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63      IF (LMAT.EQ.LABMCL(IMATE)) GO TO 45
64      12 CONTINUE
65 C
66 C      *** ASSIGN EOS PRIVATE FILES TO PROGRAM IF AVAILABLE
67      IF(LU45.EQ.4HNONE) GO TO 31
68      IMATE=NMAT
69      IF(ICFASP .GT. 0 ) GO TO 15
70      ICFASP=1
71      CALL EOSFAS(3)
72      15 CONTINUE
73 C
74 C      THE CURRENT PRIVATE LIST DIRECTORY (MIXDIR) IS ON UNIT LU45
75 C      CHECK IF LF45 EXISTS IN LOCAL FILE SPACE
76      CALL FEXIST(LF45,IFFLAG)
77      IF(IFFLAG .EQ. 0 ) GO TO 30
78 C      IFFLAG = 0 FILE NOT IN LOCAL FILE SPACE
79 C      IFFLAG = 1 FILE LOCAL
80 C
81      REWIND LU45
82      20 READ (LU45,80) LABEL,ID
83      IMATE=IMATE+1
84      IF (LMAT.EQ.LABEL) GO TO 50
85      IF (EOF(LU45)) 30,20
86      30 CONTINUE
87      31 CONTINUE
88 C
89 C      CHECK IF THE LMAT IS A SESAME NUMBER
90      IMAT1=AND(SHIFT(LMAT,6),77B)
91 CRAY CODE IMAT1=AND(SHIFT(LMAT,8),377B)
92 C
93      IF(IMAT1.LT.20B) GO TO 35
94      IF(IMAT1.GT.31B) GO TO 35
95 C
96      DECODE(10,32,LMAT) ID
97      32 FORMAT(I4)
98 C
99      DO 33 IMATE=1,IMATEL
100     IF(ID.EQ.IDMAT(IMATE)) GO TO 40
101     33 CONTINUE
102 C
103     IMATEL=IMATEL+1
104     IMATE=IMATEL
105     LABMAT(IMATE)=LMAT
106     IDMAT(IMATE)=ID
107 C
108 C      ASSUME THE MATERIAL IS IN THE STANDARD SESAME LIST
109 C      IF IT IS NOT, A NONFATAL ERROR WILL OCCUR AT A LATER STEP
110     GO TO 40
111 C
112 C      THE MATERIAL WAS NOT FOUND. PRINT AN ERROR MESSAGE
113     35 IMATE=0
114     WRITE(LOUT,75) LMAT
115     GO TO 999
116 C
117     40 ID=IDMAT(IMATE)
118 C
119 C      *** ASSIGN EOS FILES TO PROGRAM
120     IF(ICFASE .GT. 0 ) GO TO 44
121     ICFASE=1
122     CALL EOSFAS(1)
123     44 CONTINUE
124 C

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```

125          GO TO 999
126 C
127          45 ID=IDMCL(IMATE)
128 C
129 C          *** ASSIGN CLASSIFIED EDS FILES TO PROGRAM
130          IF(ICFASCL .GT. 0 ) GO TO 46
131          ICFASCL=1
132          CALL EOSFAS(4)
133          46 CONTINUE
134 C
135          50 CONTINUE
136          IF (IMATE.LE.IRDIM) GO TO 60
137          IMATE=0
138          WRITE(LOUT,90) LMAT
139          60 CONTINUE
140 C
141          999 CONTINUE
142          RETURN
143 C
144          75 FORMAT (" MATERIAL LMAT = ",A10," NOT FOUND")
145          80 FORMAT (A10,I3)
146          90 FORMAT (" IMATE EXCEEDS UPPER BOUND IN SUBROUTINE EOSEFD "
147          1 ,/, " FOR MATERIAL LMAT=",A10)
148          END

```

```

1      SUBROUTINE EOSFAS(KTABLE)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      * TO ASSIGN FILE NAMES TO THE EOS AND OPACITY DATA FILES
7 C      *
8 C      * INPUT VARIABLES-
9 C      * KTABLE = 1 EOS TABLE
10 C     *           2 OPACITY TABLE
11 C     *           3 PRIVATE TABLES
12 C     *           4 SES2CL TABLES
13 C     *
14 C     * OUTPUT VARIABLES-
15 C     * NONE
16 C     *
17 C     * LOCAL VARIABLES-
18 C     * INITE, INITECL, INITO AND INITP ARE SET TO 1 AFTER THE EOS, OPACITY
19 C     * AND PRIVATE FILES HAVE BEEN INITIALIZED
20 C     *
21 C     * EXTERNALS AND COMMON BLOCKS-
22 C     * EOSMOD COMMON BLOCKS- EOSC1, EOSC2
23 C     * FTN SUBROUTINES- QASSIGN, ASSIGN
24 C     *
25 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
26 C     *
27 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
28 C     *
29 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
30 C     *           EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
31 C     *           EQUATIONS-OF-STATE AND OPACITIES
32 C     *           LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
33 C     *
34 C     * DATE- MARCH 6, 1980
35 C     *
36 C     *****
37 C
38     COMMON /EOSCZ/ LOUT
39     COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
40     COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
41     DATA INITE/O/, INITO/O/, INITP/O/, INITECL/O/
42 C
43     GO TO (10,20,30,40), KTABLE
44 C
45 C     EOS TABLE ASSIGNMENT CODING
46     10 CONTINUE
47     IF(INITE.NE.O) GO TO 999
48     IF((INITO.NE.O).AND.(LF42.EQ.LF43)) GO TO 999
49     INITE=1
50     CALL QASSIGN (LU42,LF42,O,O)
51     GO TO 999
52 C
53 C     OPACITY TABLE ASSIGNMENT CODING
54     20 CONTINUE
55     IF(INITO.NE.O) GO TO 999
56     IF((INITE.NE.O).AND.(LF42.EQ.LF43)) GO TO 999
57     INITO=1
58     CALL QASSIGN (LU43,LF43,O,O)
59     GO TO 999
60 C
61 C     PRIVATE TABLES
62     30 CONTINUE

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```
63     IF(INITP.NE.O) GO TO 999
64     INITP=1
65     CALL QASSIGN (LU44,LF44,O,O)
66     CALL ASSIGN (LU45,LF45,4000B)
67     GO TO 999
68 C
69 C     CLASSIFIED EOS TABLE ASSIGNMENT CODING
70     40 CONTINUE
71     IF(INITECL.NE.O) GO TO 999
72     INITECL=1
73     CALL QASSIGN (LU41,LF41,O,O)
74     GO TO 999
75 C
76     999 RETURN
77     END
```

```

1      SUBROUTINE EOSGET(LMAT,KUNIT,KREP,IMAT,IDT,IERR)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      * LOAD THE SESAME EOS DATA FILES
7 C      *
8 C      * INPUT VARIABLES-
9 C      *   LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
10 C     *   THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
11 C     *   THE MATERIAL BY SETTING LMAT TO THE SESAME
12 C     *   NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
13 C     *
14 C     *   KUNIT= KIND OF UNITS
15 C     *   0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
16 C     *   1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
17 C     *   2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
18 C     *   3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/GM,O-CM**2/G
19 C     *   4 (HYDROXD) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
20 C     *   5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
21 C     *   6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
22 C     *
23 C     *   IMAT = INDICATES WHETHER TO LOAD THE DATA FILE IF
24 C     *   IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
25 C     *   PREVIOUSLY LOADED FILE.
26 C     *   =0 CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
27 C     *   IF NOT, SEARCH FOR THE FILE, CONVERT IT TO THE PROPER UNITS
28 C     *   AND COPY IT INTO LCM .
29 C     *   >0 EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
30 C     *   BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSDRE,
31 C     *   EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMAT = 0
32 C     *   BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
33 C     *
34 C     * OUTPUT VARIABLES-
35 C     * IERR = 0 SUCCESSFULL
36 C     *       .NE.O UNSUCCESSFUL
37 C     *
38 C     * TBLS = LCM FILE SPACE WHERE THE EOS TABLES ARE WRITTEN
39 C     *
40 C     * LOCAL VARIABLES-
41 C     *
42 C     * EXTERNALS AND COMMON BLOCKS-
43 C     *   EOSMOD COMMON BLOCKS- EOSC1,EOSC3
44 C     *
45 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
46 C     *
47 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
48 C     *
49 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
50 C     *   EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
51 C     *   EQUATIONS-OF-STATE AND OPACITIES
52 C     *   LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
53 C     *
54 C     * DATE- MARCH 6, 1980
55 C     *
56 C     *****
57 C
58 C     LOAD THE SESAME EOS TABLES IN THE INVERTED FORMAT
59 C
60 C     COMMON BLOCKS FOR THE SESAME EOS ROUTINES
61 C     LEVEL 2, TBLS
62 C     COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)

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63      COMMON /SESDATX/ TBLS(11000)
64      COMMON /SESINX/ DUM(4), KBR, DUM1
65      COMMON /INTORDX/ KFN
66 C
67 C      COMMON BLOCKS FOR THE EOSMOD ROUTINES
68      COMMON /EOSCZ/ LOUT
69      COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
70      COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
71      COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
72 C
73      DIMENSION ZB(3)
74 C
75      IERR=0
76 C
77 C      CALL THE FILE ASSIGNMENT ROUTINE TO ASSIGN READ AND WRITE
78 C      UNIT NUMBERS TO THE INPUT DATA FILES
79      IF(IDT.NE.2) CALL EOSEFD (LMAT, ID, IMAT)
80      IF(IDT.EQ.2) CALL EOSOFD (LMAT, ID, IMAT)
81 C
82      IF (IMAT.LE.0) IERR=-1
83      IF (IMAT.LE.0) GO TO 75
84 C
85 C      CHECK IF THE TABLES HAVE BEEN INITIALIZED
86      IF (IR(IMAT, IDT).GT.0) GO TO 70
87 C
88 C      CONVERT TABLES TO APPROPRIATE UNITS
89      CALL EOSCON(KUNIT, KREP, LMAT)
90 C
91      MIXTST=ID/1000
92 C
93      GO TO (10, 20, 30), IDT
94 C
95 C      LOAD THE EOS TABLES IN THE INVERTED FORMAT (IDT=1)
96 10 CONTINUE
97      IF(MIXTST.NE.0)CALL GETINVX (NTABLE, ID, IDT, TBLS, LCNT, LU42, IERR, ZB)
98      IF(MIXTST.EQ.0)CALL GETINVX (NTABLE, ID, IDT, TBLS, LCNT, LU44, IERR, ZB)
99      GO TO 40
100 C
101 C      LOAD THE OPACITY TABLES (IDT=2)
102 20 CONTINUE
103 C
104      IF (MIXTST.EQ.0) CALL GETRPOX (NTABLO, ID, IDT, TBLS, LCNT, LU44, IERR)
105      IF (MIXTST.NE.0) CALL GETRPOX (NTABLO, ID, IDT, TBLS, LCNT, LU43, IERR)
106      GO TO 40
107 C
108 C      LOAD THE EOS TABLES IN THE STANDARD FORMAT (IDT=3)
109 30 CONTINUE
110      IF(MIXTST.NE.0)CALL GETEOSX (NTABLE, ID, IDT, TBLS, LCNT, LU42, IERR, ZB)
111      IF(MIXTST.EQ.0)CALL GETEOSX (NTABLE, ID, IDT, TBLS, LCNT, LU44, IERR, ZB)
112 40 CONTINUE
113 C
114 C      IERR RETURNS NEGATIVE IF THERE IS AN INITIALIZATION ERROR
115      IF (IERR.GT.0) GO TO 60
116      IF(IERR.LT.0) WRITE(LOUT, 90) IERR
117      IF(IERR.EQ.0) WRITE(LOUT, 100)LMAT
118      IF(IERR.EQ.0) IERR=-2
119      GO TO 75
120 C
121 C      THE TABLES HAS BEEN LOADED, SET THE EOSMOD VARIABLES
122 60 IERR=0
123      IF(IDT.NE.2) GO TO 65
124 C

```

```

125 C      OPACITY TABLE UPDATE
126      IR(IMAT, IDT)=NTABLO
127      KUP(IMAT, IDT)=10*KUNIT+KREP
128      NTABLO=NTABLO+1
129      GO TO 70
130 C
131 C      EOS TABLE UPDATE
132      65 CONTINUE
133      IR(IMAT, IDT)=NTABLE
134      KUP(IMAT, IDT)=10*KUNIT+KREP
135      NTABLE=NTABLE+1
136      70 CONTINUE
137 C
138 C      CHECK IF THE UNITS ARE VALID
139      IF(10*KUNIT+KREP.NE.KUP(IMAT, IDT)) IERR=-6
140 C
141      IF(IERR.EQ.-6) WRITE(LOUT, 80)KUNIT, KREP, KUP(IMAT, 3)
142      80 FORMAT(" THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE"
143      2./, " THE CURRENT VALUES OF KUNIT AND KREP ARE ", 2I4
144      3./, " THE PREVIOUS VALUES OF KUNIT AND KREP WERE", I5)
145 C
146      75 CONTINUE
147      IF(IERR.LT.0) IMAT=IERR
148 C
149      RETURN
150 C
151      90 FORMAT(" INSUFFICIENT STORAGE IN LCM"
152      1 ./, " LACK", I10, " WORDS")
153      100 FORMAT(" UNABLE TO LOCATE MATERIAL ", A10./,
154      1 " IN SUBROUTINE EOSGET")
155      END

```

```

1      SUBROUTINE EOSKUT(KPARM,KBR,KUNIT,KREP,KFN,KEOSS,KBRS,KFNS,IMAT,
2      IDT,IERR)
3 C
4 C      *****
5 C      *
6 C      * PURPOSE-
7 C      * TO CHECK THE VALIDITY OF THE INPUT VALUE FOR KPARM
8 C      * AND TO SEPARATE OUT THE INTERNAL PARTS
9 C      *
10 C     * INPUT VARIABLES-
11 C     * KPARM = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
12 C     *       AND RETRIEVE THE DATA FILE. KPARM HAS FOUR DECIMAL DIGITS.
13 C     *
14 C     * KPARM = 1000*KBR + 100*KUNIT + 10*KREP + KFN WHERE
15 C     *
16 C     * OUTPUT VARIABLES-
17 C     * KBR = COMPUTATIONAL MODE FLAG TO INDICATE WHICH
18 C     *       QUANTITIES AND THEIR PARTIAL DERIVATIVES ARE TO
19 C     *       BE CALCULATED AND RETURNED BY THE PACKAGE.
20 C     *
21 C     * KUNIT= KIND OF UNITS
22 C     *   0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
23 C     *   1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
24 C     *   2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
25 C     *   3 (HYDROXE) R-G/CC,T-DEG.K,P=MBR,E-MBR*CC/GM,O-CM**2/G
26 C     *   4 (HYDROXD) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
27 C     *   5 (SESAMEO) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
28 C     *   6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
29 C     *
30 C     * IF KREP REFERS TO EOS TABLE UNITS
31 C     * KREP = COMPUTATION FLAG TO INDICATE WHETHER E IS
32 C     *       IS TO BE REPRESENTED AS ENERGY PER UNIT MASS OR ENERGY
33 C     *       PER UNIT VOLUME
34 C     *   0 ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-
35 C     *       UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
36 C     *   1 ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
37 C     *       UNITS OF ERGS/CM**3 WHEN KUNIT = 1. THIS IS THE ENERGY
38 C     *       DENSITY RHO*E COMMONLY COMPUTED IN HYDRODYNAMIC
39 C     *       COMPUTER CODES.
40 C     *
41 C     * IF KREP (KREPO) REFERS TO OPACITY TABLE UNITS
42 C     * KREPO = COMPUTATIONAL FLAG TO INDICATE WHICH REPRESENTATION
43 C     *       TO USE FOR THE OPACITY VARIABLE.
44 C     *   0 OPACITY REPRESENTED AS KAPPA IN DIMENSIONAL
45 C     *       UNITS OF LENGTH**2/MASS
46 C     *   1 OPACITY REPRESENTED AS A MEAN-FREE PATH.
47 C     *       LAMBDA = 1/(KAPPA*RHO), IN DIMENSIONAL
48 C     *       UNITS OF LENGTH.
49 C     *
50 C     * KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES
51 C     *       = 0 RATIONAL APPROXIMATIONS (ACCURATE)
52 C     *       = 1 BILINEAR APPROXIMATIONS (FAST)
53 C     *
54 C     * LOCAL VARIABLES-
55 C     *
56 C     * EXTERNALS AND COMMON BLOCKS-
57 C     *
58 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
59 C     *
60 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
61 C     *
62 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN

