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Subroutine Package for Calculating

Submous of State and Opacities

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LA-8502-M Manual

UC-34

Issued: October 1981

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

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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 1-3 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 ρ 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 (ρ) .

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.

- 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.

- O 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.

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

- Energy in units of energy per unit volume (for example, ergs/cm 3). This is the energy density ρE commonly computed in hydrodynamic computer codes.
- KFN Indicates the form of the function used to interpolate the data tables.
 - O 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.
 - O 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>O 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.
 - O LMAT not found.
 - N>O LMAT table number (success).
 - N<O 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

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.

- O 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.

- O Energy in units of energy per unit mass (for example, ergs/g). This is the usual E.
- Energy in units of energy per unit volume (for example, ergs/cm³). This is the energy density ρΕ commonly computed in hydrodynamic computer codes.

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

- O 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.

O 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>O 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.

O LMAT not found or the iteration failed to converge.

N>0 LMAT table number (success).

N<O 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 ρ 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.

- O 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 3). This is the energy density ρE commonly computed in hydrodynamic computer codes.

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

- O 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.

O 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>O 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.

O Material not found or iteration failed to converge.

N>0 LMAT table number (success).

N<O 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 ρ and T are independent variables (input) and P(ρ ,T) and E(ρ ,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 (ρ) .

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.

- O 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.

O 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 3). This is the energy density ρE commonly computed in hydrodynamic computer codes.
- KFN Indicates the form of the function used to interpolate the data tables.
 - O 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.
 - O 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>O 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.
 - O LMAT not found.
 - N>O LMAT table number (success).
 - N<O 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 0)

The Rosseland mean opacity⁸ 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 ρ and T are independent variables (input) and 0 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 (ρ) .

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.

- O 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.

- Opacity represented as K in dimensional units of length²/mass.
- 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.
 - O Accurate rational 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.
 - O 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>O 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

O Opacity.

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

O LMAT not found.

N>O LMAT table number (success).

N<O 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,

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

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

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

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^{2,10} 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.⁵ 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 $0.01~g/cm^3$.

```
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
     DECLARE THE COMMON BLOCK WITH THE FILE LABELS
C
     COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
     DIMENSION P(3), E(3)
     INCREASE THE LCM STORAGE AVAILABLE TO EOSMOD
С
     THE MAXIMUM LCM STORAGE IN /SESDAT/ IS LCMX WORDS
C
     LCMX = 20000
     SET THE DENSITY IN KILOGRAMS
C
     AND THE TEMPERATURE IN DEGREES KELVIN
     R = 1.E-5
     T = 300.0
     KEOS = 110
     THE TABLE FOR DEUTERIUM IS CONVERTED BY EOSMOD TO A MIXTURE BY
C
     SCALING THE DENSITY IN SUBROUTINE EOSSLL.
     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
     LMAT = "HELIUM"
     IMATE = 0
     CALL EOSDRT(LMAT,R,T,P,E,KEOS,IMATE)
     PRINT 20, LMAT, P(1)
C
```

```
DECLARE THE NAME OF THE PRIVATE EOS DATA TABLES AND DIRECTORY
C
     LF44 = "MIXLIB"
     LF45 = "MIXDIR"
C
     FIND EOS PRESSURE OF A 90% DEUTERIUM 10% NEON MIXTURE.
C
     THE EOS IS CONTAINED IN THE PRIVATE TABLES MIXLIB AND MIXDIR
C
     LMAT = "D90NE10"
     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")
     CALL EXIT
     END
     SUBROUTINE EOSSCL (LMAT, DSFAC)
     COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KPE
C
     SET UP A NEW SET OF UNITS TO BE USED BY THE CODE
C
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
     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
                          PRESSURE = 5.6817E+04 BARS
     HELIUM
                          PRESSURE = 7.3926E+05 BARS
     D90NE10
```

VI. MATERIALS AVAILABLE

The following materials are currently available using EOSMOD. 11

INC TOTTOWI	_		m	D:	Danaita	SESAME		
Material	EOS	Opacity		Density	Density Minimum	Material		
Name	File	File	Maximum	Minimum		Number		
(LMAT)	Name	<u>Name</u>	(K)	(g/cm^3)	(g/cm^3)	Mumber		
ALLUVIUM (Nevada)	SESAME		4×10 ⁸	0.018	4.7×10 ⁴	7111		
ALUMINUM	SESAME	SESAME	4×10 ⁸	0.021	2.7×10 ³	3710		
$AL203 (= Al_20_3)$	SESAME	000.00	4×10 ⁸	0.031	4.0×10 ⁸	7410		
ARGON		SESAME	. 20	5		5170		
BERYLLIUM	SESAME		4×10 ⁸	0.014	4.0×10 ⁴	2020		
BORON		SESAME	. 10			2330		
BORON CARB(ide)	SESAME	020.22	6×10 ⁴	0.0002	3.2	7081		
BRASS	SESAME		4×10 ⁸	0.066	1.7×10 ⁵	4100		
CALCIUM	DEDIRE	SESAME	420	0.000	21. 25	2030		
CARBON		SESAME				2180		
CH	SESAME	DECIME	4×10 ⁸	0.0082	2.1×10 ⁴	7590		
(= polystyrene)			. 10	0.000		, 52 -		
CH2	SESAME		4×10 ⁸	0.082	1.8×10 ⁴	7170		
(= polyethylene)								
CHLORINE		SESAME				5020		
CHROMIUM		SESAME				3070		
COPPER	SESAME		4×10 ⁸	0.070	1.8×10 ⁵	3330		
DEUTERIUM	SESAME	SESAME	4×10 ⁸	0.0	3.5×10 ³	5263		
GOLD	SESAME		4×10 ⁸	0.15	3.9×10 ⁵	2700		
GRANI TE	SESAME		4×10 ⁸	0.021	5.3×10 ⁴	7390		
HELIUM	SESAME	SESAME	1×10 ⁸	0.0018	4.7×10 ³	5760		
HE (= High	SESAME		4×10 ⁸	0.014	3.7×10 ⁴	8180		
Explosive)								
IRON	SESAME	SESAME	4×10 ⁸	0.061	1.6×10 ⁵	2140		
IRON2	SESAME		1.2×10 ⁴	0.0	12.5	2145		
LEAD	SESAME		4×10 ⁸	0.088	2.3×10 ⁵	3200		
LITHIUM		SESAME				2290		
6LID (= ⁶ LiD)	SESAME		4×10 ⁸	0.0062	1.6×10 ⁴	7240		
6LIH (= ⁶ LiH)	SESAME		4×10 ⁸	0.0053	1.4×10 ⁴	7370		
MAGNESIUM		SESAME	_		_	3080		
MOLYBDENUM	SESAME		4×10 ⁸	0.08	0.2×10 ⁵	2980		
NEON	SESAME		4×10 ⁸	0.011	2.9×10 ⁴	5410		
NICKEL	SESAME		4×10 ⁸	0.069	1.8×10 ⁵	3100		
NITROGEN		SESAME				5000		
OXYGEN		SESAME				5010		
PBX-9502		SESAME				8200		
PHOSPHORUS		SESAME	_			3910		
PLATINUM	SESAME		4×10 ⁸	0.17	2.1×10 ⁴	3730		
POLYE	SESAME		4×10 ⁸	0.0072	1.8×10 ⁴	7170		
(= polyethylene)								