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63 C      *           EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
64 C      *           EQUATIONS-OF-STATE AND OPACITIES
65 C      *           LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-B502-M,1980
66 C      *
67 C      * DATE- MARCH 6, 1980
68 C      *
69 C      *****
70 C
71      COMMON /EOSCZ/ LOUT
72      COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
73 C
74      IERR=0
75 C
76      IF(INIT.EQ.0) CALL EOSBEG
77 C
78 C      UNSCRAMBLE MULTIPLE FLAG KPARAM
79 C
80      KBR=KPARAM/1000
81      ITEMP=KPARAM-KBR*1000
82 C
83      KUNIT=ITEMP/100
84      ITEMP=ITEMP-KUNIT*100
85 C
86      KREP=ITEMP/10
87      KFN=ITEMP-10*KREP
88 C
89      KEOSS=KPARAM
90      KFNS=KFN
91      KBR5=KBR
92 C
93 C      CHECK IF KPARAM IS A VALID INPUT PARAMATER
94      IF(KPARAM.LT.0) IERR=-2
95      IF(KBR.GT.2) IERR=-2
96      IF(KUNIT.GT.6) IERR=-2
97      IF(KREP.GT.1) IERR=-2
98      IF(KFN.GT.1) IERR=-2
99 C
100 C      PRINT AN ERROR MESSAGE IF KUNIT IS NOT VALID
101      IF(IERR.LT.0) WRITE(LOUT,10)KPARAM,KBR,KUNIT,KREP,KFN
102 10 FORMAT(" ERROR DETECTED IN KPARAM VALUE IN SUBROUTINE EOSKUT"
103 1 ./.," KPARAM=",I5," KBR=",I5," KUNIT=",I5," KREP=",I5," KFN=",I5)
104 C
105 C      CHECK IF THE UNITS HAVE CHANGED
106      IF(IMAT.LE.0) GO TO 90
107      IF(10*KUNIT+KREP.NE.KUP(IMAT,1DT)) IERR=-6
108      IF (IERR.GE.0) GO TO 90
109 C
110      WRITE(LOUT,30)KUNIT,KREP,KUP(IMAT,1DT)
111 30 FORMAT(" THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE"
112 2./," THE CURRENT VALUES OF KUNIT AND KREP ARE ",2I2
113 3./," THE PREVIOUS VALUES OF KUNIT AND KREP WERE",I5)
114 C
115      90 CONTINUE
116 C
117      RETURN
118      END

```

```

1      SUBROUTINE EOSOFD (LMAT,IO,IMATO)
2 C
3 C
4 C      *****
5 C      *
6 C      * PURPOSE-
7 C      * TO OBTAIN MATERIAL NUMBERS FOR OPACITY TABLES
8 C      *
9 C      * INPUT VARIABLES-
10 C     * LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
11 C     * THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
12 C     * THE MATERIAL BY SETTING LMAT TO THE SESAME
13 C     * NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
14 C     *
15 C     * OUTPUT VARIABLES-
16 C     * ID= SESAME OR MIXTUREID NUMBER AS STORED
17 C     * IN SESAME OR MIXDIR(MIXLIB)
18 C     * IMATO = LOCATION OF MATERIAL IN ARRAY LABMO + MIXDIR
19 C     * PROVIDED MATERIAL HAS BEEN LOCATED
20 C     * = 0 IF MATERIAL HAS NOT BEEN LOCATED
21 C     *
22 C     * LOCAL VARIABLES-
23 C     * EOSMOD COMMON BLOCKS- EOSC1,EOSC3
24 C     *
25 C     * EXTERNALS AND COMMON BLOCKS-
26 C     *
27 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
28 C     *
29 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
30 C     * EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
31 C     * EQUATIONS-OF-STATE AND OPACITIES
32 C     * LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
33 C     *
34 C     * DATE- MARCH 6, 1980
35 C     *
36 C     *****
37     COMMON /EOSC2/ LOU1, LOU2, LOU3, LOU4, LOU5
38     COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
39     COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
40     COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
41     COMMON /EOSC7/ NMATO, LABMO(60), IDMATO(60), IMATOL
42 C
43     DATA ICFASO,ICFASP/2*0/
44 C     **** ASSIGN OPACITY FILES TO PROGRAM
45     IF(ICFASO .GT. 0) GO TO 5
46     ICFASO=1
47     CALL EOSFAS(2)
48     5 CONTINUE
49 C
50 C     CHECK IF THE MATERIAL IS IN THE STANDARD SESAME TABLES
51     DO 10 IMATO=1,IMATOL
52     IF (LMAT.EQ.LABMO(IMATO)) GO TO 40
53     10 CONTINUE
54     IMATO=IMATOL
55 C
56 C     *** ASSIGN PRIVATE OPACITY FILES TO PROGRAM
57     IF(ICFASP .GT. 0) GO TO 15
58     ICFASP=1
59     CALL EOSFAS(3)
60     15 CONTINUE
61 C
62 C     THE CURRENT PRIVATE LIST DIRECTORY (MIXDIR) IS ON UNIT LU45

```

```

63 C      CHECK IF LF45 EXISTS IN LOCAL FILE SPACE
64      CALL FEXIST(LF45,IFFLAG)
65      IF(IFFLAG .EQ. 0 ) GO TO 30
66 C      IFFLAG = 0 FILE NOT IN LOCAL FILE SPACE
67 C      IFFLAG = 1 FILE LOCAL
68      REWIND LU45
69      20 READ (LU45,80) LABEL,ID
70      IMATO=IMATO+1
71      IF (LMAT.EQ.LABEL) GO TO 50
72      IF (EOF(LU45)) 30,20
73      30 CONTINUE
74 C
75 C      CHECK IF THE LMAT IS A SESAME NUMBER
76      IMAT1=AND(SHIFT(LMAT,6),77B)
77 CRAY CODE IMAT1=AND(SHIFT(LMAT,8),377B)
78 C
79      IF(IMAT1.LT.20B) GO TO 35
80      IF(IMAT1.GT.31B) GO TO 35
81 C
82      DECODE(10,32,LMAT) ID
83      32 FORMAT(I5)
84 C
85      DO 33 IMATO=1,IMATOL
86      IF(ID.EQ.IDMATO(IMATO)) GO TO 40
87      33 CONTINUE
88 C
89      IMATOL=IMATOL+1
90      IMATO=IMATOL
91      LABMO(IMATO)=LMAT
92      IDMATO(IMATO)=ID
93 C
94 C      ASSUME THE MATERIAL IS IN THE STANDARD SESAME LIST
95 C      IF IT IS NOT, A NONFATAL ERROR WILL OCCUR AT A LATER STEP
96      GO TO 40
97 C
98 C
99 C      THE MATERIAL WAS NOT FOUND. PRINT AN ERROR MESSAGE
100      35 CONTINUE
101      IMATO=0
102      WRITE(LOUT,70) LMAT
103      GO TO 999
104 C
105      40 ID=IDMATO(IMATO)
106      50 CONTINUE
107 C
108      IF (IMATO.LE.IRDIM) GO TO 60
109      IMATO=0
110      WRITE(LOUT,90) LMAT
111      60 CONTINUE
112 C
113      999 CONTINUE
114      RETURN
115 C
116 C***** IMPROVE THESE DIAGNOSTICS*****
117      70 FORMAT (" MATERIAL LMAT = ",A10," NOT FOUND")
118      80 FORMAT (A10,I3)
119      90 FORMAT (" IMATO EXCEEDS UPPER BOUND IN SUBROUTINE EOSOFD "
120      1 ,/, " FOR MATERIAL LMAT=",A10)
121      END

```

## T-4 SUBROUTINES USED BY EOSMOD

DPACKX (packs real numbers) . . . . .	64
GETEOSX (loads the total EOS tables) . . . . .	65
GETINVX (gets inverted EOS tables) . . . . .	67
GETRPOX (loads Rosseland/Planck opacity tables) . . . . .	69
INBUFRX (sequential read) . . . . .	71
INV301X (inverts a 301 table) . . . . .	72
ISRCHKX (index search) . . . . .	74
MATCHKX (checks if material table is loaded) . . . . .	75
RATFN1X (one-dimensional interpolator) . . . . .	76
TABRANX (fetches a given table for a given material from a Sesame II library) . . . . .	78
T4DATIX (interpolates the inverted tables) . . . . .	80
T4DATX (search/interpolate for atomic data as functions of region, density, and temperature) . . . . .	83
T4INTPX (interpolates for a function $z(x,y)$ and its derivatives) . . . . .	86
T4PTREX (computes R and E from inverted table) . . . . .	89
T4RTPEX (computes P and E from inverted table) . . . . .	91

```

1      FUNCTION DPACKX(A,B)
2 C-----
3 C
4 C  FUNCTION  DPACKX
5 C
6 C  PURPOSE   TO DOUBLE PACK ARGUMENTS A AND B INTO A SINGLE WORD
7 C
8 C  REMARKS   SYSTEM DEPENDENT SHIFT FUNCTION
9 C
10 C PROGRAMMER J.ABDALLAH,JR.
11 C
12 C DATE      1 MAY 1979
13 C-----
14 C
15      EQUIVALENCE (I1,X1),(I2,X2)
16      DATA MASK/77777777770000000000B/
17      X1=A
18      X2=B
19      I1=I1.AND.MASK
20      I2=I2.AND.MASK
21      I2=SHIFT(I2,30)
22      I1=I1.OR.I2
23      DPACKX=X1
24      RETURN
25      END

```

```

1      SUBROUTINE GETEOSX(IR,MID,IDT,TBLS,LCNT,LU,IFL,ZB)
2 C*****
3 C
4 C  SUBROUTINE  GETEOSX(IR,MID,IDT,TBLS,LCNT,LU,IFL,ZB)
5 C
6 C  PURPOSE    TO LOAD THE TOTAL EOS TABLES
7 C
8 C  ARGUMENTS  IR      (INPUT)  REGION NO.
9 C            MID     (INPUT)  MATERIAL ID.
10 C           IDT     (INPUT)  DATA TYPE INDICATOR
11 C           TBLS    (OUTPUT)  ARRAY FOR TABLE STORAGE
12 C           LCNT    (I/O)    POSITION IN ARRAY FOR STORING TABLES
13 C           LU      (INPUT)  SESAME LIBRARY UNIT NUMBER
14 C           IFL     (OUTPUT)  ERROR FLAG
15 C                                     = 2 FOR MATERIAL ALREADY LOADED
16 C                                     = 1 FOR SUCCESSFUL LOADING
17 C                                     = 0 FOR DATA NOT FOUND
18 C                                     = - NO. OF EXTRA WORDS NEEDED FOR
19 C                                     STORAGE
20 C           ZB      (OUTPUT)  ATOMIC CHARGE,CHARGE**2,AND MASS
21 C                                     ZB(1) = Z
22 C                                     ZB(2) = Z**2
23 C                                     ZB(3) = A
24 C
25 C
26 C  REMARKS    THIS IS THE LASNEX VERSION OF GETEOS
27 C
28 C            PRESSURES AND ENERGIES ARE DOUBLE PACKED
29 C
30 C            ENERGY DENSITIES ARE PER UNIT VOLUME (NOT MASS)
31 C
32 C  EXTERNALS  MATCHKX,TABRANX,DPACKX
33 C
34 C  PROGRAMMER R.C. ALBERS, T-4
35 C
36 C  DATE      25 APRIL 79
37 C
38 C*****
39      LEVEL 2,TBLS
40      DIMENSION TBLS(1),ZB(3)
41 C  REPLACE FOLLOWING LINE BY USER COMMON BLOCKS
42      COMMON/S2DIRX/LCMX,NRS,LCFW(10,3)
43      COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
44 C
45 C  CHECK TO SEE IF TABLE HAS BEEN LOADED
46      CALL MATCHKX(MID,NRS,LCFW(1,IDT),TBLS(1),IFLG)
47      IF(IFLG.EQ.0) GO TO 10
48      LCFW(IR,IDT) = IFLG
49      IFL=2
50      RETURN
51      10 NLEFT = LCMX - LCNT - 1
52 C
53 C  FETCH THE 201 TABLE
54      CALL TABRANX(MID,201.,LU,TBLS(LCNT+2),NLEFT,IFL)
55      IF(IFL.LE.0) RETURN
56      ZB(1) = TBLS(LCNT+2)
57      ZB(2) = ZB(1)*ZB(1)
58      ZB(3) = TBLS(LCNT+3)
59      RHOO=TBLS(LCNT+4)
60 C
61 C  FETCH THE 301 TABLE
62      CALL TABRANX(MID,301.,LU,TBLS(LCNT+2),NLEFT,IFL)

```

```

63      IF(IFL.LE.O) RETURN
64 C
65 C      CONVERT TO LASNEX UNITS AND DOUBLE PACK
66      NR = TBLS(LCNT+2)
67      NT = TBLS(LCNT+3)
68      DO 20 I=1,NT
69      LOCT = I + (LCNT + NR + 3)
70 20    TBLS(LOCT)=TFACE+TBLS(LOCT)
71      NWDS = NR*NT
72      DO 30 J=1,NR
73      RHO = TBLS(J + LCNT + 3)*RFACE
74      TBLS(J+LCNT+3)=RHO
75      DO 40 I=1,NT
76      LOCP = (I-1)*NR + J + (NT + NR + LCNT + 3)
77      LOCE = LOCP + NWDS
78      PTEM=TBLS(LOCP)*PFACE
79      ETEM=TBLS(LOCE)*EFACE
80      IF(KREPE.EQ.1)ETEM=ETEM+RHO
81      TBLS(LOCP) = DPACKX(PTEM,ETEM)
82 40    CONTINUE
83 30    CONTINUE
84 C
85 C      RESET INPUT PARAMETERS AND END
86      TBLS(LCNT)=FLOAT(MID)
87      TBLS(LCNT+1)=RHOO
88      LCFW(IR, IDT)=LCNT
89      LCNT = LCNT + 2 + IFL - NWDS
90      IFL = 1
91      RETURN
92      END

```

```

1      SUBROUTINE GETINX(IR,MID,IDT,TBLS,LCNT,LU,IFL,ZB)
2 C-----
3 C
4 C  SUBROUTINE  GETINX(IR,MID,IDT,TBLS,LCNT,LU,IFL,ZB)
5 C
6 C  PURPOSE      TO LOAD INVERTED (ENERGY BASED) SESAME II
7 C                EOS TABLES
8 C
9 C  ARGUMENTS   IR          (INPUT)   REGION NO.
10 C            MID         (INPUT)   SESAME MATERIAL ID
11 C            IDT         (INPUT)   DATA TYPE INDICATOR
12 C            TBLS        (INPUT)   TABLE STORAGE ARRAY
13 C            LCNT        (IN/OUT)   POSITION IN ARRAY FOR STORING TABLES
14 C            LU          (INPUT)   SESAME LIBRARY UNIT NO.
15 C            IFL         (OUTPUT)  ERROR FLAG
16 C                                     2=MATERIAL ALREADY LOADED
17 C                                     1=SUCCESSFUL LOADING
18 C                                     0=DATA NOT FOUND
19 C                                     LT.0 FOR - THE NO. OF EXTRA WORDS
20 C                                     NEEDED FOR LOADING
21 C            ZB          (OUTPUT)  ATOMIC CHARGE,CHARGE**2,AND MASS
22 C                                     ZB(1)=Z
23 C                                     ZB(2)=Z**2
24 C                                     ZB(3)=A
25 C
26 C  REMARKS     UNITS - ENERGY      MBAR*CC/GM
27 C                TEMP              DEGREES KELVIN
28 C                DENSITY           GRAMS/CC
29 C                PRESSURE          MBAR
30 C
31 C                THIS ROUTINE WAS ORIGINALLY NAMED GETINV BEFORE THE
32 C                MODIFICATIONS WERE MADE SO IT WOULD INTERFACE WITH EOSMOD
33 C
34 C  EXTERNALS   MATCHKX,TABRANX,INV301X
35 C
36 C  PROGRAMMER  J.ABDALLAH, JR.
37 C
38 C  DATE        13 JUNE 1979
39 C
40 C-----
41 C
42 C      LEVEL 2,TBLS
43 C      COMMON/S2DIRX/LCMX,NRS,LCFW(10,3)
44 C      DIMENSION ZB(3),TBLS(1)
45 C
46 C      OBTAIN THE UNIT CONVERSION FACTORS FROM THE EOSMOD ROUTINES
47 C      COMMON/EOSCCCE/TFACE,RFACE,PFACE,EFACE, KREPE
48 C
49 C      CALL MATCHKX(MID,NRS,LCFW(1,IDT),TBLS(1),IFL)
50 C      IF(IFL.EQ.0) GO TO 10
51 C      LCFW(IR,IDT)=IFL
52 C      IFL=2
53 C      RETURN
54 C 10  NL=LCMX-LCNT-1
55 C . .  FETCH EOS TABLES
56 C      CALL TABRANX(MID,201.,LU,TBLS(LCNT+2),NL,IFL)
57 C      IF(IFL.LE.0) RETURN
58 C      ZB(1)=TBLS(LCNT+2)
59 C      ZB(2)=ZB(1)*ZB(1)
60 C      ZB(3)=TBLS(LCNT+3)
61 C      TBLS(LCNT+1)=TBLS(LCNT+4)
62 C      CALL TABRANX(MID,301.,LU,TBLS(LCNT+2),NL,IFL)

```



```

63      IF(IFL.LE.O) RETURN
64      TBLS(LCNT)=FLOAT(MIO)
65 C    CALL PERTCB(IR,TBLS(LCNT),ZB(1),ZB(3))
66      NR=TBLS(LCNT+2)
67      NT=TBLS(LCNT+3)
68      NRT=NR*NT
69      LOCP=LCNT+3+NR+NT
70 C
71 C . . CONVERT TO DESIRED UNITS
72      DO 30 I=1,NT
73 C
74      TBLS(3+I+LCNT+NR)=TFACE*TBLS(3+I+LCNT+NR)
75 C
76      DO 30 J=1,NR
77 C
78      IF(I.GT.1) GO TO 20
79      TBLS(3+J+LCNT)=TBLS(3+J+LCNT)*RFACE
80      RHO=TBLS(3+J+LCNT)
81 20   LOCP=LOCP+1
82 C
83      TBLS(LOCP)=PFACE*TBLS(LOCP)
84      TBLS(LOCP+NRT)=EFACE*TBLS(LOCP+NRT)
85      IF (KREPE.EQ.1) TBLS(LOCP+NRT)=TBLS(LOCP+NRT)*RHO
86 30   CONTINUE
87 C
88 C . . WINDOW TABLES HERE AND RESET VALUES OF NR NT AND
89 C    NRT IF WINDOWING IS NEEDED
90 C . . INVERT TABLES
91 C . . CHECK TO SEE IF THERE IS ENOUGH ROOM TO INVERT THE TABLES
92 C    NINV IS THE LAST LOCATION NEEDED FOR TABLE INVERSION
93      NINV=LCNT+3+2*NRT+2*NR+4*NT
94      IF(NINV.LE.LCMX) GO TO 40
95      IFL=LCMX-NINV
96      RETURN
97 40   RO=TBLS(LCNT+1)
98      LOC=LCNT+2
99      CALL INV301X(TBLS,LOC,RO,LDS)
100 C . . DOUBLE PACK DEPENDENT VARIABLES
101      LOCP=LCNT+3+NR+NT+NR
102      DO 50 I=1,NRT
103      LOCP=LOCP+1
104      PTEM=TBLS(LOCP)
105      TTEM=TBLS(LOCP+NRT)
106      TBLS(LOCP)=DPACKX(PTEM,TTEM)
107 50   CONTINUE
108 C . . WRAP UP
109      LCFW(IR, IDT)=LCNT
110      LCNT=LCNT+2+LDS-NRT
111      IFL=1
112      RETURN
113      END

```

```

1      SUBROUTINE GETRPOX(IR,MID,IDT,TBLS,LCNT,LU,IFL)
2 C-----
3 C
4 C SUBROUTINE GETRPOX(IR,MID,IDT,TBLS,LCNT,LU,IFL)
5 C
6 C PURPOSE      TO LOAD THE ROSSELAND/PLANCK OPACITY TABLE
7 C
8 C ARGUMENTS   IR      (INPUT)  REGION NO.
9 C            MID     (INPUT)  SESAME MATERIAL ID
10 C           IDT     (INPUT)  DATA TYPE INDICATOR
11 C           TBLS    (OUTPUT)  ARRAY FOR TABLE STORAGE
12 C           LCNT    (I/O)    POSITION IN ARRAY FOR
13 C                               STORING TABLES
14 C           LU      (INPUT)  SESAME LIBRARY UNIT NO.
15 C           IFL     (OUTPUT)  ERROR FLAG
16 C                               =1 FOR SUCCESSFUL LOADING
17 C                               =0 FOR DATA NOT FOUND
18 C                               =-NO. OF EXTRA WORDS NEEDED
19 C                               TO STORE DATA
20 C
21 C REMARKS     THE ROSSELAND/PLANCK TABLE IS DOUBLE PACKED ON DISK.
22 C             THIS VERSION OF GETRPOX IS SPECIALLY DESIGNED FOR
23 C             USE IN HYDROX. IF NECESSARY, MODIFICATIONS
24 C             MAY BE MADE HERE FOR ADAPTATION TO OTHER CODES.
25 C
26 C             THIS ROUTINE WAS ORIGINALLY NAMED GETRPO BEFORE THE
27 C             MODIFICATIONS WERE MADE SO IT WOULD INTERFACE WITH EOSMOD
28 C
29 C EXTERNALS   MATCHKX,TABRANX,DPACKX
30 C             COMMON/EOSCCO/ FROM THE EOSMOD PACKAGE
31 C
32 C PROGRAMMER   J.ABDALLAH, JR.
33 C
34 C MODIFIED BY M. KLEIN, GROUP T-7, 11 DECEMBER 1979
35 C
36 C DATE        24 APRIL 1979
37 C
38 C-----
39           LEVEL 2,TBLS
40           DIMENSION TBLS(1)
41           COMMON/S2DIRX/LCMX,NRS,LCFW(10,3)
42 C
43 C THE COMMON BLOCK EOSCCO PROVIDES THE UNIT CONVERSION FACTORS
44 C FROM THE EOSMOD PACKAGE
45 C COMMON/EOSCCO/ TFACO,RFACO,OFACO,KREPO
46 C
47 C UNITS..TEMP..DEG.K,RHO IN G/CC,OPACITY IN CM**2/G
48 C . . CHECK TO SEE IF TABLE HAS BEEN LOADED ALREADY
49 C CALL MATCHKX(MID,NRS,LCFW(1,IDT),TBLS(1),IFL)
50 C IF(IFL.EQ.0) GO TO 10
51 C LCFW(IR,IDT)=IFL
52 C IFL=2
53 C RETURN
54 10 NLEFT=LCMX-LCNT-1
55 C . . FETCH THE 502 TABLE
56 C CALL TABRANX(MID,502.,LU,TBLS(LCNT+2),NLEFT,IFL)
57 C IF(IFL.LE.0) RETURN
58 C . . CONVERT TO DESIRED UNITS
59 C . . LINES THROUGH STATEMENT 60 MAY BE DELETED IF NO CONVERSION IS
60 C . . REQUIRED
61 C NR=TBLS(LCNT+2)
62 C NT=TBLS(LCNT+3)

```

```

63      IPT=LCNT+3+NR+NT
64      DO 60 K=1,NT
65      TBLS(LCNT+3+NR+K)=TBLS(LCNT+3+NR+K) + TFACO
66      DO 60 J=1,NR
67      IF(K.GT.1) GO TO 50
68      TBLS(LCNT+3+J)=TBLS(LCNT+3+J)+RFACO
69 50    IPT=IPT+1
70      ROP=TBLS(IPT)
71      POP=SHIFT(ROP,30)
72      ROP=ROP+TBLS(LCNT+3+J)*KREPO+DFACO
73      POP=POP+TBLS(LCNT+3+J)*KREPO+DFACO
74      ROP=DPACKX(ROP,POP)
75      TBLS(IPT)=ROP
76 60    CONTINUE
77      TBLS(LCNT)=FLOAT(MID)
78      TBLS(LCNT+1)=FLOAT(IDT)
79      LCFW(IR, IDT)=LCNT
80      LCNT=LCNT+IFL+2
81      IFL=1
82      RETURN
83      END

```

```

1      SUBROUTINE INBUFRX(LU,Z,NW,IAD,IFLG)
2 C -----
3 C
4 C SUBROUTINE INBUFRX(LU,Z,NW,IAD,IFLG)
5 C
6 C PURPOSE      RANDOM I/O READ
7 C
8 C ARGUMENTS   LU   (INPUT)  UNIT NO.
9 C             Z   (OUTPUT)  STORAGE AREA WHERE DAT IS RETURNED
10 C            NW  (INPUT)  NO. OF WORDS TO BE READ
11 C            IAD (INPUT)  STARTING DISK ADDRESS OF DATA
12 C            IFLG (OUTPUT) 0=NORMAL
13 C                        1=EOF ENCOUNTERED
14 C                        -1=ERROR
15 C
16 C REMARKS     NONE
17 C
18 C EXTERNALS   RDISK
19 C
20 C PROGRAMMER  J.ABDALLAH, JR.
21 C
22 C DATE       1 MAY 1979
23 C
24 C -----
25      LEVEL 2,Z
26      CALL RDISK(LU,Z,NW,IAD)
27      IF(UNIT(LU)) 10,20,30
28 10  IFLG=1
29      RETURN
30 20  IFLG=0
31      RETURN
32 30  IFLG=-1
33      RETURN
34      END

```

```

1      SUBROUTINE INV301X(DSTR,LOC,RO,LDS)
2 C-----
3 C
4 C SUBROUTINE: INV301X(DSTR,LOC,RO,LDS)
5 C
6 C PURPOSE: INVERT DATA STRING OF TYPE 301 TO TYPE 302.
7 C
8 C ARGUMENTS: DSTR (INPUT) - TABLE STORAGE ARRAY
9 C LOC (INPUT) - STARTING LOCATION OF DATA STRING
10 C IN DSTR
11 C RO (INPUT) - APPROXIMATE DENSITY OF SOLID
12 C LDS (OUTPUT) - LENGTH OF NEW DATA STRING
13 C
14 C REMARKS: DSTR CAN BE DECLARED LCM ON THE CDC 7600.
15 C THIS ROUTINE OVERWRITES LOCATIONS FOLLOWING THE
16 C DATA STRING. IT EXPANDS THE STRING BY NR WORDS,
17 C WHERE NR IS THE NUMBER OF DENSITIES. IT ALSO
18 C USES 3*NT WORDS AS TEMPORARY STORAGE, WHERE NT
19 C IS THE NUMBER OF TEMPERATURES.
20 C
21 C EXTERNALS: ISRCHKX, RATFN1X
22 C
23 C PROGRAMMER: G. I. KERLEY, T-4.
24 C
25 C DATE: 4 OCTOBER 1977
26 C
27 C-----
28 LEVEL 2,DSTR
29 DIMENSION DSTR(1)
30 COMMON/INTORDX/IFN
31 COMMON/RTBLK1X/LOCX,NR,LOCY,KY,JX,NT,INT,ET,Z(2)
32 INT=1
33 IFNS=IFN
34 IFN=0
35 NR = DSTR(LOC)
36 NT = DSTR(LOC+1)
37 LOCT = 2+NR+LOC
38 LCEC = LOCT+NT
39 LOCP = LCEC+NR
40 LDCE = LOCP+NR+NT
41 LOCN = LOCE+NR+NT
42 IMAX = 2*NR+NT
43 DO 1 I=1,IMAX
44 1 DSTR(LOCN-I) = DSTR(LOCN-I-NR)
45 DO 2 I=1,NR
46 JJ = LOCE+I-1
47 Q = 1.E-12*ABS(DSTR(JJ))
48 DSTR(LCEC+I-1) = DSTR(JJ)
49 DSTR(JJ) = 0.
50 DO 2 J=2,NT
51 JJ = JJ+NR
52 DSTR(JJ) = DSTR(JJ)-DSTR(LCEC+I-1)
53 IF(DSTR(JJ)-DSTR(JJ-NR).LT.Q) DSTR(JJ)=DSTR(JJ-NR)+Q
54 2 CONTINUE
55 I = ISRCHKX(RO,DSTR(LOC+3),NR-2,1,0)+1
56 DO 3 J=1,NT
57 DSTR(LOCN+J-1) = DSTR(LOCT+J-1)
58 3 DSTR(LOCT+J-1) = DSTR(LOCE+I-1+NR*(J-1))
59 DO 5 I=1,NR
60 LOCX = LOCE+I-1
61 DO 4 J=1,NT
62 ET = DSTR(LOCT+J-1)

```

```
63     JX = ISRCHKX(ET,DSTR(LOCX+NR),NT-2,NR,0)+1
64     LOCY = LOCP+I-1
65     KY = NR
66     CALL RATFN1X
67     DSTR(LOCN+NT+J-1) = Z(1)
68     LOCY = LOCN
69     KY = 1
70     CALL RATFN1X
71     4  DSTR(LOCN+NT+NT+J-1) = Z(1)
72     DO 5 J=1,NT
73     DSTR(LOCP+I-1+NR*(J-1)) = DSTR(LOCN+NT+J-1)
74     5  DSTR(LOCX+NR*(J-1)) = DSTR(LOCN+NT+NT+J-1)
75     LDS = LOCN-LOC
76     IFN=IFNS
77     RETURN
78     END
```

```

1      FUNCTION ISRCHKX(X,TBLS,N,K,NSFT)
2 C -----
3 C
4 C  FUNCTION:      ISRCHKX(X,TBLS,N,K,NSFT)
5 C
6 C  PURPOSE:      FIND INDEX OF X IN AN ARRAY TBLS.  TABLE VALUES
7 C                NEED NOT BE CONTIGUOUS AND CAN BE IN EITHER
8 C                ASCENDING OR DESCENDING ORDER.
9 C
10 C ARGUMENTS:   X      (INPUT) - VALUE TO BE LOCATED
11 C              TBLS (INPUT) - TABLE TO BE SEARCHED
12 C              N      (INPUT) - NUMBER OF VALUES TO BE SEARCHED
13 C              K      (INPUT) - SPACING BETWEEN VALUES IN TABLE
14 C              THE VALUE OF THE FUNCTION = INDEX I, WHERE
15 C                TBLS(1+K*(I-1)).LE.X.LT.TBLS(1+K*I), OR
16 C                TBLS(1+K*(I-1)).GE.X.GT.TBLS(1+K*I), OR
17 C                I=0 OR I=N IF X IS OUTSIDE RANGE OF TABLE.
18 C              NSFT (INPUT) - NO. OF BITS THE TABLE VALUES ARE
19 C                TO BE SHIFTED
20 C
21 C REMARKS:      TBLS CAN BE DECLARED LCM ON THE CDC 7600.
22 C
23 C EXTERNALS:    SHIFT.
24 C
25 C PROGRAMMER:   G. I. KERLEY, T-4, J.ABDALLAH, JR.
26 C
27 C DATE:        19 NOVEMBER 1976, REVISED 6 JULY 1979
28 C -----
29 C
30      LEVEL 2, TBLS
31      DIMENSION TBLS(1)
32      ISRCHKX = 0
33      J = N+1
34      KI = 1-K
35      S1=TBLS(1)
36      S1=SHIFT(S1,NSFT)
37      S=TBLS(KI+K*N)
38      S=SHIFT(S,NSFT)
39      S=S-S1
40  1  IF(J-ISRCHKX.EQ.1) RETURN
41      JP = .5*(J+ISRCHKX)
42      S1=TBLS(KI+K*JP)
43      S1=SHIFT(S1,NSFT)
44      IF(S*(X-S1).LT.O.O) GO TO 2
45      ISRCHKX = JP
46      GO TO 1
47  2  J = JP
48      GO TO 1
49      END

```

```

1      SUBROUTINE MATCHKX(MID,NRS,LOC,TBLS,IFLG)
2 C -----
3 C
4 C SUBROUTINE MATCHKX(MID,NRS,LOC,TBLS,IFLG)
5 C
6 C PURPOSE      TO CHECK IF A MATERIAL HAS BEEN
7 C              PREVIOUSLY LOADED
8 C
9 C ARGUMENTS   MID      (INPUT)   SESAME MATERIAL ID
10 C            NRS      (INPUT)   NUMBER OF REGIONS
11 C            LOC      (INPUT)   ARRAY OF FIRST WORD LOCATIONS
12 C                                     IN TABLE STORAGE ARRAY FOR
13 C                                     FOR EACH REGION
14 C            TBLS     (INPUT)   TABLE STORAGE ARRAY
15 C            IFLG     (OUTPUT)  =0 MATERIAL NOT PREVIOUSLY LOADED
16 C                                     GT.0 LOCATION OF TABLE IF LOADED
17 C                                     ALREADY
18 C
19 C REMARKS     NONE
20 C
21 C EXTERNALS   NONE
22 C
23 C PROGRAMMER  J.ABDALLAH, JR.
24 C
25 C DATE       26 APRIL 1979
26 C -----
27 C
28      LEVEL 2, TBLS
29      DIMENSION LOC(1), TBLS(1)
30      IFLG=0
31      DO 100 J=1, NRS
32      LC=LOC(J)
33      IF(LC.LE.0) GO TO 100
34      ITEST=TBLS(LC)
35      IF(MID.EQ.ITEST) GO TO 200
36 100 CONTINUE
37      RETURN
38 200 IFLG=LC
39      RETURN
40      END

```