Material Name	EOS File	Opacity File	Temperature Maximum	Density Minimum	Density Minimum	SESAME , Material
(LMAT)	Name	<u>Name</u>	(K)	(g/cm^3)	(g/cm^3)	Number
POLYS (= polystyrene)	SESAME		4×10 ⁸	0.0082	2.1×10 ⁴	7590
POTASSIUM		SESAME				2460
$SIO2 (= SiO_2)$	SESAME	SESAME	4×10 ⁸	0.017	4.4×10 ⁴	7380
SILICON		SESAME				3810
SODIUM	SESAME	SESAME	1×10 ⁴	0.0	1.3	2448
SS (Steel) STAINLESS	SESAME	SESAME	4×10 ⁸	0.062	1.6×10 ⁵	4270
(Steel)	SESAME		4×10 ⁸	0.062	1.6×10 ⁵	4270
STEAM	SESAME		1300	0.0	0.9	7151
SULPHUR		SESAME				4010
TITANIUM		SESAME				2960
TITANIUM N						
(Nitride)		SESAME				6000
$U02 (= U0_2)$	SESAME		3×10 ⁴	0.0	14.3	7432
URANIUM	SESAME		4×10 ⁸	0.15	4.0×10 ⁵	1540
URETHANE	SESAME		4×10 ⁹	0.0099	2.5×10 ⁴	7560
VERMICULIT	SESAME		4×10 ⁸	0.021	5.4×10 ⁴	7520
WATER	SESAME	SESAME	1.8×10 ⁸	2.0×10 ⁻⁶	4.0×10^{2}	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/EODMOD/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 EOSINFO	FORTRAN source of EOSMOD User information	/EOSMOD/EOSFTN /EOSMOD/EOSINFO					
EOSLIB	Compiled FTN Library file of EOSMOD	/EOSMOD/EOSLIB					

File Name	Description	CFS File Location					
MIXDATA MIXDIR	T-7 mixture EOS and opacity data file directory of MIXLIB	/EOSMOD/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	In hydrodynamic codes	/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/SEMV2					
S2DV3	plots SESAME data	/SESAME/S2DV3					
S2DHELP	help package for SES2D	/SESAME/S2DHELP					
DSPLX	computes Hugoniots, isentropes and						
	isobars ¹²	/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

SESAME EOS Units 0 KUNIT R - grams/cm³ E - megajoules/kilogram (= 10¹⁰ ergs/gram) P - gigapascals (= 10¹⁰ dyne/cm²) T - degrees Kelvin $0 - cm^2/gram^1$ 1 CGS Units R - grams/cm³ E - ergs/gram P - microbars (= 1 dyne/cm²) T - degrees Kelvin 0 - cm²/gram Standard International Units (SIU) 2 R - kilograms/meter³ E - joules/kilogram (= 10 ergs/gram) P - pascals (= 10 dyne/cm²)

```
T - degrees Kelvin
0 - meter<sup>2</sup>/kilogram<sup>2</sup>
```

Hydrox EOS Units

```
R - grams/cm<sup>3</sup>
```

E - megabar $cm^3/gram$ (= $10^{12} ergs/gram$)

P - megabar (= 10^{12} dyn/cm^2)

T - degrees Kelvin

 $0 - gram/cm^2$

4 Hydrox Opacity Units

E - megabar $cm^2/gram$ (= $10^{12} ergs/gram$)

P - megabars (= 10^{12} dyne/cm²)

T - electron volts

 $0 - gram/cm^2$

SESAME Opacity Units 5

 $R - grams/cm^3$

E - megajoules/kilogram (= 10¹⁰ ergs/gram)

P - gigapascals (= 10^{10} dyne/cm²)

T - electron volts

 $0 - cm^2/gram^1$

6 LASNEX Units

R - grams/cm³

E - jerks (= 1 erg/gram) P - jerks/cm³ (= 1 dyne/cm²)

T - keV

 $0 - cm^2/gram$

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 This subroutine can be changed easily by the user to write the Appendixes. tables in units other than those provided automatically by the package.

ACKNOWLEDGMENTS

We wish to thank J. Abdallah, Jr., M. Argo, S. Colgate, W. Huebner, J. D. Johnson, G. Kerley, and S. Lyon for their constructive criticism, advice, and help in developing this package.

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APPENDIX A

SUBROUTINE LISTING

User Callable Routines

EOSDRE	(input I	R and	Ε,	output	P	and	T)							24
EOSDRT	(input I	R and	Τ,	output	P	and	E)							28
	(input 1													32
EOSIRT	(input I	R and	Т,	output	P	and	E)							35
EOSORT	(input I	R and	T.	output	0)			_	_	_	_	_		3,5

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

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

```
125 C
                KEDS = 110
126 C
                IMATE = O
127 C
                CALL EDSORE(LMAT, R, E, P, T. KEDS, IMATE)
128 C
                PRINT 10,P(1)
             10 FORMAT(" PRESSURE = ",E10.2," MICROBARS")
129 C
130 C
                CALL EXIT
131 C
                END
132 C
          * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
133 C
134 C
135 C
          * REFERENCE- J. M. HYMAN, M. M. KLEIN
136 C
                       EDSMOD- 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
          LEVEL 2, TBLS
          COMMON /S20IRX/ LCMX, NRS, LCFW(10.3)
146
          COMMON /SESDATX/ TBLS(11000)
147
148
          COMMON /INTOROX/ KFN
149
          COMMON /SESINX/ IRC, IDT, RHO, ENERGY, KBR, IFL
          COMMON /SESOUTX/ PRES(3), TEMP(3)
150
151 C
          COMMON BLOCKS FOR THE EOSMOD ROUTINES
152 C
          COMMON /EDSCZ/ LOUT
153
          COMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
154
          COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
155
156 C
157
          DIMENSION T(3), P(3)
          DATA KEDSS /-99/, KBRS/O/, KFNS/O/, LMATS/1H /
158
159 C
160 C
161 C
          IDT=1 LOCATOR OF DATA TYPE FOR IR, GETINVX(,, IOT,...)
162 C
163 C
          FOR THE INVERTED SESAME FORMAT
164
          IOT=1
165 C
166 C
          CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
          IF(KEOSS.NE.KEDS.OR.LMAT.NE_LMATS) GO TO 5
167
168
          LMATS=LMAT
          KBR=KBRS
169
          KFN=KFNS
170
          GD TD 10
171
        5 CONTINUE
172
173 C
174 C
          CHECK THE VALIDITY OF THE INPUT PARAMETERS
          CALL EOSKUT(KEOS, KBR, KUNIT, KREPE, KFN, KEOSS, KBRS, KFNS. IMATE. IDT
175
176
          1 , IERR)
          IF(IERR.LT.O) GD TD 80
177
178
       10 CONTINUE
179 C
180 C
          FIND THE MATERIAL
          IF (IMATE.GT.O) GO TO 60
181
          CALL EDSGET(LMAT, KUNIT, KREPE, IMATE, IDT, IERR)
182
          IF(IMATE.LE.O.DR.IERR.LT.O) GD TO 80
183
184
       60 CONTINUE
185 C
           TRANSFER INPUT CALL PARAMETERS TO COMMON BLOCK
186 C
```