```

1      SUBROUTINE RATFN1X
2 C-----
3 C
4 C  SUBROUTINE:  RATFN1X
5 C
6 C  PURPOSE:    INTERPOLATE FOR A FUNCTION Y(X) AND ITS
7 C             DERIVATIVE FROM TABLES LOCATED IN ARRAY TBLS.
8 C
9 C             THE ROUTINE ALSO REQUIRES COMMON BLOCKS.
10 C            COMMON/RTBLK1X/LOCX,KX,LOCY,KY,I,N,IP,X,Y(2)
11 C            LOCX = LOCATION OF X VECTOR
12 C            KX  = SPACING OF X VECTOR
13 C            LOCY = LOCATION OF Y VECTOR
14 C            KY  = SPACING OF Y VECTOR
15 C            I   = INDEX OF X AND Y VECTORS
16 C            N   = LENGTH OF X AND Y VECTORS
17 C            X   (INPUT) - INDEPENDENT VARIABLE
18 C            Y   (OUTPUT) - VECTOR OF LENGTH 2, WHERE
19 C            Y(1) = VALUE OF FUNCTION
20 C            Y(2) = DERIVATIVE OF FUNCTION
21 C            IP  (INPUT) - BRANCH PARAMETER
22 C            IP.EQ.0, USE INPUT COEFFICIENTS IN YY
23 C            IP.NE.0, CALCULATE YY VECTOR FIRST
24 C            COMMON/INTORDX/IFN
25 C            IFN (INPUT) - INTERPOLATION TYPE
26 C            IFN.NE.1, RATIONAL FUNCTION
27 C            IFN.EQ.1, LINEAR
28 C            COMMON/SESDATX/TBLS
29 C            TBLS (INPUT) - TABLE STORAGE ARRAY
30 C
31 C
32 C  REMARKS:    UNLESS LINEAR FORM IS SPECIFIED, ROUTINE
33 C             USES RATIONAL FUNCTION METHOD WITH QUADRATIC
34 C             ESTIMATE OF DERIVATIVES AT THE MESH POINTS.
35 C             TBLS CAN BE DECLARED LCM ON THE CDC 7600.
36 C
37 C  EXTERNALS:  NONE, BUT A SEARCH ROUTINE MUST BE CALLED
38 C             FIRST, TO COMPUTE INDEX I.
39 C
40 C  PROGRAMMER: G. I. KERLEY, T-4.
41 C
42 C  DATE:       18 JULY 1979
43 C
44 C-----
45 C            LEVEL 2,TBLS
46 C            DIMENSION YY(6)
47 C            COMMON/SESDATX/TBLS(10000)
48 C            COMMON/INTORDX/IFN
49 C            COMMON/RTBLK1X/LOCX,KX,LOCY,KY,I,N,IP,X,Y(2)
50 C            IF(IFN.EQ.1) GO TO 6
51 C            IF(IP.EQ.0) GO TO 3
52 C  CALCULATE COEFFICIENTS FOR RATIONAL FUNCTION INTERPOLATION
53 C            IX = LOCX+KX*(I-1)
54 C            IY = LOCY+KY*(I-1)
55 C            YY(3) = TBLS(IX)
56 C            YY(4) = TBLS(IX+KX)-YY(3)
57 C            YY(1) = TBLS(IY)
58 C            YY(2) = (TBLS(IY+KY)-YY(1))/YY(4)
59 C            IF(I.EQ.N-1) GO TO 1
60 C            SP = (TBLS(IY+KY+KY)-TBLS(IY+KY))/(TBLS(IX+KX+KX)-TBLS(IX+KX))
61 C            YY(6) = (SP-YY(2))/(TBLS(IX+KX+KX)-YY(3))
62 C            IF(I.GT.1) GO TO 1

```

```

63     IF(YY(2)+((YY(2)-YY(4)+YY(6)).LE.O.) YY(6)=YY(2)/YY(4)
64     YY(5) = YY(6)
65     GO TO 2
66 1    DM = YY(3)-TBLS(IX-KX)
67     SM = (YY(1)-TBLS(IY-KY))/DM
68     YY(5) = (YY(2)-SM)/(YY(4)+DM)
69     IF(I.EQ.N-1) YY(6)=YY(5)
70     IF(I.GT.2) GO TO 2
71     IF(SM+(SM-DM*YY(5)).LE.O.) YY(5)=(YY(2)-SM-SM)/YY(4)
72 2    IF(YY(6).NE.O.) YY(5)=YY(5)/YY(6)
73 C   EVALUATE RATIONAL FUNCTION FROM PRECALCULATED COEFFICIENTS
74 3    Q = X-YY(3)
75     R = YY(4)-Q
76     IF(R.NE.O.) GO TO 4
77     W = 1.
78     GO TO 5
79 4    W = 1.-1./((1.+ABS(YY(5)+Q/R))
80 5    F = YY(6)*(W+YY(5)*(1.-W))
81     Y(1) = YY(1)+Q*(YY(2)-R*F)
82     Y(2) = YY(2)+(Q-R)*F+YY(4)*W*(F-YY(6))
83     RETURN
84 C   CALCULATE COEFFICIENTS FOR LINEAR INTERPOLATION
85 6    IF(IP.EQ.O) GO TO 7
86     IX = LOCX+KX*(I-1)
87     IY = LOCY+KY*(I-1)
88     YY(3) = TBLS(IX)
89     YY(1) = TBLS(IY)
90     YY(2) = (TBLS(IY+KY)-YY(1))/(TBLS(IX+KX)-YY(3))
91 C   CALCULATE LINEAR ESTIMATE FROM PRECALCULATED COEFFICIENTS
92 7    Y(1) = YY(1)+YY(2)*(X-YY(3))
93     Y(2) = YY(2)
94     RETURN
95     END

```

```

1      SUBROUTINE TABRANX(MID,TID,LIB,A,LEN,IFLAG)
2 C-----
3 C
4 C SUBROUTINE TABRANX(MID,TID,LIB,A,LEN,IFLAG)
5 C
6 C PURPOSE TO FETCH A GIVEN TABLE FOR A GIVEN MATERIAL
7 C FROM A SESAME II LIBRARY
8 C
9 C ARGUMENTS MID (INPUT) MATERIAL ID
10 C TID (INPUT) TABLE NO. - IF 0.0 MATERIAL INDEX
11 C IS RETURNED
12 C LIB (INPUT) LIBRARY FILE UNIT NO.
13 C A (OUTPUT) ARRAY FOR TABLE STORAGE
14 C LEN (INPUT) NO. OF WORDS IN A AVAILABLE
15 C IFLAG (OUTPUT) =0 IF TABLE COULD NOT BE LOCATED
16 C GT. 0=NO. OF WORDS IN TABLE RETURNED
17 C LT. 0 - NO. OF ADDITIONAL
18 C WORDS NEEDED
19 C
20 C REMARKS A RANDOM I/O TECHNIQUE IS USED TO LOCATE AND LOAD
21 C THE SPECIFIED TABLE FROM THE SESAME II LIBRARY.
22 C THE MATERIAL INDEX AND ITS ADDRESS ARE TO SAVED
23 C TO HASTEN THE FETCHING OF ANOTHER TABLE FOR THE SAME
24 C MATERIAL AND LIBRARY FILE IN SUBSEQUENT CALLS TO
25 C TABFCH.
26 C
27 C EXTERNALS INBUFRX
28 C
29 C PROGRAMMER J.ABDALLAH.,JR.
30 C
31 C DATE 24 APRIL 1979
32 C
33 C-----
34 LEVEL 2,A
35 DIMENSION A(1),HINDEX(50)
36 DATA HINDEX(1)/0.0/
37 DATA LIBLST/0/
38 IFLAG=0
39 C . . FIND NO. MATERIALS ON LIBRARY
40 IF(LIB.NE.LIBLST) GO TO 50
41 IDLAST=HINDEX(1)
42 IF(IDLAST.NE.MID) GO TO 50
43 IF(TID.NE.O.O) GO TO 230
44 NW=HINDEX(5)
45 NW=NW+NW+5
46 IF(LEN.LT.NW) GO TO 999
47 DO 30 J=1,NW
48 A(J)=HINDEX(J)
49 30 CONTINUE
50 IFLAG=NW
51 RETURN
52 50 LIBLST=LIB
53 NW=1
54 IF(LEN.LT.NW) GO TO 999
55 CALL INBUFRX(LIB,A,1,O,IER)
56 N=A(1)
57 NW=N+N+N
58 IF(LEN.LT.NW) GO TO 999
59 CALL INBUFRX(LIB,A,NW,3,IER)
60 C . . FIND ADDRESS OF MATERIAL FILE
61 DO 100 J=1,N
62 ITTEST=A(J)

```

```

63     IF(ITEST.NE.MID) GO TO 100
64     NW=A(J+N)
65     IAD=A(J+N+N)
66     GO TO 200
67 100 CONTINUE
68     RETURN
69 C . . GET MATERIAL INDEX
70 200 IF(LEN.LT.NW) GO TO 999
71     IADX=IAD
72     CALL INBUFRX(LIB,A,NW,IADX,IER)
73     DO 210 J=1,NW
74     HINDEX(J)=A(J)
75 210 CONTINUE
76     IF(TID.EQ.O.O) GO TO 500
77 230 N=HINDEX(5)
78     DO 300 J=1,N
79     IF(TID.NE.HINDEX(5+J)) GO TO 300
80     NW=HINDEX(5+J+N)
81     IAD=HINDEX(5+J+N+N)
82     IAD=IADX+IAD
83     GO TO 400
84 300 CONTINUE
85     RETURN
86 400 IF(LEN.LT.NW) GO TO 999
87 C . . READ REQUESTED TABLE
88     CALL INBUFRX(LIB,A,NW,IAD,IER)
89 500 IFLAG=NW
90     RETURN
91 999 IFLAG=LEN-NW
92     RETURN
93     END

```

```

1      SUBROUTINE T4DATIX
2 C -----
3 C
4 C SUBROUTINE: T4DATIX
5 C
6 C PURPOSE: SEARCH/INTERPOLATE FOR PRESSURE AND TEMPERATURE
7 C AS FUNCTIONS OF REGION, DENSITY AND ENERGY,
8 C USING PACKED SESAME 2 DATA STRING OF TYPE 302
9 C
10 C COMMON/SESINX/IR, IDT, R, E, IBR, IFL
11 C COMMON/SESOUTX/P(3), T(3)
12 C IR (INPUT) - MATERIAL REGION NUMBER
13 C IDT (INPUT) - DATA TYPE INDICATOR
14 C R (INPUT) - DENSITY
15 C E (INPUT) - INTERNAL ENERGY
16 C P, T (OUTPUT) - PRESSURE, TEMPERATURE VECTORS
17 C P(1), T(1) = PRESSURE AND TEMPERATURE
18 C P(2), T(2) = DENSITY DERIVATIVES
19 C P(3), T(3) = ENERGY DERIVATIVES
20 C IBR (INPUT) - 0=COMPUTE BOTH P AND T
21 C 1=COMPUTE P ONLY
22 C 2=COMPUTE T ONLY
23 C COMMON/SESDATX/TBLS
24 C TBLS (INPUT) - TABLE STORAGE ARRAY
25 C
26 C REMARKS: ADAPTED FROM T-4 SESAME 2 ROUTINES S2EOSI AND
27 C LA302A. PRESSURE AND TEMPERATURE ARE PACKED.
28 C THE SEARCH INDICES AND INTERPOLATION CONSTANTS
29 C ARE SAVED AND REUSED, IF POSSIBLE.
30 C
31 C ***** SYSTEM DEPENDENT FEATURE. THE CONSTANT NSFT
32 C ***** IN STATEMENT 60 SHOULD BE SET TO 1/2 THE BIT
33 C ***** LENGTH. FOR A CDC 7600, NSFT = 30.
34 C
35 C EXTERNALS: RATFN1X (1-D INTERPOLATION ROUTINE)
36 C T4INTPX (2-D INTERPOLATION ROUTINE)
37 C
38 C PROGRAMMER: G. I. KERLEY AND B. I. BENNETT, T-4.
39 C J. ABDALLAH, JR.
40 C
41 C DATE: 2 AUGUST 1978
42 C
43 C -----
44 C LEVEL 2, TBLS
45 C COMMON/S2DIRX/LCMX, NRS, LCFW(10, 3)
46 C COMMON/RTBLK1X/LOCR, KX, LOCE, KY, IRX, N, ISAME, RX1, PX1(2)
47 C COMMON/RTBLK2X/LOCX, IX, NX, LOCY, IY, NY, LOCZ, NZ, NSFT,
48 C $ RX2, ET, PX2(3), INT, IDS, ZZ(96)
49 C COMMON/SESINX/IR, IDT, R, E, IBR, IFL
50 C COMMON/SESOUTX/P(3), T(3)
51 C COMMON/SESDATX/TBLS(10000)
52 C DATA LOCLST, IP, IT/O, 1, 1/
53 C LOC IS POINTER TO START OF DATA STRING FOR REGION IR
54 C LOC = LCFW(IR, IDT)+2
55 C . . THE FOLLOWING LINES OF CODE (THRU NZ=1) CAN BE
56 C MOVED AFTER THE IF(LOC.EQ.LOCLST) GO TO 5
57 C STATEMENT TO MAKE THE SUBROUTINE QUICKER FOR CODES WHICH
58 C DO NOT ALSO USE TEMPERATURE BASED EOS TABLES.
59 C NX = TBLS(LOC)
60 C NY = TBLS(LOC+1)
61 C N = NX
62 C LOCR = LOC+2

```

```

63      KX = 1
64      LOCX = LOCR
65      LOCY = LOCX+NX
66      LOCE = LOCY+NY
67      KY = 1
68      LOCZ = LOCE+NX
69      NZ = 1
70 C   TEST TO SEE IF THE MATERIAL IS THE SAME AS LAST CALL
71      IF(LOC.EQ.LOCLST) GO TO 5
72 C   THE FOLLOWING OPERATIONS DO NOT NEED TO BE REPEATED
73 C   UNLESS A NEW REGION HAS BEEN ENTERED
74      LOCLST=LOC
75      IXLAST = 0
76      IYLAST = 0
77      LOCI = LOCX+NX/2-1
78      LOCJ = LOCY+NY/2-1
79      LOCNX=LOCX+NX-2
80      LOCNY=LOCY+NY-2
81 C   SEARCH FOR DENSITY INDEX
82 5    IF(R.LT.TBLS(LOCI)) GO TO 15
83 10   IF(R.LT.TBLS(LOCI+1)) GO TO 20
84     IF(LOCI.EQ.LOCNX) GO TO 20
85     LOCI=LOCI+1
86     GO TO 10
87 15   IF(LOCI.EQ.LOCX) GO TO 20
88     LOCI=LOCI-1
89     IF(R.LT.TBLS(LOCI)) GO TO 15
90 20   IX=LOCI-LOCX+1
91 C   INTERPOLATE FOR ENERGY ON COLD CURVE. IF ISAME = 0, DENSITY
92 C   INDEX IS THE SAME AS IN THE LAST CALL TO THIS ROUTINE
93     IRX = IX
94     ISAME = IABS(IX-IXLAST)
95     RX1=R
96     CALL RATFN1X
97     ET = AMAX1(0.,E-PX1(1))
98     DECDR = PX1(2)
99     RX2=R
100 C  SEARCH FOR ENERGY INDEX
101     IF(ET.LT.TBLS(LOCJ)) GO TO 35
102 30   IF(ET.LT.TBLS(LOCJ+1)) GO TO 40
103     IF(LOCJ.EQ.LOCNY) GO TO 40
104     LOCJ=LOCJ+1
105     GO TO 30
106 35   IF(LOCJ.EQ.LOCY) GO TO 40
107     LOCJ=LOCJ-1
108     IF(ET.LT.TBLS(LOCJ)) GO TO 35
109 40   IY=LOCJ-LOCY+1
110 C  IF ISAME = 0, DENSITY AND TEMPERATURE INDICES ARE
111 C  THE SAME AS IN THE LAST CALL TO THIS ROUTINE
112     ISAME = ISAME+IABS(IY-IYLAST)
113     IP = MINO(1,IP+ISAME)
114     IT = MINO(1,IT+ISAME)
115     IXLAST = IX
116     IYLAST = IY
117     IDS=(IDT-1)*32+1
118     IF(IBR.EQ.2) GO TO 50
119 C  PRESSURE CALCULATION
120     NSFT = 0
121     INT=IP
122     CALL T4INTPX
123     P(1)=PX2(1)
124     P(2)=PX2(2)-DECDR*PX2(3)

```

```
125     P(3)=PX2(3)
126     IP = 0
127     IF(IBR.EQ.1) RETURN
128 C   TEMPERATURE CALCULATION
129 50   NSFT = 30
130     INT=IT
131     IDS=IDS+16
132     CALL T4INTPX
133     T(1)=PX2(1)
134     T(2)=PX2(2)-DECDR+PX2(3)
135     T(3)=PX2(3)
136     IT = 0
137     RETURN
138     END
```

```

1      SUBROUTINE T4DATX
2 C-----
3 C
4 C  SUBROUTINE:  T4DATX
5 C
6 C  PURPOSE:     SEARCH/INTERPOLATE FOR ATOMIC DATA AS
7 C              FUNCTIONS OF REGION, DENSITY AND TEMPERATURE,
8 C              USING PACKED SESAME 2 DATA STRING
9 C
10 C            COMMON/SESINX/IR, IDT, AR, AT, IBR, IFL
11 C            IR  (INPUT) - MATERIAL REGION NUMBER
12 C            IDT (INPUT) - DATA TYPE INDICATOR
13 C            AR  (INPUT) - DENSITY
14 C            AT  (INPUT) - TEMPERATURE
15 C            IBR (INPUT) - SPECIFIES VARIABLES REQUIRED
16 C                IBR = 0, BOTH VARIABLES
17 C                IBR = 1, FIRST HALF VARIABLE ONLY
18 C                IBR = 2, SECOND HALF VARIABLE ONLY
19 C            IFL (NOT USED)
20 C            COMMON/SESOUTX/P(3),E(3)
21 C            P,E (OUTPUT) - VARIABLES OF FIRST AND SECOND HALF
22 C                OF PACKED DATA STRING
23 C                P(1),E(1) = VALUE OF THE VARIABLES
24 C                P(2),E(2) = DENSITY DERIVATIVES
25 C                P(3),E(3) = TEMPERATURE DERIVATIVES
26 C
27 C  REMARKS:     ADAPTED FROM T-4 SESAME 2 ROUTINES S2EOS AND
28 C              LA301A. TABLES OF 2 VARIABLES ARE DOUBLE PACKED.
29 C              THE SEARCH INDICES AND INTERPOLATION CONSTANTS
30 C              ARE SAVED AND REUSED, IF POSSIBLE.
31 C
32 C            ***** SYSTEM DEPENDENT FEATURE.  THE CONSTANT NSFT
33 C            ***** IN STATEMENT 60 SHOULD BE SET TO 1/2 THE BIT
34 C            ***** LENGTH.  FOR A CDC 7600, NSFT = 30.
35 C
36 C  EXTERNALS:  T4INTPX (RATIONAL FUNCTION AND BI LINEAR INTERPOLATION)
37 C              INTERPOLATION COEFFICIENTS FROM A PREVIOUS
38 C              CALL TO THE ROUTINE CAN BE REUSED.
39 C
40 C  PROGRAMMER:  G. I. KERLEY, T-4., J. ABDALLAH, T-4
41 C
42 C  DATE:       11 JULY 1978, REVISED 27 APRIL 1979
43 C-----
44 C
45 C            LEVEL 2, TBLS
46 C            DIMENSION LOCLST(3), IXLAST(3), IYLAST(3),
47 C            1 IPLAST(3), IELAST(3)
48 C            COMMON/S2DIRX/LCMX, NRS, LCFW(10,3)
49 C            COMMON/RTBLK2X/LOCX, IX, NX, LOCY, IY, NY, LOCZ, NZ, NSFT,
50 C            1 R, T, Z(3), INT, IDS, ZZ(96)
51 C            COMMON/SESDATX/TBLS(10000)
52 C            COMMON/SESINX/IR, IDT, AR, AT, IBR, IFL
53 C            COMMON/SESOUTX/P(3), E(3)
54 C            DATA IPLAST/3*0/
55 C            DATA IELAST/3*1/
56 C            DATA LOCLST/3*0/
57 C  LOC IS POINTER TO START OF DATA STRING FOR REGION IR
58 C  LOC = LCFW(IR, IDT)+2
59 C  NZ=1
60 C  NX=TBLS(LOC)
61 C  NY=TBLS(LOC+1)
62 C  LOCX=LOC+2

```



```

63     LOCY=LOCX+NX
64     LOCZ=LOCY+NY
65     LOCNX=LOCX+NX-2
66     LOCNY=LOCY+NY-2
67     IF(LOC.EQ.LOCLST(IDT)) GO TO 2
68     LOCLST(IDT)=LOC
69     IX=NX/2
70     IY=NY/2
71     IXLAST(IDT)=0
72     IYLAST(IDT)=0
73     GO TO 3
74 2   IX=IXLAST(IDT)
75     IY=IYLAST(IDT)
76 3   R=AR
77     T=AT
78 C   SEARCH FOR DENSITY INDEX
79 5   LOCI=LOCX+IX-1
80     IF(R.LT.TBLS(LOCI)) GO TO 15
81 10  IF(R.LT.TBLS(LOCI+1)) GO TO 20
82     IF(LOCI.EQ.LOCNX) GO TO 20
83     LOCI=LOCI+1
84     GO TO 10
85 15  IF(LOCI.EQ.LOCX) GO TO 20
86     LOCI=LOCI-1
87     IF(R.LT.TBLS(LOCI)) GO TO 15
88 20  IX=LOCI-LOCX+1
89 C   SEARCH FOR TEMPERATURE INDEX
90     LOCI=LOCY+IY-1
91     IF(T.LT.TBLS(LOCI)) GO TO 35
92 30  IF(T.LT.TBLS(LOCI+1)) GO TO 40
93     IF(LOCI.EQ.LOCNY) GO TO 40
94     LOCI=LOCI+1
95     GO TO 30
96 35  IF(LOCI.EQ.LOCY) GO TO 40
97     LOCI=LOCI-1
98     IF(T.LT.TBLS(LOCI)) GO TO 35
99 40  IY=LOCI-LOCY+1
100 C IF ISAME = 0, DENSITY AND TEMPERATURE INDICES ARE
101 C THE SAME AS IN THE LAST CALL TO THIS ROUTINE
102     ISAME = IABS(IX-IXLAST(IDT))+IABS(IY-IYLAST(IDT))
103     IXLAST(IDT) = IX
104     IYLAST(IDT) = IY
105     IDS=(IDT-1)*32+1
106     IPLAST(IDT)=MINO(1,IPLAST(IDT)+ISAME)
107     IELAST(IDT)=MINO(1,IELAST(IDT)+ISAME)
108     IF(IBR.EQ.2) GO TO 50
109     INT=IPLAST(IDT)
110     NSFT=0
111     CALL T4INTPX
112     P(1)=Z(1)
113     P(2)=Z(2)
114     P(3)=Z(3)
115     IPLAST(IDT)=0
116     IF(IBR.EQ.1) RETURN
117 50  INT=IELAST(IDT)
118     IDS=IDS+16
119     NSFT=30
120     CALL T4INTPX
121     E(1)=Z(1)
122     E(2)=Z(2)
123     E(3)=Z(3)
124     IELAST(IDT)=0

```

125      RETURN  
126      END

```

1      SUBROUTINE T4INTPX
2 C-----
3 C
4 C  SUBROUTINE:  T4INTPX
5 C
6 C  PURPOSE:    INTERPOLATE FOR A FUNCTION Z(X,Y) AND ITS
7 C              DERIVATIVES FROM TABLES LOCATED IN ARRAY TBL5.
8 C
9 C              THE ROUTINE REQUIRES COMMON BLOCKS,
10 C             COMMON/RTBLK2X/LOCX,IX,NX,LOCY,IY,NY,LOCZ,NZ,NSFT,
11 C              X,Y,Z(3),IP,IDS,ZZ
12 C             LOCX = LOCATION OF X VECTOR
13 C             IX  = INDEX OF X VECTOR
14 C             NX  = LENGTH OF X VECTOR
15 C             LOCY = LOCATION OF Y VECTOR
16 C             IY  = INDEX OF Y VECTOR
17 C             NY  = LENGTH OF Y VECTOR
18 C             LOCZ = LOCATION OF Z(X,Y) ARRAY
19 C             NZ  = SPACING OF Z ARRAY
20 C             NSFT = BIT SHIFT PARAMETER
21 C             X,Y (INPUT) - INDEPENDENT VARIABLES
22 C             Z   (OUTPUT) - VECTOR OF LENGTH 3, WHERE
23 C             Z(1) = VALUE OF FUNCTION
24 C             Z(2) = X DERIVATIVE OF FUNCTION
25 C             Z(3) = Y DERIVATIVE OF FUNCTION
26 C             ZZ (IN/OUT) - COEFFICIENT VECTOR OF LENGTH 16
27 C             IP  (INPUT) - BRANCH PARAMETER
28 C             IP.EQ.O, USE INPUT COEFFICIENTS IN ZZ
29 C             IP.NE.O, CALCULATE ZZ VECTOR FIRST
30 C             IDS (INPUT) - DISPLACEMENT INTO ZZ FOR COEFFS.
31 C             TO BE USED
32 C             COMMON/INTORDX/IFN.
33 C             IFN (INPUT) - INTERPOLATION TYPE
34 C             IFN.NE.1, RATIONAL FUNCTION
35 C             IFN.EQ.1, BILINEAR
36 C             COMMON/SES DATX/TBL5
37 C             TBL5 IS THE TABLE STORAGE ARRAY
38 C
39 C
40 C  REMARKS:    UNLESS BILINEAR FORM IS SPECIFIED, ROUTINE
41 C              USES RATIONAL FUNCTION METHOD WITH QUADRATIC
42 C              ESTIMATE OF DERIVATIVES AT THE MESH POINTS.
43 C              TBL5 CAN BE DECLARED LCM ON THE CDC 7600.
44 C
45 C             ***** SYSTEM DEPENDENT FEATURE.  THE Z-ARRAY CAN BE
46 C             ***** DOUBLE PACKED.  PARAMETER NSFT SPECIFIES THE
47 C             ***** NUMBER OF BITS TO BE SHIFTED WHEN UNPACKING THE
48 C             ***** RIGHT HALF OF THE WORD.  THIS ROUTINE USES
49 C             ***** THE LASL SHIFT FUNCTION
50 C
51 C  EXTERNALS:  NONE, BUT A SEARCH ROUTINE MUST BE CALLED
52 C              FIRST, TO COMPUTE INDICES IX AND IY.
53 C
54 C  PROGRAMMER: G. I. KERLEY, T-4., J. ABDALLAH,T-4.
55 C
56 C  DATE:      01 AUG 1979
57 C
58 C-----
59      LEVEL 2,TBL5
60      COMMON/RTBLK2X/LOCX,IX,NX,LOCY,IY,NY,LOCZ,NZ,NSFT,X,Y,Z(3),
61      $ IP,IDS,ZZ(96)
62      COMMON/INTORDX/IFN

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63      COMMON/SESDATX/TBLS(10000)
64 C   CALCULATE COEFFICIENTS FOR RATIONAL INTERPOLATION
65     IF(IFN.EQ.1) GO TO 13
66     IF(IP.EQ.0) GO TO 8
67     I = LOCX+IX-1
68     IZ = LOCZ+NZ*(IX-1+NX*(IY-1))
69     KZ = NZ
70     IBR = IX
71     NBR = NX-IX
72     ZZ(IDS+4) = TBLS(I)
73     DO 7 K=1,4
74     KI=IDS+K-1
75     IF(K.LT.4) GO TO 1
76     IZ = IZ+NZ
77     GO TO 4
78 1   IF(K.LT.3) GO TO 2
79     ZZ(IDS+6) = D
80     I = LOCY+IY-1
81     KZ = KZ+NX
82     IZ = IZ-KZ
83     IBR = IY
84     NBR = NY-IY
85     ZZ(IDS+5) = TBLS(I)
86     GO TO 3
87 2   IF(K.LT.2) GO TO 3
88     IZ = IZ+NX*NZ
89     GO TO 4
90 3   D = TBLS(I+1)-TBLS(I)
91 4   ZZ(KI)=SHIFT(TBLS(IZ),NSFT)
92     S=SHIFT(TBLS(IZ+KZ),NSFT)
93     S = (S-ZZ(KI))/D
94     IF(NBR.EQ.1) GO TO 5
95     SP=SHIFT(TBLS(IZ+KZ+KZ),NSFT)
96     SP = (SP-D*S-ZZ(KI))/(TBLS(I+2)-TBLS(I+1))
97     G2 = (SP-S)/(TBLS(I+2)-TBLS(I))
98     IF(IBR.GT.1) GO TO 5
99     IF(S*(S-D*G2).LE.O.) G2=S/D
100    G1 = G2
101    GO TO 6
102 5   DM = TBLS(I)-TBLS(I-1)
103     SM=SHIFT(TBLS(IZ-KZ),NSFT)
104     SM = (ZZ(KI)-SM)/DM
105     G1 = (S-SM)/(D+DM)
106     IF(NBR.EQ.1) G2=G1
107     IF(IBR.GT.2) GO TO 6
108     IF(SM*(SM-DM*G1).LE.O.) G1=(S-SM-SM)/D
109 6   IF(G2.NE.O.) G1=G1/G2
110     ZZ(KI+8) = G1
111 7   ZZ(KI+12) = G2
112     ZZ(IDS+7)=D
113     ZZ8=ZZ(IDS+7)
114     ZZ7=ZZ(IDS+6)
115     ZZ(IDS+2)=(ZZ(IDS+1)-ZZ(IDS))/ZZ8
116     ZZ(IDS+1)=(ZZ(IDS+3)-ZZ(IDS))/ZZ7
117     ZZ(IDS+3)=(S-ZZ(IDS+2))/ZZ7
118     ZZ(IDS+12)=ZZ(IDS+12)/ZZ8
119     ZZ(IDS+13)=ZZ(IDS+13)/ZZ8
120     ZZ(IDS+14)=ZZ(IDS+14)/ZZ7
121     ZZ(IDS+15)=ZZ(IDS+15)/ZZ7
122 C   EVALUATE RATIONAL FUNCTION FROM PRECALCULATED COEFFICIENTS
123 8   QX = X-ZZ(IDS+4)
124     RX = ZZ(IDS+6)-QX