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

```
SUBROUTINE EOSORT (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) DF A MATERIAL (LMAT)
           THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
7 C
8 C
           ENERGY (E) USING THE LASL T-4 SESAME EDS ROUTINES
9 C
10 C
        * INPUT VARIABLES-
11 C
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
                  NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
16 C
17 C
           R = DENSITY (RHD)
18 C
19 C
           T = TEMPERATURE
20 C
21 C
22 C
           KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
23 C
                  AND RETRIEVE THE DATA FILE. KEDS HAS FOUR DECIMAL DIGITS.
24 C
25 C
           KEDS = 1000+KBR + 100+KUNIT + 10+KREPE + KFN WHERE
26 C
            KBR = COMPUTATIONAL MODE FLAG TO INDICATE WHICH
27 C
28 C
                  QUANTITIES AND THEIR PARTIAL DERIVATIVES ARE TO
29 C
                  BE CALCULATED AND RETURNED BY THE PACKAGE.
30 C
                         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
               O (SESAMEE) R-G/CC,T-DEG.K,D-CM++2/G,P-GPA,E-MJ/KG
36 C
               1 (CGS) R-G/CC, T-DEG.K, D-CM++2/GM, P-MUBR, E-ERGS/GM
37 C
               2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,D-M**2/KG
38 C
               3 (HYDROXE) R-G/CC.T-DEG.K.P=MBR.E-MBR+CC/GM.D-CM++2/G
               4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR+CC/G,D-CM++2/G
39 C
40 C
               5 (SESAMED) R-G/CC, T-EV. D-CM++2/G.P-GPA, E-MJ/KG
               6 (LASNEX) R-G/CC,T-KEV,D-CM++2/GM,P-JRKS/CC,ED-JRKS/CC
41 C
42 C
43 C
               LEGEND-
                       R = DENSITY
44 C
45 C
                       T = TEMPERATURE
46 C
                       O = OPACITY
47 C
                       P = PRESSURE
48 C
                       E = INTERNAL ENERGY
49 C
50 C
                       CC = CUBIC CENTIMETER
                       CM = CENTIMETER
51 C
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
                       KEV = KILO ELECTRON VOLTS
58 C
                       KG = KILOGRAM
59 C
60 C
         *
                       M = METER
61 C
                       MBR = MEGABAR
62 C
                       MUBR = MICROBAR
```

```
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
                    PER UNIT VOLUME
67 C
68 C
                O ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-
                    UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
69 C
                 1 ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
70 C
71 C
                    UNITS OF ERGS/CM++3 WHEN KUNIT = 1. THIS IS THE ENERGY
                    DENSITY RHO+E COMMONLY COMPUTED IN HYDRODYNAMIC
72 C
73 C
                    COMPUTER CODES.
74 C
75 C
            KFN = KINO OF FUNTION INTERPOLATION IN THE TABLES
76 C
              = O 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.
              =O CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
82 C
83 C
                 IF NOT, SEARCH FOR THE FILE, COMVERT IT TO THE PROPER UNITS
84 C
                 AND COPY IT INTO LCM USING THE STANDARD SESAME FORMAT.
85 C
              >O EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
86 C
                 BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EDSORE,
87 C
                 EOSIPT OR EOSIRT. THIS DPTION 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
                 ITS PARTIAL DERIVATIVES. THIS ARRAY MUST BE DIMENSIONED
93 C
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 (OP/OR)
            P(3) = TEMPERATURE DERIVATIVE OF THE PRESSURE (OP/DT)
98 C
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/OT)
107 C
108 C
          * IMATE = INDICATES THE SUCCESS DR FAILURE OF
109 C
                    LOCATING AND LOADING THE DATA FILE FOR LMAT.
110 C
111 C
                   = N>O MATERIAL TABLE NUMBER (SUCCESS)
112 C
                    0
                         MATERIAL (LMAT) NOT IN LIBRARY
113 C
                        (N>1) INSUFFICIENT STORAGE
114 C
                        THE LCM STORAGE MUST BE INCREADED BY AT LEAST
115 C
                        N STORAGE LOCATIONS. SEE THE EDSMOD MANUAL
116 C
117 C
          * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
118 C
119 C
          * SAMPLE ORIVER PROGRAM-
120 C
121 C
                PROGRAM TST(OUTPUT)
                DIMENSION P(3),E(3)
122 C
123 C
                LMAT = "HELIUM"
124 C
                R = 0.001
```

```
125 C
                T = 300.0
                KEDS = 110
126 C
                IMATE = O
127 C
                CALL EDSORT (LMAT.R.T.P.E.KEGS, IMATE)
128 C
129 C
                PRINT 10,P(1)
             10 FORMAT( PRESSURE = ",E10.2, MICROBARS")
130 C
131 C
                CALL EXIT
132 C
                FNO
133 C
          * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOO PACKAGE
134 C
135 C
          * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
136 C
137 C
138 C
            REFERENCE- J. M. HYMAN, M. M. KLEIN
                       EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
139 C
140 C
                        EQUATIONS-OF-STATE AND OPACITIES
                       LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
141 C
142 C
143 C
          + DATE- MARCH 6, 1980
144 C
145 C
          _____
146 C
147 C
          COMMON BLOCKS FOR THE SESAME EDS ROUTINES
148
          LEVEL 2, TBLS
149
          COMMON /S2DIRX/ LCMX, NRS., LCFW(10,3)
          COMMON /SESDATX/ TBLS(11000)
150
151
          COMMON /INTOROX/ KFN
          COMMON /SESINX/ IRC, IOT, RHO, TEMP, KBR, IFL
152
          COMMON /SESOUTX/ PRES(3), ENERGY(3)
153
154 C
          COMMON BLOCKS FOR THE EOSMOD ROUTINES
155 C
          COMMON /EDSCZ/ LOUT
COMMON /EDSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
156
157
          COMMON /EDSC1/ LU41, LU42, LU43, LU44, LU45
158
          COMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
159
          COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
160
161 C
          DIMENSION E(3), P(3)
162
          DATA KEDSS /-99/, KBRS/O/, KFNS/O/, LMATS/1H /
163
164 C
165 C
166 C
          IOT=3 LOCATOR OF DATA TYPE FOR IR, GETEOSX(,, IOT,...)
167 C
168 C
          FOR THE STANDARD SESAME FORMAT
169
          IOT = 3
170 C
          CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
171 C
          IF(KEDSS.NE.KEDS.OR.LMAT.NE.LMATS) GO TO 5
172
          LMATS=LMAT
173
174
          KBR=KBRS
175
          KFN=KFNS
          GD TD 10
176
        5 CONTINUE
177
178 C
          CHECK THE VALIDITY OF THE INPUT PARAMETERS
179 C
          CALL EDSKUT(KEDS, KBR, KUNIT, KREPE, KFN, KEDSS, KBRS, KFNS, IMATE, IDT
180
          1 , IERR)
181
182
          IF(IERR.LT.O) GO TO 80
183
        10 CONTINUE
184 C
185 C
          FIND THE MATERIAL
           IF (IMATE_GT.O) GD TD 60
186
```

```
187
          CALL EDSGET(LMAT, KUNIT, KREPE, IMATE, 10T, IERR)
188
          IF(IMATE_LE.O.DR.IERR.LT.O) GO TO 80
       60 CONTINUE
189
190 C
          TRANSFER INPUT CALL PARAMETERS TO COMMON BLOCK
191 C
          TEMP=T
192
          RHO=R
193
194
          IRC=IR(IMATE,3)
195 C
196 C
          CALCULATE THE EQUATION OF STATE
          CALL T40ATX
197
            * T40ATX DOES NOT RETURN AN EROR FLAG FOR DATA OUT OF RANGE
198 C
199 C
200
       75 CONTINUE
          RESTORE OUTPUT VARIABLES FOR RETURN TO CALL
201 C
202
          P(1)=PRES(1)
          P(2)=PRES(2)
203
204
          P(3)=PRES(3)
          E(1)=ENERGY(1)
205
          E(2)=ENERGY(2)
E(3)=ENERGY(3)
206
207
208 C
209
       80 CONTINUE
210
          IFLP=IERR
          RETURN
211
212
          ENO
```

```
SUBROUTINE EDSIPT (LMAT, P.T.R.E.KEDS, IMATE)
2 C
 3 C
         4 C
5
  С
         * PURPOSE-
6 C
            GIVEN THE PRESSURE (P) AND TEMPERATURE (T) OF A MATERIAL (LMAT)
            THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
7
  С
8 C
            ENERGY (E) USING THE LASL T-4 SESAME EQUATION OF STATE ROUTINES
9
  C
         * AN ITERATIVE METHOO IS USED TO INTERPOLATE THE TABLES
10 C
11 C
12 C
         * INPUT VARIABLES-
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
            P = PRESSURE
19 C
20 C
21 C
            T = TEMPERATURE
22 C
            KEDS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
23 C
                  AND RETRIEVE THE DATA FILE. KEOS HAS FOUR DECIMAL DIGITS.
24 C
25 C
26 C
            KEDS = 100+KUNIT + 10+KREPE WHERE
27 C
28 C
            KUNIT= KIND OF UNITS
               O (SESAMEE) R-G/CC,T-DEG.K,D-CM++2/G,P-GPA,E-MJ/KG
29 C
30 C
               1 (CGS) R-G/CC,T-DEG.K,D-CM++2/GM,P-MUBR,E-ERGS/GM
               2 (SIU) R-KG/M++3,T-DEG_K,P-PA,E-J/KG,D-M++2/KG
31 C
               3 (HYDROXE) R-G/CC,T-DEG.K,P=MBR,E-MBR+CC/GM,D-CM++2/G
4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR+CC/G,D-CM++2/G
32 C
33 C
               5 (SESAMED) R-G/CC,T-EV,D-CM++2/G,P-GPA,E-MJ/KG
34 C
               6 (LASNEX) R-G/CC,T-KEV,D-CM++2/GM,P-JRKS/CC,ED-JRKS/CC
35 C
36 C
37 C
                LEGENO-
38 C
                       R = DENSITY
                       T = TEMPERATURE
39 C
                       D = OPACITY
40 C
41 C
                       P = PRESSURE
42 C
                       E = INTERNAL ENERGY
43 C
44 C
                       CC = CUBIC CENTIMETER
45
   С
                       CM = CENTIMETER
46 C
                       DEG. K = DEGREES KELVIN
47 C
                        EV = ELECTRON VOLT
48 C
                        G = GRAM
                        GPA = GIGA PASCALS
49 C
50 C
                        J = JOULES
                        JRKS = JERKS
51 C
52 C
                       KEV = KILO ELECTRON VOLTS
                        KG = KILDGRAM
53 C
                        M = METER
54 C
55 C
                        MBR = MEGABAR
                        MUBR = MICROBAR
56 C
                        PA = PASCAL
57 C
58 C
            KREPE = COMPUTATION FLAG TO INDICATE WHETHER E IS
59 C
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-
```

```
UNITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL E.
63 C
                1 ENERGY IN UNITS OF ENERGY PER UNIT VOLUME. FOR EXAPMLE-
64 C
                   UNITS OF ERGS/CM++3 WHEN KUNIT = 1. THIS IS THE ENERGY
                   DENSITY RHO+E COMMONLY COMPUTED IN HYDRODYNAMIC
66 C
                   COMPUTER CODES.
67 C
68 C
           IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
69 C
                  IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
70 C
71 C
                  PREVIOUSLY LDAGED FILE.
             =O CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
72 C
73 C
                IF NOT, SEARCH FOR THE FILE, COMVERT IT TO THE PROPER UNITS
74 C
                AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
75 C
             >O EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
                BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSORE,