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125      QY = Y-ZZ(IDS+5)
126      RY = ZZ(IDS+7)-QY
127      IF(RX.NE.O.) GO TO 9
128      W1 = 1.
129      W2 = 1.
130      GO TO 10
131  9    W1 = 1.-1./(1.+ABS(ZZ(IDS+8)*QX/RX))
132      W2 = 1.-1./(1.+ABS(ZZ(IDS+9)*QX/RX))
133  10   F1 = ZZ(IDS+12)*(W1+ZZ(IDS+8))*(1.-W1)
134      F2 = ZZ(IDS+13)*(W2+ZZ(IDS+9))*(1.-W2)
135      Z(2) = ZZ(IDS+6)*(RY*(F1-ZZ(IDS+12))+W1+QY*(F2-ZZ(IDS+13))+W2)
136      G1 = RY*F1+QY*F2
137      IF(RY.NE.O) GO TO 11
138      W1 = 1.
139      W2 = 1.
140      GO TO 12
141  11   W1 = 1.-1./(1.+ABS(ZZ(IDS+10)*QY/RY))
142      W2 = 1.-1./(1.+ABS(ZZ(IDS+11)*QY/RY))
143  12   F3 = ZZ(IDS+14)*(W1+ZZ(IDS+10))*(1.-W1)
144      F4 = ZZ(IDS+15)*(W2+ZZ(IDS+11))*(1.-W2)
145      Z(3) = ZZ(IDS+7)*(RX*(F3-ZZ(IDS+14))+W1+QX*(F4-ZZ(IDS+15))+W2)
146      G2 = RX*F3+QX*F4
147      ZZ2=ZZ(IDS+1)
148      ZZ3=ZZ(IDS+2)
149      ZZ4=ZZ(IDS+3)
150      Z(1) = ZZ(IDS)+(ZZ2+ZZ4*QY-RX*G1)*QX+(ZZ3-RY*G2)*QY
151      Z(2) = Z(2)+ZZ2+QY*(ZZ4+RY*(F3-F4))+(QX-RX)*G1
152      Z(3) = Z(3)+ZZ3+QX*(ZZ4+RX*(F1-F2))+(QY-RY)*G2
153      RETURN
154 C    CALCULATE COEFFICIENTS FOR BILINEAR INTERPOLATION
155  13   IF(IP.EQ.O) GO TO 14
156      I=LOCX+IX
157      IND=IDS+4
158      ZZ(IND)=TBLS(I-1)
159      DX=TBLS(I)-ZZ(IND)
160      J=LOCY+IY
161      IND=IDS+5
162      ZZ(IND)=TBLS(J-1)
163      DY=TBLS(J)-ZZ(IND)
164      IZ=LOCZ+NZ*(IX-1+NX*(IY-1))
165      ZZ(IND)=SHIFT(TBLS(IZ),NSFT)
166      IND=IDS+1
167      ZZ(IND)=SHIFT(TBLS(IZ+NZ),NSFT)
168      ZZ(IND)=(ZZ(IND)-ZZ(IDS))/DX
169      IZ=IZ+NZ*NX
170      IND=IDS+2
171      ZZ(IND)=SHIFT(TBLS(IZ),NSFT)
172      ZZ(IND)=(ZZ(IND)-ZZ(IDS))/DY
173      IND=IDS+3
174      ZZ(IND)=SHIFT(TBLS(IZ+NZ),NSFT)
175      ZZ(IND)=(ZZ(IND)-ZZ(IDS)-ZZ(IDS+1)+DX-ZZ(IDS+2)+DY)/(DX+DY)
176 C    EVALUATE BILINEAR FUNCTION FROM PRECALCULATED COEFFICIENTS
177  14   QX = X-ZZ(IDS+4)
178      QY = Y-ZZ(IDS+5)
179      Z(2) = ZZ(IDS+1)+ZZ(IDS+3)*QY
180      Z(3) = ZZ(IDS+2)+ZZ(IDS+3)*QX
181      Z(1) = ZZ(IDS)+Z(2)+QX+ZZ(IDS+2)*QY
182      RETURN
183      END

```

```

1      SUBROUTINE T4PTREX(IR, IDT, TBLS, P, T, R, E, IFL)
2 C-----
3 C
4 C  SUBROUTINE:  T4PTREX(IR, IDT, TBLS, P, T, R, E, IFL)
5 C
6 C  PURPOSE:    FIND DENSITY AND INTERNAL ENERGY AS FUNCTIONS
7 C             OF PRESSURE AND TEMPERATURE FROM A 302
8 C             SESAME TABLE.  USES DOUBLE BINARY SEARCH TO
9 C             FIND INITIAL GUESS OF R AND E, THEN USES
10 C            DOUBLE NEWTONS METHOD.
11 C
12 C  ARGUMENTS:  IR   (INPUT) - REGION NO.
13 C            IDT  (INPUT) - DATA TYPE CORRESPONDING TO E BASED EOS
14 C            TBLS (INPUT) - TABLE STORAGE ARRAY
15 C            P    (INPUT) - PRESSURE
16 C            T    (INPUT) - TEMPERATURE
17 C            R    (OUTPUT) - DENSITY
18 C            E    (OUTPUT) - ENERGY
19 C            IFL  (OUTPUT) - ERROR FLAG
20 C            IFL=1, IF CALCULATION IS SUCCESSFUL
21 C            IFL=0, IF CALCULATION FAILS
22 C
23 C  REMARKS:    TBLS CAN BE DECLARED LCM ON THE CDC 7600.
24 C
25 C  EXTERNALS:  T4DATIX, ISRCHKX.
26 C
27 C  PROGRAMMER: G. I. KERLEY, T-4.
28 C
29 C  DATE:       3 MARCH 1978
30 C
31 C-----
32      LEVEL 2, TBLS
33      DIMENSION TBLS(1)
34      COMMON/S2DIRX/LCMX, NRS, LCFW(10, 3)
35      COMMON/SESINX/IRX, IDTX, RX, EX, IBR, IFLX
36      COMMON/SESOUTX/ZP(3), ZT(3)
37      IBR=0
38      IFLX=1
39      IRX=IR
40      IDTX=IDT
41      LOC=LCFW(IR, IDT)+1
42      NR = TBLS(LOC+1)
43      NT = TBLS(LOC+2)
44      ILO = 1
45      IHI = NR
46  1    I = .5*(ILO+IHI)
47      LOCT = LOC+2+NR+NR+NT+I+NR
48      J = ISRCHKX(T, TBLS(LOCT), NT-2, NR, 30)+1
49      LOCP = LOC+2+NR+NT+I+NR*(J)
50      IF(IHI-I.EQ.1) GO TO 3
51      IF(P.LT.TBLS(LOCP)) GO TO 2
52      ILO = I
53      GO TO 1
54  2    IHI = I
55      GO TO 1
56  3    RX = TBLS(LOC+2+I)
57      EX = TBLS(LOC+2+NR+J)+TBLS(LOC+2+NR+NT+I)
58      K = 0
59      IFL = 1
60  4    K = K+1
61      IF(K.EQ.50) GO TO 6
62      CALL T4DATIX

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```

63      R=RX
64      E=EX
65      PTEST = ABS(P-ZP(1))-1.E-05*(ABS(P)+1.E-05)
66      IF(PTEST.GT.O.) GO TO 5
67      TTEST = ABS(T-ZT(1))-1.E-05*(ABS(T)+1.E-02)
68      IF(TTEST.LT.O) RETURN
69  5    DNOMR = ZT(3)*ZP(2)-ZP(3)*ZT(2)
70      IF(DNOMR.EQ.O.) GO TO 6
71      RX = RX+(ZT(3)*(P-ZP(1))-ZP(3)*(T-ZT(1)))/DNOMR
72      DNOMR = ZT(2)*ZP(3)-ZP(2)*ZT(3)
73      IF(DNOMR.EQ.O.) GO TO 6
74      EX = EX+(ZT(2)*(P-ZP(1))-ZP(2)*(T-ZT(1)))/DNOMR
75      GO TO 4
76  6    IFL = 0
77      RETURN
78      END

```

```

1      SUBROUTINE T4RTPEX(IR, IDT, TBLS, R, T, P, E, IFL)
2 C -----
3 C
4 C      SUBROUTINE T4RTPEX(IR, IDT, TBLS, R, T, P, E, IFL)
5 C
6 C      PURPOSE      TO FIND PRESSURE AND ENERGY AS FUNCTIONS
7 C                  OF DENSITY AND TEMPERATURE FROM A
8 C                  SESAME TYPE 302 TABLE USING NEWTONS METHOD.
9 C
10 C     ARGUMENTS    IR          (INPUT)    REGION NO.
11 C                IDT         (INPUT)    DATA TYPE FOR 302 TABLES
12 C                TBLS        (INPUT)    TABLE STORAGE ARRAY
13 C                T           (INPUT)    TEMPERATURE
14 C                P           (OUTPUT)   PRESSURE
15 C                E           (OUTPUT)   ENERGY
16 C                IFL         (OUTPUT)   OUTPUT FLAG
17 C                                     =1 FOR SUCCESS
18 C                                     =0 FOR FAILURE
19 C
20 C     REMARKS      NONE
21 C
22 C
23 C     PROGRAMMER   J. ABDALLAH, JR.
24 C
25 C     DATE         5 JULY 1979
26 C
27 C -----
28      LEVEL 2, TBLS
29      COMMON/S2DIRX/LCMX, NRS, LCFW(10, 3)
30      DIMENSION TBLS(1)
31      COMMON/SESINX/IRXX, IDTX, RX, EX, IBR, IFLX
32      COMMON/SESOUTX/ZP(3), ZT(3)
33      IBR=0
34      IFLX=1
35      RX=R
36      IRXX=IR
37      IDTX=IDT
38      LOC=LCFW(IR, IDT)
39      NR=TBLS(LOC+2)
40      NE=TBLS(LOC+3)
41 C . . GET INITIAL GUESS ON ENERGY
42 C . . FIND CLOSEST DENSITY INDEX
43      LOCX=LOC+4
44      IRX=1
45      DELS=ABS(R-TBLS(LOCX))
46      IF(NR.EQ.1) GO TO 20
47      DO 10 J=2, NR
48      LOCX=LOCX+1
49      DEL=ABS(R-TBLS(LOCX))
50      IF(DEL.GT.DELS) GO TO 10
51      IRX=J
52      DELS=DEL
53 10  CONTINUE
54 C . . FIND THE ENERGY INDEX ASSOCIATED WITH THE CLOSEST TEMP
55 20  LOCX=LOC+3+NR+NE+NR+IRX
56      DELS=TBLS(LOCX)
57      DELS=SHIFT(DELS, 30)
58      DELS=ABS(T-DELS)
59      IEX=1
60      IF(NE.EQ.1) GO TO 40
61      DO 30 J=2, NE
62      LOCX=LOCX+NR

```



```

63     DEL=TBLS(LOCK)
64     DEL=SHIFT(DEL,30)
65     DEL=ABS(T-DEL)
66     IF(DEL.GT.DELS) GO TO 30
67     IEX=J
68     DELS=DEL
69 30   CONTINUE
70 C . . INITIAL GUESS ON ENERGY
71 40   EX=TBLS(LOC+3+NR+IEX)+TBLS(LOC+3+NR+NE+IRX)
72 C . . ITERATE USING NEWTONS METHOD
73     K=0
74     IFL=1
75 50   K=K+1
76     IF(K.EQ.50) GO TO 90
77     CALL T4DATIX
78     E=EX
79     P=ZP(1)
80     TTEST=ABS(T-ZT(1))-1.OE-05+(ABS(T)+1.OE-02)
81     IF(TTEST.LT.O.) RETURN
82     D=-ZT(3)
83     IF(D.EQ.O.O) GO TO 90
84     EX=EX-(T-ZT(1))/D
85     GO TO 50
86 90   IFL=0
87     RETURN
88     END

```

APPENDIX B

CROSS-REFERENCE DIRECTORY OF EOSLIB

NO UNUSED SPACE

	ROUTINE	INDEX	RECORD LENGTH	DSKAD	EXTERNAL SYMBOLS		COMMON BLOCKS	
1.	DPACKX DPACKX	18	15	017113				
2.	EOSBEG EOSBEG	5	7	002354			S2DIRX SESINX EDSC2 EDSC2 EDSC4 EDSC6 EOSCCE	SESDATX INTORDX EOSC1 EOSC3 EOSC5 EOSC7 EOSCC0
3.	EOSCON EOSCON	1	81	000000	EOSDSL	GOTOER.	EOSCCE	EOSCC0
4.	EOSDRE EOSDRE	6	81	005404	T4DATX EOSKUT	EOSGET	S2DIRX INTORDX SESOUTX EOSC3	SESDATX SESINX EOSC7 EOSC4
5.	EOSDRT EOSDRT	7	80	006173	T4DATX EOSKUT	EOSGET	S2DIRX INTORDX SESOUTX EOSCCE EOSC3	SESDATX SESINX EOSC2 EOSC1 EOSC4
6.	EOSDSL EOSDSL	2	6	000454			EOSCCE	EOSCC0
7.	EOSEFD EOSEFD	4	166	001320	OUTCI. EOF REWIND. EOSFAS	DECODI. INPCI. FEXIST	EOSC2 EOSC2 EOSC5	EOSC1 EOSC3 EOSC6
8.	EOSFAS EOSFAS	3	74	000644	ASSIGN GOTOER.	OASSIGN	EOSC2 EOSC2	EOSC1
9.	EOSGET EOSGET	11	231	011374	OUTCI. GETRPOX GOTOER. EOSOFD	GETEOSX GETINX EOSCON EOSEFD	S2DIRX SESINX EDSC2 EDSC3	SESDATX INTORDX EOSC1 EOSC4
10.	EOSIPT EOSIPT	9	128	007722	OUTCI. EOSGET	T4PTREX EOSKUT	S2DIRX SESINX EDSC2 EDSC4	SESDATX INTORDX EOSC3
11.	EOSIRT EOSIRT	8	128	007020	OUTCI.	T4RTPEX	S2DIRX	SESDATX

					EOSGET	EOSKUT	SESINX EOSCZ EOSC4	INTORDX EOSC3
12.	EOSKUT EOSKUT	10	123	010624	OUTCI.	EOSBEG	EOSC2	EOSC3
13.	EOSOFD EOSOFD	12	145	012524	OUTCI. EOF REWIND. EOSFAS	DECDI INPCI. FEXIST	EOSCZ EOSC2 EOSC7	EOSC1 EOSC3
14.	EOSORT EOSORT	13	106	013464	XTOYS OLOGIO EOSKUT	T4DATX EOSGET OUTCI.	S2DIRX INTORDX SESOUTX EOSCCO EOSC3	SESDATX SESINX EOSCZ EOSC1 EOSC4
15.	GETEOSX GETEOSX	14	171	014330	DPACKX MATCHKX	TABRANX	S2DIRX	EOSCCE
16.	GETIN VX GETIN VX	21	201	021107	DPACKX TABRANX	INV301X MATCHKX	S2DIRX	EOSCCE
17.	GETRPOX GETRPOX	26	139	025611	DPACKX MATCHKX	TABRANX	S2DIRX	EOSCCO
18.	INBUFRX INBUFRX	17	29	016627	UNIT	RDISK		
19.	INV301X INV301X	24	166	023711	RATFN1X	ISRCHKX	INTORDX	RTBLK1X
20.	ISRCHKX ISRCHKX	19	55	017303				
21.	MATCHKX MATCHKX	16	22	016437				
22.	RATFN1X RATFN1X	22	128	022237			SESDATX RTBLK1X	INTORDX
23.	T4DATIX T4DATIX	23	124	022770	T4INTPX	RATFN1X	S2DIRX RTBLK2X SESOUTX	RTBLK1X SESINX SESDATX
24.	T4DATX T4DATX	27	130	026551	T4INTPX		S2DIRX SESDATX SESOUTX	RTBLK2X SESINX
25.	T4INTPX T4INTPX	20	289	017702			RTBLK2X SESDATX	INTORDX

26.	T4PTREX T4PTREX	15	156	015403	T4DATIX	ISRCHKX	S2DIRX SESOUTX	SESINX	-
27.	T4RTPEX T4RTPEX	25	128	024613	T4DATIX		S2DIRX SESOUTX	SESINX	-
28.	TABRANX TABRANX	28	188	027566	INBUFRX				

NO.	ENTRY PT:	CALLED BY:				
1	EOSCON	EOSGET				
2	EOSDSL	EOSCON				
3	EOSFAS	EOSEFD	EOSOFD			
4	EOSEFD	EOSGET				
5	EOSBEG	EOSKUT				
6	EOSDRE					
7	EOSDRT					
8	EOSIRT					
9	EOSIPT					
10	EOSKUT	EOSDRE	EOSDRT	EOSIRT	EOSIPT	EOSORT
11	EOSGET	EOSDRE	EOSDRT	EOSIRT	EOSIPT	EOSORT
12	EOSOFD	EOSGET				
13	EOSORT					
14	GETEOSX	EOSGET				
15	T4PTREX	EOSIPT				
16	MATCHKX	GETEOSX	GETIN VX	GETRPOX		
17	INBUFRX	TABRANX				
18	DPACKX	GETEOSX	GETIN VX	GETRPOX		
19	ISRCHKX	T4PTREX	INV301X			
20	T4INTPX	T4DATIX	T4DATX			
21	GETIN VX	EOSGET				
22	RATFN1X					

	T4DATIX	INV301X	
23 T4DATIX	EOSDRE	T4PTREX	T4RTPEX
24 INV301X	GETINVX		
25 T4RTPEX	EOSIRT		
26 GETRPOX	EOSGET		
27 T4DATX	EOSDRT	EOSORT	
28 TABRANX	GETEOSX	GETINVX	GETRPOX

1  
COMMON BLOCK: USED BY:

EOSCCE	EOSCON	EOSDSL	EOSBEG	EOSDRT	GETEOSX	GETINVX		
EOSCCD	EOSCON	EOSDSL	EOSBEG	EOSDRT	GETRPOX			
EOSCZ	EOSFAS EOSGET	EOSEFD EOSOFD	EOSBEG EOSDRT	EOSDRE	EOSORT	EOSIRT	EOSIPT	EOSKUT
EOSC1	EOSFAS	EOSEFD	EOSBEG	EOSDRT	EOSGET	EOSOFD	EOSORT	
EOSC2	EOSFAS	EOSEFD	EOSBEG	EOSOFD				
EOSC3	EOSEFD EOSOFD	EOSBEG EOSORT	EOSDRE	EOSDRT	EOSIRT	EOSIPT	EOSKUT	EOSGET
EOSC5	EOSEFD	EOSBEG						
EOSC6	EOSEFD	EOSBEG						
S2DIRX	EOSBEG T4PTREX	EOSDRE GETINVX	EOSDRT T4DATIX	EOSIRT T4RTPEX	EOSIPT GETRPOX	EOSGET T4DATX	EOSORT	GETEOSX
SES DATX	EOSBEG RATFN1X	EOSDRE T4DATIX	EOSDRT T4DATX	EOSIRT	EOSIPT	EOSGET	EOSORT	T4INTPX
SESINX	EOSBEG T4DATIX	EOSDRE T4RTPEX	EOSDRT T4DATX	EOSIRT	EOSIPT	EOSGET	EOSORT	T4PTREX
INTORDX	EOSBEG RATFN1X	EOSDRE INV301X	EOSDRT	EOSIRT	EOSIPT	EOSGET	EOSORT	T4INTPX
EOSC4	EOSBEG	EOSDRE	EOSDRT	EOSIRT	EOSIPT	EOSGET	EOSORT	
EOSC7	EOSBEG	EOSOFD						
SESOUTX	EOSDRE	EOSDRT	EOSORT	T4PTREX	T4DATIX	T4RTPEX	T4DATX	
RTBLK2X	T4INTPX	T4DATIX	T4DATX					
RTBLK1X	RATFN1X	T4DATIX	INV301X					



APPENDIX C  
TEST PROGRAM