76 C
                EDSIPT OR EDSIRT. THIS OPTION IS FASTER THAN IMATE = O
77 C
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
           E = INTERNAL ENERGY
85 C
86 C
         * IMATE = INDICATES THE SUCCESS OR FAILURE OF
                   LOCATING AND LOADING THE DATA FILE FOR LMAT.
87 C
88 C
                   - N>O MATERIAL TABLE NUMBER (SUCCESS)
89 C
90 C
                   0
                        MATERIAL (LMAT) NOT IN LIBRARY
91 C
                       (N>1) INSUFFICIENT STORAGE
                        THE LCM STORAGE MUST BE INCREADED BY AT LEAST
92 C
93 C
                        N STORAGE LOCATIONS. SEE THE EOSMOO MANUAL
94 C
95 C
          * REMARKS- THIS SUBROUTINE IS PART DF THE EOSMOO PACKAGE
96 C
97 C
           SAMPLE DRIVER PROGRAM-
98 C
99 C
                PROGRAM TST(OUTPUT)
               DIMENSION P(3),E(3)
100 C
101 C
                LMAT = "HELIUM"
                R = 0.001
102 C
103 C
                T = 300.0
104 C
               KEDS = 110
105 C
                IMATE = O
106 C
                CALL EDSIPT(LMAT, P, T, R, E, KEOS, 1MATE)
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
                       EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
                       EQUATIONS-OF-STATE AND OPACITIES
118 C
                       LDS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
119 C
120 C
121 C
          * DATE- MARCH 6, 1980
122 C
123 C
          124 C
```

```
125 C
          COMMON BLOCKS FOR THE SESAME EDS ROUTINES
          LEVEL 2, TBLS
126
127
          COMMON /S20IRX/ LCMX, NRS, LCFW(10,3)
          COMMON /SESDATX/ TBLS(11000)
128
          COMMON /SESINX/ DUM(4), KBR, DUM1
129
          COMMON /INTOROX/ KFN
130
131 C
          COMMON BLOCKS FOR THE EOSMOD ROUTINES
132 C
          COMMON /EOSCZ/ LOUT
133
          COMMON /EDSC3/ INIT. IRDIM, IR(60,3), KUP(60,3)
134
          COMMON /EOSC4/ NTABLE, NTABLO, IFLP, LCNT
135
136 C
137
          DIMENSION R(3), E(3)
          DATA KEDSS /-99/,KBRS/O/,KFNS/O/,LMATS/1H /
138
139 C
140 C
141 C
           IOT=1 LOCATOR OF DATA TYPE FOR IR, GETINVX(,, IOT,...)
142 C
          FOR THE INVERTED SESAME FORMAT
143 C
144
           IDT=1
145 C
           CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
146 C
           IF(KEOSS.NE.KEOS.OR.LMAT.NE.LMATS) GO TO 5
147
148
           LMATS=LMAT
149
           KBR=KBRS
150
          KFN=KFNS
151
           GD TD 10
        5 CONTINUE
152
153 C
           CHECK THE VALIDITY OF THE INPUT PARAMETERS
154 C
           CALL EDSKUT(KEDS, KBR, KUNIT, KREPE, KFN, KEDSS, KBRS, KFNS, IMATE, IDT
155
156
          1 , IERR)
157
           IF(IERR.LT.O) GD TD 75
158
        10 CONTINUE
159 C
160 C
           FIND THE MATERIAL
           IF (IMATE.GT.O) GD TD 60
161
           CALL EDSGET(LMAT, KUNIT, KREPE, IMATE, IOT, IERR)
162
           IF(IMATE.LE.O.OR.IERR.LT.O) GO TO 75
163
164
        60 CONTINUE
165 C
           CALCULATE THE EQUATION OF STATE
166 C
           CALL T4PTREX (IR(IMATE, 1), 1, TBLS, P, T, R, E, IERR)
167
168 C
           PRINT AN ERROR MESSAGE IF TAPTREX FAILES TO CONVERGE
169 C
           IF (IERR_EQ.O) WRITE(LOUT,80) LMAT,P,T
170
           IF (IERR.EQ.O) IMATE=O
171
172 C
        75 CONTINUE
173
174
           IFLP=IERR
           RETURN
175
176 C
        80 FORMAT(" FAILED TO CONVERGE WHEN ITERATING ON THE INVERTED",
177
          1 /." EOS TABLES IN SUBROUTINE TAPTREX CALLED BY EOSIPT"./.
178
         * 2 " THE REQUESTED VALUES FOR RHO, PRESSURE, TEMPERATURE AND ENERGY"
179
          2 ./." MAY BE OUT OF RANGE OR NEAR THE EDGE OF THE TABLE"./.
3 " CHECK THE EDSMOD WRITEUP FOR THE DATA RANGE"./.
180
181
182
          1 " LMAT =",A10,
          4 " PRESSURE =", 1PE12_4." TEMPERATURE =", 1PE12_4)
183
184
           ENO
```

```
SUBROUTINE EOSIRT (LMAT,R,T,P,E,KEOS,IMATE)
2 C
         ______
3 C
4 C
5 C
         * PURPDSE -
           GIVEN THE DENSITY (R) AND TEMPERATURE (T) OF A MATERIAL )
6 C
            (LMAT), THIS SUBROUTINE RETURNS THE PRESSURE (P) AND INTERNAL
7
  C
            ENERGY (T) USING THE LASL E-4 SESAME EQUATION OF STATE ROUTINES
8
  C
9
  C
         * AN ITERATIVE METHOD IS USED TO INTERPOLATE THE TABLES
10 C
          SUBROUTINE EDSORT USES A FASTER DIRECT METHOD
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
20 C
            R = DENSITY (RHD)
21 C
22 C
            T = TEMPERATURE
23 C
            KEOS = MULTIPLE PARAMETER FLAG TO DESCRIBE HOW TO WRITE
24 C
25 C
                  AND RETRIEVE THE DATA FILE. KEDS HAS FOUR DECIMAL DIGITS,
26 C
            KEDS = 100+KUNIT + 10+KREPE WHERE
27 C
28 C
29 C
            KUNIT= KIND OF UNITS
               O (SESAMEE) R-G/CC,T-DEG.K.D-CM++2/G,P-GPA,E-MJ/KG
30 C
               1 (CGS) R-G/CC.T-DEG.K.D-CM*+2/GM.P-MUBR.E-ERGS/GM
31 C
               2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,D-M**2/KG
32 C
33 C
               3 (HYDROXE) R-G/CC,T-DEG_K,P=MBR,E-MBR+CC/GM,D-CM++2/G
               4 (HYDROXD) R-G/CC, T-KEV, P-MBR, E-MBR+CC/G.D-CM++2/G
34 C
               5 (SESAMED) R-G/CC, T-EV, D-CM++2/G, P-GPA, E-MJ/KG
35 C
               6 (LASNEX) R-G/CC, T-KEV, D-CM++2/GM, P-JRKS/CC, ED-JRKS/CC
36 C
37 C
38 C
                LEGEND -
39 C
                       R = DENSITY
40 C
                       T = TEMPERATURE
41
   С
         *
                       D = OPACITY
42 C
                       P = PRESSURE
                       E = INTERNAL ENERGY
43 C
44 C
                       CC = CUBIC CENTIMETER
45 C
         .
                       CM = CENTIMETER
46 C
                       DEG. K = DEGREES KELVIN
47 C
                       EV = ELECTRON VDLT
48 C
                       G = GRAM
49 C
         *
                       GPA = GIGA PASCALS
50 C
51 C
                       J = JOULES
52 C
                       JRKS = JERKS
                       KEV = KILO ELECTRON VOLTS
53 C
54 C
                       KG = KILDGRAM
                       M = METER
55 C
56 C
                       MBR = MEGABAR
57 C
                       MUBR = MICROBAR
                        PA = PASCAL
58 C
59 C
            KREPE = COMPUTATION FLAG TO INDICATE WHETHER T 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-
63 C
                    LINITS OF ERGS/GRAM WHEN KUNIT = 1. THIS IS THE USUAL T.
64 C
                 I 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+T COMMONLY COMPUTED IN HYDRODYNAMIC
67 C
                    COMPUTER CODES.
68 C
69 C
         * IMATE = INDICATES WHETHER TO LOAD THE DATA FILE IF
70 C
                   IT ODES NOT EXIST FOR LMAT DR GO DIRECTLY TO A PREVIOUSLY LOADED FILE.
71 C
72 C
             =O CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
73 C
                 IF NOT, SEARCH FOR THE FILE, COMVERT IT TO THE PROPER UNITS
74 C
                 AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
75 C
             >O EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
76 C
                 BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSORE, EOSIPT OR EOSIRT. THIS OPTION IS FASTER THAN IMATE = 0
77 C
78 C
                 BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
79 C
80 C
         * OUTPUT VARIABLES-
81 C
82 C
83 C
          * P = PRESSURE
84 C
85 C
         * E = INTERNAL ENERGY
86 C
          * IMATE = INDICATES THE SUCCESS OR FAILURE OF
87 C
                    LOCATING AND LOADING THE DATA FILE FOR LMAT.
88 C
89 C
                   = N>O MATERIAL TABLE NUMBER (SUCCESS)
90 C
                         MATERIAL (LMAT) NOT IN LIBRARY
91 C
                    0
                        (N>1) INSUFFICIENT STORAGE
92 C
                        THE LCM STORAGE MUST BE INCREADED BY AT LEAST
93 C
                        N STORAGE LOCATIONS. SEE THE EDSMOD MANUAL
94 C
95 C
          * REMARKS- THIS SUBROUTINE IS PART OF THE EDSMOD PACKAGE
96 C
97 C
          * SAMPLE DRIVER PROGRAM-
99 C
                PROGRAM TST(OUTPUT)
100 C
                DIMENSION P(3),T(3)
101 C
                LMAT = "HELIUM"
102 C
103 C
                R = 0.001
                T = 300.0
104 C
105 C
                KEOS = 110
                IMATE .= 0
106 C
                CALL EDSIRT(LMAT,R,T,P,E,KEDS,IMATE)
107 C
                PRINT 10,P(1)
108 C
109 C
             10 FORMAT(" PRESSURE = ",E10.2," MICROBARS")
                CALL EXIT
110 C
111 C
                ENO
112 C
            REMARKS- THIS SUBROUTINE IS PART OF THE EDSMOD 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
                        EDSMOD- 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
```

```
125 C
126 C
          COMMON BLOCKS FOR THE SESAME EOS ROUTINES
127
          LEVEL 2. TBLS
          COMMON /S2DIRX/ LCMX, NRS, LCFW(10.3)
128
          COMMON /SESDATX/ TBLS(11000)
129
          COMMON /SESINX/ DUM(4), KBR, DUM1
130
          COMMON /INTORDX/ KFN
131
132 C
          COMMON BLOCKS FOR THE EOSMOD ROUTINES
133 C
134
          COMMON /EOSCZ/ LOUT
          CDMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
CDMMON /EDSC4/ NTABLE, NTABLO, FIFLP, LCNT
135
136
137 C
138
          DIMENSION P(3), E(3)
139
          DATA KEOSS /-99/, KBRS/O/, KFNS/O/, LMATS/1H /
140 C
141 C
           *****************************
142 C
143 C
           IDT=1 LOCATOR OF DATA TYPE FOR IR.GETINVX(., IDT,...)
144 C
          FOR THE INVERTED SESAME FORMAT
145
           IOT=1
146 C
           CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
147 C
           IF(KEOSS.NE.KEOS.OR.LMAT, NE.LMATS) GO TO 5
148
149
           LMATS=LMAT
150
          KBR=KBRS
151
           KFN=KFNS
152
           GD TD 10
153
        5 CONTINUE
154 C
           CHECK THE VALIDITY OF THE INPUT PARAMETERS
155 C
           CALL EOSKUT(KEOS, KBR, KUNIT, KREPE, KFN, KEOSS, KBRS, KFNS, IMATE, IOT
156
          1 , IERR)
157
158
           IF(IERR_LT.O) GO TO 75
        10 CDNTINUE
159
160 C
           FIND THE MATERIAL
161 C
           IF (IMATE.GT_O) GD TD 60
162
           CALL EDSGET(LMAT.KUNIT, KREPE, IMATE, IDT, IERR)
163
164
           IF(IMATE.LE.O.DR.IERR.LT.O) GO TO 75
165
        60 CONTINUE
166 C
           CALCULATE THE EQUATION DF STATE
167 C
           CALL TARTPEX (IR(IMATE, 1), 1, TBLS, R, T, P, E, IERR)
168
169 C
           PRINT AN ERROR MESSAGE IF TARTPEX FAILED TO CONVERGE
170 C
171
           IF (IERR.EQ.O) WRITE(LOUT,80) LMAT,R,T
           IF (IERR.EQ.O) IMATE=O
172
173 C
        75 CONTINUE
174
175
        IFLP=IERR
           RETURN
176
177 C
        80 FORMAT(" FAILED TO CONVERGE WHEN ITERATING ON THE INVERTED".
178
          1 /," EDS TABLES IN SUBROUTINE TAPTREX CALLED BY EDSIRT"./.
179
              THE REQUESTED VALUES FOR RHD, PRESSURE, TEMPERATURE AND ENERGY"
180
          2 ,/," MAY BE OUT OF RANGE OR NEAR THE EDGE OF THE TABLE"./.
181
          3 " CHECK THE EDSMOD WRITEUP FOR THE DATA RANGE",/,
182
            " LMAT =",A10,
183
          4 " DENSITY =", 1PE12.4," TEMPERATURE =", 1PE12.4)
184
185
           ENO
```