```

1      PROGRAM SES (INPUT,OUTPUT,TAPE6=OUTPUT,TAPE59=TTY,TAPE3)
2 C
3 C      *****
4 C      *
5 C      * PURPOSE-
6 C      *   TO PROVIDE THE APPROPRIATE EOS SCALE FACTORS FOR THE
7 C      *   SYSTEM OF UNITS CHOSEN BY KUNIT (SEE BELOW)
8 C      *
9 C      * INPUT VARIABLES-
10 C     *
11 C     *   LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
12 C     *   THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
13 C     *   THE MATERIAL BY SETTING LMAT TO THE SESAME
14 C     *   NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
15 C     *
16 C     *   R = DENSITY (RHO)
17 C     *
18 C     *   E = INTERNAL EN
19 C     *
20 C     *   KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
21 C     *   AND RETRIEVE THE DATA FILE. KEOS HAS FOUR DECIMAL DIGITS.
22 C     *
23 C     *   KEOS = 1000*KBR + 100*KUNIT + 10*KREPE + KFN WHERE
24 C     *
25 C     *   KBR = COMPUTATIONAL MODE FLAG TO INDICATE WHICH
26 C     *   QUANTITIES AND THEIR PARTIAL DERIVATIVES ARE TO
27 C     *   BE CALCULATED AND RETURNED BY THE PACKAGE.
28 C     *       = 0  COMPUTE PRESSURE AND TEMPERATURE
29 C     *       = 1  COMPUTE PRESSURE ONLY
30 C     *       = 2  COMPUTE TEMPERATURE ONLY
31 C     *
32 C     *   KUNIT= KIND OF UNITS
33 C     *       0 (SESAMEE) R-G/CC,T-DEG.K,O-CM**2/G,P-GPA,E-MJ/KG
34 C     *       1 (CGS) R-G/CC,T-DEG.K,O-CM**2/GM,P-MUBR,E-ERGS/GM
35 C     *       2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,O-M**2/KG
36 C     *       3 (HYDROXE) R-G/CC,T-DEG.K,P-MBR,E-MBR*CC/GM,O-CM**2/G
37 C     *       4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR*CC/G,O-CM**2/G
38 C     *       5 (SESAMED) R-G/CC,T-EV,O-CM**2/G,P-GPA,E-MJ/KG
39 C     *       6 (LASNEX) R-G/CC,T-KEV,O-CM**2/GM,P-JRKS/CC,ED-JRKS/CC
40 C     *
41 C     *   LEGEND-
42 C     *       R = DENSITY
43 C     *       T = TEMPERATURE
44 C     *       O = OPACITY
45 C     *       P = PRESSURE
46 C     *       E = INTERNAL EN
47 C     *
48 C     *       CC = CUBIC CENTIMETER
49 C     *       CM = CENTIMETER
50 C     *       DEG. K = DEGREES KELVIN
51 C     *       EV = ELECTRON VOLT
52 C     *       G = GRAM
53 C     *       GPA = GIGA PASCALS
54 C     *       J = JOULES
55 C     *       JRKS = JERKS
56 C     *       KEV = KILO ELECTRON VOLTS
57 C     *       KG = KILOGRAM
58 C     *       M = METER
59 C     *       MBR = MEGABAR
60 C     *       MUBR = MICROBAR
61 C     *       PA = PASCAL
62 C

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63 C * KREPE = COMPUTATION FLAG TO INDICATE WHETHER E IS
64 C * IS TO BE REPRESENTED AS EN PER UNIT MASS OR EN
65 C * PER UNIT VOLUME
66 C * 0 EN IN UNITS OF EN PER UNIT MASS. FOR EXAMPLE-
67 C * UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
68 C * 1 EN IN UNITS OF EN PER UNIT VOLUME. FOR EXAPMLE-
69 C * UNITS OF ERGS/CM**3 WHEN KUNIT = 1. THIS IS THE EN
70 C * DENSITY RHO*E COMMONLY COMPUTED IN HYDRODYNAMIC
71 C * COMPUTER CODES.
72 C *
73 C * KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES
74 C * = 0 RATIONAL APPROXIMATIONS (ACCURATE)
75 C * = 1 BILINEAR APPROXIMATIONS (FAST)
76 C *
77 C * IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
78 C * IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
79 C * PREVIOUSLY LOADED FILE.
80 C * =0 CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
81 C * IF NOT, SEARCH FOR THE FILE, CONVERT IT TO THE PROPER UNITS
82 C * AND COPY IT INTO LCM USING THE STANDARD SESAME FORMAT.
83 C * >0 EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
84 C * BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSDRE,
85 C * EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMATE = 0
86 C * BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
87 C *
88 C * OUTPUT VARIABLES-
89 C *
90 C * P = ARRAY OF DIMENSION 3 CONTAINING THE PRESSURE AND
91 C * ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
92 C * EVEN IF THE PARTIAL DERIVATIVES ARE NOT COMPUTED.
93 C *
94 C * P(1) = PRESSURE
95 C * P(2) = DENSITY DERIVATIVE OF THE PRESSURE (DP/DR)
96 C * P(3) = TEMPERATURE DERIVATIVE OF THE PRESSURE (DP/DE)
97 C *
98 C * T = ARRAY OF DIMENSION 3 CONTAINING THE TEMPERATURE AND
99 C * ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
100 C * EVEN IF THE PARTIAL DERIVATIVES ARE NOT COMPUTED
101 C *
102 C * T(1) = INTERNAL TEMPERATURE
103 C * T(2) = DENSITY DERIVATIVE OF THE TEMPERATURE (DT/DR)
104 C * T(3) = EN DERIVATIVE OF THE TEMPERATURE (DT/DE)
105 C *
106 C * IMATE = INDICATES THE SUCCESS OR FAILURE OF
107 C * LOCATING AND LOADING THE DATA FILE FOR LMAT.
108 C *
109 C * = N>0 MATERIAL TABLE NUMBER (SUCCESS)
110 C * 0 MATERIAL (LMAT) NOT IN LIBRARY
111 C * -N (N>1) INSUFFICIENT STORAGE
112 C * THE LCM STORAGE MUST BE INCREASED BY AT LEAST
113 C * N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
114 C *
115 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
116 C *
117 C * SAMPLE DRIVER PROGRAM-
118 C *
119 C * PROGRAM TST(OUTPUT)
120 C * DIMENSION P(3),E(3)
121 C * LMAT = "HELIUM"
122 C * R = 0.001
123 C * E = 1.0
124 C * KEOS = 110

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125 C * IMATE = 0
126 C * CALL EOSDRE(LMAT,R.E.P.T,KEOS,IMATE)
127 C * PRINT 10,P(1)
128 C * 10 FORMAT(" PRESSURE = ",E10.2," MICROBARS")
129 C * CALL EXIT
130 C * END
131 C *
132 C * OUTPUT VARIABLES- IN THE COMMON BLOCKS EOSCCE AND EOSCCO
133 C * TFACE = TEMPERATURE EOS SCALING FACTOR
134 C * RFACE = DENSITY EOS SCALING FACTOR
135 C * PFACE = PRESSURE EOS SCALING FACTOR
136 C * EFACE = EN EOS SCALING FACTOR
137 C *
138 C * TFACO = TEMPERATURE OPACITY SCALING FACTOR
139 C * RFACO = DENSITY OPACITY SCALING FACTOR
140 C * OFACO = OPACITY SCALING FACTOR
141 C *
142 C * TBLS = ARRAY FOR STORAGE OF THE EOS TABLES
143 C * LCMX = LENGTH OF THE TBLS ARRAY
144 C * NRS = UPPER BOUND ON THE NUMBER OF MAT REGIONS LCFW(NRS,)
145 C * LCFW = ARRAY USED AS A DIRECTORY BY THE SESAME ROUTINES
146 C * IR = MATERIAL REGION NUMBER
147 C * IRC = IR (DEFINED TO PERMIT SUBROUTINE CALL
148 C * IDS2 = SESAME MATERIAL NUMBER
149 C * TBLS = NAME OF AN ARRAY DESIGNATED FOR THE STORAGE OF TABLES
150 C * LCNT = CRRRENT WORD IN THE ARRAY TBLS
151 C * LU41 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SES2CL
152 C * LU42 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SES2L
153 C * LU43 = UNIT NUMBER ASSIGNED TO SES2OP/8 FILES
154 C * LU44 = UNIT NUMBER ASSIGNED TO MIXLIB (MIXTURES)
155 C * LU45 = UNIT NUMBER ASSIGNED TO MIXLIB DIRECTORY.
156 C * KFN = 0 RATIONAL APPROXIMATIONS (ACCURATE)
157 C * KFN = 1 BILINEAR APPROXIMATIONS (FAST)
158 C * ZB (OUTPUT FROM GETINX) AT. CHARGE,AT. CHG**2,MASS
159 C * IDT = DATA TYPE INDICATOR
160 C * MID (ID) MATERIAL ID =1 INVERSE TABLES =2 OPACITY
161 C *
162 C * EXTERNAL FILES TO HANDLE EOS, OPACITIES AND MIXTURES
163 C * SES2CL - CLASSIFIED SESAME LIBRARY
164 C * SES2L - CUCLASSIFIED SESAME LIBRARY
165 C * SES2OP - OPACITY TABLE FROM T4
166 C * MIXLIB - PRIVATE (EOS,OPC) TABLES CREATED BY MIXB(OR MIXER)
167 C * MIXDIR - DIRECTORY OF MIXTURES ON MIXLIB ( NAME,NO (A10,I3))
168 C *
169 C * EXTERNALS AND COMMON BLOCKS-
170 C * SESAME ROUTINES- S2GET,S2EOS
171 C * SESAME ROUTINES MATCHKX,TABFCHX,INBUFRX,DPACKX,ISRCHKX,
172 C * T4INTPX,GETINX,RATFN1X,T4DATIX,INV301X,T4RTPEX
173 C * SESAME COMMON BLOCKS-S2DIRX,RTBLK2X,SESDATX,SESINX,SESOUTX,INTO
174 C * EOSMOD COMMON BLOCKS- EOSC1,-7
175 C * EOSMOD COMMON (ALSO INSERTED INTO GETINX) EOSCCE, EOSCCO
176 C *
177 C * LOCAL VARIABLES-
178 C * NONE
179 C *
180 C * EXTERNALS AND COMMON BLOCKS-
181 C * EOSMOD COMMON BLOCKS- EOSCCE,EOSCCO
182 C *
183 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
184 C *
185 C * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
186 C *

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187 C * REFERENCE- J. M. HYMAN, M. M. KLEIN
188 C *
189 C * EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
190 C * EQUATIONS-OF-STATE AND OPACITIES
191 C *
192 C * LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
193 C *
194 C *
195 C *****
196 C LEVEL 2, TBLS
197 C COMMON /S2DIR/ LCMX, NRS, LCFW(10.3)
198 C COMMON /SESDAT/ TBLS(11000)
199 C COMMON /SESIN/ IRC, IDT, DUM(2), KBR, DUM1
200 C COMMON /INTORD/ KFN
201 C
202 C COMMON BLOCKS FOR THE EOSMOD ROUTINES
203 C COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
204 C COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
205 C COMMON /EOSC3/ INIT, IRDIM, IR(60.3), KUT(60.3)
206 C COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
207 C COMMON /EOSC5/ NMAT, LABMAT(60), IDMAT(60)
208 C COMMON /EOSC6/ NMCL, LABMCL(60), IDMCL(60)
209 C COMMON /EOSC7/ NMATO, LABMO(60), IDMATO(60)
210 C
211 C EOSMOD COMMON BLOCKS USED BY THE MODIFIED SESAME ROUTINES
212 C COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
213 C COMMON /EOSCCO/ TFACO, RFACO, OFACO, KREPO
214 C
215 C NAMELIST /INP/ KUNIT, KREP, NLMAT, NBR, NFN, IIPT, IIRT, IDRT, IDRE, LCMX
216 C 1 ,NRS, DUM, KBR, DUM1, KFN, INIT, IRDIM, NTABLE, NTABLO, IFLP, LCNT, NMAT
217 C 2 ,NMCL, NMATO, TFACE, RFACE, EFACE, KREPE, TFACO, RFACO, OFACO, KREPO, RHO
218 C 3 ,TEMP, PR, EN, IRC, IDT, IORT, NGO
219 C DATA RHO /0.16/, TEMP /5.E4/, PR /19.2/, EN /310./
220 C
221 C DATA KUNIT /0/, KREP /0/, NLMAT /2/, NBR /1/, NFN /1/
222 C DATA IIPT /1/, IDRT /1/, IIRT /1/, IDRE /1/, IORT /1/, NGO /0/
223 C
224 C WRITE (3,210)
225 C DO 10 I=1, NMAT
226 C WRITE (3,220) LABMAT(I), IDMAT(I)
227 C 10 CONTINUE
228 C
229 C WRITE (3,230)
230 C DO 20 I=1, NMATO
231 C WRITE (3,220) LABMO(I), IDMATO(I)
232 C 20 CONTINUE
233 C
234 C 30 CONTINUE
235 C** READ (59, INP)
236 C
237 C WRITE (6, 160)
238 C
239 C DO 60 LMATP=1, NLMAT
240 C LMAT=6HHELIUM
241 C LMATO=LMAT
242 C IF (LMATP.EQ.2) LMAT="5760"
243 C IF (LMATP.EQ.2) LMATO="15760"
244 C
245 C DO 50 KBRP=1, NBR
246 C KBR=KBRP-1
247 C
248 C DO 40 KFNP=1, NFN

```

```

249      KFN=KFNP-1
250 C
251      KEOS=1000*KBR+100*KUNIT+10*KREP+KFN
252 C
253      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE,IORT,1
254      1 )
255 C
256      40 CONTINUE
257      50 CONTINUE
258      60 CONTINUE
259 C
260      WRITE (59,170)
261 C**   READ (59,180) LANS
262      IF (LANS.EQ.1HY) GO TO 30
263 C
264      IF (NGO.GT.0) GO TO (70,80,90,100,110,130), NGO
265 C
266 C   CHECK THE ERROR MESSAGES
267 C
268 C   CHANGE UNITS
269      70 CONTINUE
270      KEOS=KEOS+100
271      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE,IORT,1
272      1 )
273      KEOS=KEOS-100
274 C
275 C   CHANGE TABLE FORMAT FOR THE ENERGY AND OPACITY REPRESENTATION
276      80 CONTINUE
277      KEOS=KEOS+10
278      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE,IORT,1
279      1 )
280      KEOS=KEOS-10
281 C
282 C   NON MATERIAL TEST
283      90 CONTINUE
284      LMAT="NOMAT"
285      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE,IORT,1
286      1 )
287 C
288      LMAT="99999"
289      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE,IORT,1
290      1 )
291 C
292 C   NEGATIVE DENSITY TEST
293      100 CONTINUE
294      R=-RHO
295      CALL ES (LMAT,LMATO,R,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE,IORT,1)
296      GO TO 150
297 C
298 C   CHECK IF ALL THE MATERIALS ARE AVAILABLE
299 C
300 C   EOS MATERIALS CHECK
301      110 CONTINUE
302      DO 120 I=1,NMAT
303 C
304      LMAT=LABMAT(I)
305      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,0.1,0.0,0.0)
306 C
307      ENCODE (4,190,LMAT) IDMAT(I)
308 C
309      CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,0.1,0.0,0.0)
310 C

```

```

311 120 CONTINUE
312 C
313 C   OPACITY MATERIALS CHECK
314 130 CONTINUE
315   DO 140 I=1,NMATO
316 C
317   LMATO=LABMO(I)
318   CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,O,O,O,O,1,O)
319 C
320   ENCODE (5,200,LMATO) IDMATO(I)
321 C
322   CALL ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,O,1,O,O,O,O)
323 140 CONTINUE
324 150 CONTINUE
325 C
326   CALL EXITA (1)
327 C
328 160 FORMAT ("          KEOS IMATE R      T      P      E")
329 170 FORMAT (" CONTINUE?")
330 180 FORMAT (A1)
331 190 FORMAT (I4)
332 200 FORMAT (I5)
333 210 FORMAT (" THE EDS MATERIALS ARE")
334 220 FORMAT (1X,A10,I10)
335 230 FORMAT (" THE OPACITY MATERIALS ARE")
336   END

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1      SUBROUTINE ES (LMAT,LMATO,RHO,TEMP,PR,EN,KEOS,IIPT,IDRT,IIRT,IDRE
2      ,IORT,IWNL)
3 C
4 C      *****
5 C      *
6 C      * PURPOSE-
7 C      *
8 C      * INPUT VARIABLE-
9 C      *
10 C     * INPUT-OUTPUT VARIABLES IN THE COMMON BLOCKS EOSCC2 AND EOSCCO
11 C     *
12 C     * EXTERNALS AND COMMON BLOCKS-
13 C     *
14 C     * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
15 C     *
16 C     * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
17 C     *
18 C     * REFERENCE- J. M. HYMAN, M. M. KLEIN
19 C     *              EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
20 C     *              EQUATIONS-OF-STATE AND OPACITIES
21 C     *              LOS ALAMOS SCIENTIFIC LABORATORY RPT.,LA-8502-M,1980
22 C     *
23 C     * DATE- MARCH 22, 1981
24 C     *
25 C     *****
26 C
27     DIMENSION R(3), P(3), T(3), E(3)
28 C
29     LEVEL 2, TBL5
30     COMMON /S2DIR/ LCMX, NRS, LCFW(10,3)
31     COMMON /SESDAT/ TBL5(11000)
32     COMMON /SESIN/ IRC, IDT, DUM(2), KBR, DUM1
33     COMMON /INTORD/ KFN
34 C
35 C     COMMON BLOCKS FOR THE EOSMOD ROUTINES
36     COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
37     COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
38     COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUT(60,3)
39     COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
40     COMMON /EOSC5/ NMAT, LABMAT(60), IDMAT(60)
41     COMMON /EOSC6/ NMCL, LABMCL(60), IDMCL(60)
42     COMMON /EOSC7/ NMATO, LABMO(60), IDMATO(60)
43 C
44 C     EOSMOD COMMON BLOCKS USED BY THE MODIFIED SESAME ROUTINES
45     COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
46     COMMON /EOSCCO/ TFACO, RFACO, OFACO, KREPO
47 C
48     NAMELIST /INP/ KUNIT,KREP,NLMAT,NBR,NFN,IIPT,IIRT,IDRT,IDRE,LCMX
49     1 ,NRS,DUM,KBR,DUM1,KFN,INIT,IRDIM,NTABLE,NTABLO,IFLP,LCNT,NMAT
50     2 ,NMCL,NMATO,TFACE,RFACE,EFACE,KREPE,TFACO,RFACO,OFACO,KREPO,RHO
51     3 ,TEMP,PR,EN,IRC,IDT,IORT
52 C
53     R(1)=RHO
54     T(1)=TEMP
55     P(1)=PR
56     E(1)=EN
57 C     ***** EOSIPT TEST *****
58 C
59     IF (IIPT.EQ.0) GO TO 10
60     WRITE (6,70)
61     WRITE (3,70)
62     IMATE=0

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63      R(1)=R(2)=R(3)=0.0
64      E(1)=E(2)=E(3)=0.0
65      CALL EOSIPT (LMAT,P,T,R,E,KEOS,IMATE)
66      WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
67      WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
68      IF (IWNL.NE.O) WRITE (3,INP)
69      IF (IMATE.LE.O) IMATE=0
70 C
71      R(1)=R(2)=R(3)=0.0
72      E(1)=E(2)=E(3)=0.0
73      CALL EOSIPT (LMAT,P,T,R,E,KEOS,IMATE)
74      WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
75      WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
76      IF (IWNL.NE.O) WRITE (3,INP)
77      IF (IMATE.LE.O) IMATE=0
78 10 CONTINUE
79 C
80 C      ***** EOSDRT TEST *****
81 C
82      IF (IDRT.EQ.O) GO TO 20
83      WRITE (6,80)
84      WRITE (3,80)
85      IMATE=0
86      P(1)=P(2)=P(3)=0.0
87      E(1)=E(2)=E(3)=0.0
88      CALL EOSDRT (LMAT,R,T,P,E,KEOS,IMATE)
89      WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
90      WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
91      IF (IWNL.NE.O) WRITE (3,INP)
92      IF (IMATE.LE.O) IMATE=0
93 C
94      P(1)=P(2)=P(3)=0.0
95      E(1)=E(2)=E(3)=0.0
96      CALL EOSDRT (LMAT,R,T,P,E,KEOS,IMATE)
97      WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
98      WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
99      IF (IWNL.NE.O) WRITE (3,INP)
100     IF (IMATE.LE.O) IMATE=0
101 20 CONTINUE
102 C
103 C      ***** EOSIRT TEST *****
104 C
105     IF (IIRT.EQ.O) GO TO 30
106     WRITE (6,90)
107     WRITE (3,90)
108     IMATE=0
109     P(1)=P(2)=P(3)=0.0
110     E(1)=E(2)=E(3)=0.0
111     CALL EOSIRT (LMAT,R,T,P,E,KEOS,IMATE)
112     WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
113     WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
114     IF (IWNL.NE.O) WRITE (3,INP)
115     IF (IMATE.LE.O) IMATE=0
116 C
117     P(1)=P(2)=P(3)=0.0
118     E(1)=E(2)=E(3)=0.0
119     CALL EOSIRT (LMAT,R,T,P,E,KEOS,IMATE)
120     WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
121     WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
122     IF (IWNL.NE.O) WRITE (3,INP)
123     IF (IMATE.LE.O) IMATE=0
124 30 CONTINUE

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125 C
126 C ***** EOSDRE TEST *****
127 C
128 IF (IDRE.EQ.O) GO TO 40
129 WRITE (6,110)
130 WRITE (3,110)
131 IMATE=O
132 P(1)=P(2)=P(3)=O.O
133 T(1)=T(2)=T(3)=O.O
134 CALL EOSDRE (LMAT,R,E,P,T,KEOS,IMATE)
135 WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
136 WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
137 IF (IWNL.NE.O) WRITE (3,INP)
138 IF (IMATE.LE.O) IMATE=O
139 C
140 P(1)=P(2)=P(3)=O.O
141 T(1)=T(2)=T(3)=O.O
142 CALL EOSDRE (LMAT,R,E,P,T,KEOS,IMATE)
143 WRITE (6,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
144 WRITE (3,60) LMAT,KEOS,IMATE,(R(I),T(I),P(I),E(I),I=1,3)
145 IF (IWNL.NE.O) WRITE (3,INP)
146 IF (IMATE.LE.O) IMATE=O
147 40 CONTINUE
148 C
149 C ***** EOSORT TEST *****
150 C
151 IF (IQRT.EQ.O) GO TO 50
152 KOPC=KEOS
153 WRITE (6,100)
154 WRITE (3,100)
155 IMATO=O
156 OPACITY=O.O
157 CALL EOSORT (LMATO,R,T,OPACITY,KOPC,IMATO)
158 WRITE (6,60) LMATO,KOPC,IMATO,R(1),T(1),OPACITY
159 WRITE (3,60) LMATO,KOPC,IMATO,R(1),T(1),OPACITY
160 IF (IWNL.NE.O) WRITE (3,INP)
161 IF (IMATO.LE.O) IMATO=O
162 C
163 OPACITY=O.O
164 CALL EOSORT (LMATO,R,T,OPACITY,KOPC,IMATO)
165 WRITE (6,60) LMATO,KOPC,IMATO,R(1),T(1),OPACITY
166 WRITE (3,60) LMATO,KOPC,IMATO,R(1),T(1),OPACITY
167 IF (IWNL.NE.O) WRITE (3,INP)
168 IF (IMATO.LE.O) IMATO=O
169 50 CONTINUE
170 C
171 RETURN
172 C
173 60 FORMAT (1X,A10,I4,I3,12(1PE9.2))
174 70 FORMAT (" EOSIPT")
175 80 FORMAT (" EOSDRT")
176 90 FORMAT (" EOSIRT")
177 100 FORMAT (" EOSORT")
178 110 FORMAT (" EOSDRE")
179 END

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OUTPUT

	K	E	S	I	M	A	T	E	R	T	P	E								
EOSIPT																				
HELIUM	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
HELIUM	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSDRT																				
HELIUM	0	11	1.59E-01	5.00E+04	1.91E+01	3.10E+02	0.	0.	1.15E+02	-1.62E+02	0.	0.	0.	4.73E-04	1.13E-02	0.	0.	0.	0.	0.
HELIUM	0	11	1.59E-01	5.00E+04	1.91E+01	3.10E+02	0.	0.	1.15E+02	-1.62E+02	0.	0.	0.	4.73E-04	1.13E-02	0.	0.	0.	0.	0.
EOSIRT																				
HELIUM	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
HELIUM	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSDRE																				
HELIUM	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
HELIUM	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
EOSORT																				
HELIUM	0	10	1.59E-01	5.00E+04	1.27E+07															
HELIUM	0	10	1.59E-01	5.00E+04	1.27E+07															
EOSIPT																				
5760	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
5760	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
EOSDRT																				
5760	0	11	1.59E-01	5.00E+04	1.91E+01	3.10E+02	0.	1.43E+04	1.15E+02	-1.62E+02	0.	0.	0.	8.86E+01	4.73E-04	1.13E-02	0.	0.	0.	0.
5760	0	11	1.59E-01	5.00E+04	1.91E+01	3.10E+02	0.	1.43E+04	1.15E+02	-1.62E+02	0.	0.	0.	8.86E+01	4.73E-04	1.13E-02	0.	0.	0.	0.
EOSIRT																				
5760	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	0.	0.	0.	0.	0.	8.86E+01	0.	0.	0.	0.	0.	0.
5760	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	0.	0.	0.	0.	0.	8.86E+01	0.	0.	0.	0.	0.	0.
EOSDRE																				
5760	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
5760	0	11	1.59E-01	5.00E+04	1.92E+01	3.10E+02	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
EOSORT																				
5760	0	10	1.59E-01	5.00E+04	1.27E+07															
15760	0	10	1.59E-01	5.00E+04	1.27E+07															
EOSIPT																				
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE																				
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0																				
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0																				
5760	100	-8	0.	5.00E+04	1.92E+01	0.	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE																				
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0																				
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0																				
5760	100	-8	0.	5.00E+04	1.92E+01	0.	0.	1.43E+04	1.23E+02	0.	0.	0.	0.	8.86E+01	3.82E-02	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE																				
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0																				
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0																				
5760	100	-8	0.	5.00E+04	0.	0.	0.	1.43E+04	0.	0.	0.	0.	0.	8.86E+01	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE																				
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0																				
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0																				
5760	100	-8	0.	5.00E+04	0.	0.	0.	1.43E+04	0.	0.	0.	0.	0.	8.86E+01	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE																				
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0																				
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0																				
5760	100	-8	0.	5.00E+04	0.	0.	0.	1.43E+04	0.	0.	0.	0.	0.	8.86E+01	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE																				
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0																				
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0																				

5760	100 -8 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 1 0												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	100 -6 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSDRT												
THE DENSITY = 0. OR THE TEMPERATURE = 0. IS NONPOSITIVE												
5760	100 -1 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE DENSITY = 0. OR THE TEMPERATURE = 0. IS NONPOSITIVE												
15760	100 -1 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSIPT												
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	5.00E+04	1.92E+01	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	5.00E+04	1.92E+01	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSDRT												
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	5.00E+04	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	5.00E+04	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSIPT												
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	5.00E+04	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	5.00E+04	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSDRE												
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE												
THE CURRENT VALUES OF KUNIT AND KREP ARE 0 1												
THE PREVIOUS VALUES OF KUNIT AND KREP WERE 0												
5760	10 -8 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSDRT												
THE DENSITY = 0. OR THE TEMPERATURE = 0. IS NONPOSITIVE												
5760	10 -1 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
THE DENSITY = 0. OR THE TEMPERATURE = 0. IS NONPOSITIVE												
15760	10 -1 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSIPT												
MATERIAL LMAT = NOMAT NOT FOUND												
NOMAT	0 -1 0.	5.00E+04	1.92E+01	0.	0.	0.	0.	0.	0.	0.	0.	0.
MATERIAL LMAT = NOMAT NOT FOUND												
NOMAT	0 -1 0.	5.00E+04	1.92E+01	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSDRT												
MATERIAL LMAT = NOMAT NOT FOUND												
NOMAT	0 -1 0.	5.00E+04	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
MATERIAL LMAT = NOMAT NOT FOUND												
NOMAT	0 -1 0.	5.00E+04	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EDSIPT												

MATERIAL LMAT = NOMAT	NOT FOUND											
NOMAT 0 -1 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
MATERIAL LMAT = NOMAT	NOT FOUND											
NOMAT 0 -1 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSDRE												
MATERIAL LMAT = NOMAT	NOT FOUND											
NOMAT 0 -1 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
MATERIAL LMAT = NOMAT	NOT FOUND											
NOMAT 0 -1 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSORT												
THE DENSITY = 0.	OR THE TEMPERATURE = 0.											
NOMAT 0 -1 0.	0.	0.										
THE DENSITY = 0.	OR THE TEMPERATURE = 0.											
15760 0 -1 0.	0.	0.										
EOSIPT												
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 1.92E+01 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 1.92E+01 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSDRT												
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSIRT												
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSDRE												
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSORT												
THE DENSITY = 0.	OR THE TEMPERATURE = 0.											
99999 0 -1 0.	0.	0.										
THE DENSITY = 0.	OR THE TEMPERATURE = 0.											
15760 0 -1 0.	0.	0.										
EOSIPT												
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 1.92E+01 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 1.92E+01 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSDRT												
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
UNABLE TO LOCATE MATERIAL 99999												
IN SUBROUTINE EOSGET												
99999 0 -2 0.	5.00E+04 0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
EOSIRT												

```

UNABLE TO LOCATE MATERIAL 99999
IN SUBROUTINE EOSGET
99999      0 -2 0.      5.00E+04 0.      0.      0.      0.      0.      0.      0.      0.      0.
UNABLE TO LOCATE MATERIAL 99999
IN SUBROUTINE EOSGET
99999      0 -2 0.      5.00E+04 0.      0.      0.      0.      0.      0.      0.      0.
EOSORE
UNABLE TO LOCATE MATERIAL 99999
IN SUBROUTINE EOSGET
99999      0 -2 0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
UNABLE TO LOCATE MATERIAL 99999
IN SUBROUTINE EOSGET
99999      0 -2 0.      0.      0.      0.      0.      0.      0.      0.      0.      0.
EOSORT
THE DENSITY, = 0.      OR THE TEMPERATURE = 0.      IS NONPOSITIVE
99999      0 -1 0.      0.      0.
THE DENSITY = 0.      OR THE TEMPERATURE = 0.      IS NONPOSITIVE
18760      0 -1 0.      0.      0.
    
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