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

```
63 C
                      UNITS OF LENGTH.
64 C
             KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES
65 C
              = O RATIONAL APPROXIMATIONS (ACCURATE)
66 C
67 C
               = 1 BILINEAR APPROXIMATIONS (FAST)
68 C
          * IMATO = INDICATES WHETHER TO LDAD THE DATA FILE IF
69 C
                   IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
70 C
71 C
                   PREVIOUSLY LOADED FILE.
              =O CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.

IF NDT, SEARCH FOR THE FILE, COMVERT IT TO THE PROPER UNITS
72 C
73 C
74 C
                 AND COPY IT INTO LCM USING THE INVERTED SESAME FORMAT.
              >O EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
75 C
                 BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EDSORT.
76 C
                 THIS OPTION IS FASTER THAN IMATO = O
77 C
                 BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
78 C
79 C
          * DUTPUT VARIABLES-
80 C
81 C
            O = OPACITY
82 C
83 C
          * IMATO = INDICATES THE SUCCESS OR FAILURE OF
84 C
                     LOCATING AND LOADING THE DATA FILE FOR LMAT.
85 C
86 C
                   NO MATERIAL TABLE NUMBER (SUCCESS)
O MATERIAL (LMAT) NOT IN LIBRARY
87 C
88 C
                         (N>1) INSUFFICIENT STORAGE
89 C
                         THE LCM STORAGE MUST BE INCREADED BY AT LEAST
90 C
                         N STORAGE LOCATIONS. SEE THE EOSMOD MANUAL
91 C
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)
                DIMENSION P(3),E(3)
98 C
99 C
                LMAT = "HELIUM"
                R = 0.001
100 C
101 C
                T = 300.0
                KDPC = 500
102 C
                IMATO = O
103 C
104 C
                CALL EDSDRT(LMAT,R,T,D,KOPC,IMATO)
105 C
                PRINT 10.P(1)
             10 FDRMAT(" DPACITY = ".E10.2)
106 C
107 C
                CALL EXIT
108 C
                ENO
109 C
110 C
          * EXTERNALS AND COMMON BLOCKS-
             QLOG10 = QUICK VERSION OF ALDG10
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
117 C
          * REFERENCE- J. M. HYMAN, M. M. KLEIN
                        EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
118 C
119 C
                        EQUATIONS-OF-STATE AND OPACITIES
                        LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
120 C
121 C
          * DATE- MARCH 6, 1979
122 C
123 C
                ...........
124 C
```

```
125 C
           COMMON BLOCKS FOR THE SESAME EOS ROUTINES
126 C
           DIMS TBLS, LCMX, NLBUF, LCFW(,), ZZ()
127 C
           LEVEL 2. TBLS
128
129
           COMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
          COMMON /SESDATX/ TBLS(11000)
COMMON /INTORDX/ KFN
130
131
           COMMON /SESINX/ IRC, IOT, RHO, TEMP, KBR, IFL
132
           COMMON /SESOUTX/ OPACITY(3), PLANKO(3)
133
134 C
135 C
           COMMON BLOCKS FOR THE EOSMOD ROUTINES
           COMMON /EOSCZ/ LOUT
136
           COMMON /EDSCCO/ TFACD, RFACD, OFACO, KREPO
137
          COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
COMMON /EOSC3/ INIT, IROIM, IR(60,3), KUP(60,3)
138
139
           COMMON /EDSC4/ NTABLE, NTABLO, IFLP, LCNT
140
141 C
           DATA KOPCS /-99/, KFNS/O/, LMATS/1H /
142
143 C
144 C
145 C
            CHECK POSITIVITY OF INPUT PARAMETERS
146 C
           IF((T.GT.O.O).AND.(R.GT.O.O)) GO TO 4
147
148
           [MATD=-1
149 C
150
           WRITE(LOUT, 20)R, T
       20 FDRMAT(" THE DENSITY =", 1E12.4," DR THE TEMPERATURE ="
1 ,E12_4," IS NONPOSITIVE")
151
152
153 C
           GD TD 75
154
155
        4 CONTINUE
156 C
           SET INITIAL VARIABLES FOR OPACITY TABLES
157 C
158 C
           IOT=2 LOCATOR OF DATA TYPE FOR IR AND SUB. GETPRX(,,IOT,,...)
           IDT=2
159
160 C
           CHECK IF THE UNITS HAVE CHANGED SINCE THE LAST CALL
161 C
162
           IF(KOPCS.NE.KOPC.OR.LMAT.NE.LMATS) GD TO 5
           KFN=KFNS
163
164
           LMATS=LMAT
165
           KOPCS=KOPC
           GD TD 10
166
         5 CONTINUE
167
168 C
169 C
           UNSCRAMBLE MULTIPLE FLAG KOPC
170
           CALL EDSKUT(KOPC, KDUMMY, KUNIT, KREPO, KFN, KOPCS, KBRS, KFNS, IMATO, IDT
          1 , IERR)
171
172
           IF(IERR.LT.O) GD TO 75
        10 CONTINUE
173
174 C
175 C
           FIND THE MATERIAL
176
           IF (IMATD.GT.O) GD TD 60
           CALL EDSGET (LMAT, KUNIT, KREPO, IMATO, IOT, IERR)
177
           IF(IMATO.LE.O.OR.IERR.LT.O) GO TD 75
178
179 C
        60 CONTINUE
180
181 C
           TRANSFER INPUT CALL PARAMETERS TO COMMON BLOCK
182 C
           TEMP=QLDG10(T)
183
           RHO=QLOG10(R)
184
185
           KBR=1
           IRC=IR(IMATO,2)
186
```

```
187 C
188 C CALCULATE THE EQUATION OF STATE
189 CALL T40ATX
190 C T40ATIX ODES NOT RETURN AN ERROR FLAG
191 C FOR DATA OUT OF BOUNDS
192 C
193 C RESTORE OUTPUT VARIABLES FOR RETURN TO CALL
194 IFLP=IERR
195 D=10.++OPACITY(1)
196 75 CONTINUE
197 RETURN
198 END
```

INTERNAL SUBROUTINES

	(initializes all the common block variables) .			
EOSCON	(defines the table conversion factors)	•		. 46
EOSDSL	(allows the user to scale the density)			. 49
	(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

```
SUBROUTINE EDSBEG
 2 C
 3 C
 5 C
           PURPOSE -
 6
   C
               TO INITIALIZE ALL COMMON BLDCKS IN ONE PLACE OF CODE
 7
   C
 8
         * INPUT VARIABLES-
 9 C
           NONE
10 C
11 C
         * DUTPUT VARIABLES-
12 C
         * ALL DUTPUT IS AT COMPILE TIME IN THE COMMON BLOCKS.
13 C
         . THIS ALLOWS THE USER AN EASY WAY TO CHANGE THE VARIABLES
14
   C
         * BY SETTING THEM TO ANY OTHER VALUE AT EXECUTION
         * TIME IN THEIR MAIN PROGRAM
15 C
16 C
17 C
18 C
19 C
         * LOCALLY DEFINED SESAME VARIABLES-
20 C
           TBLS = ARRAY FDR STDRAGE OF THE EOS TABLES
21 C
            LCMX = LENGTH OF THE TBLS ARRAY
            NRS = UPPER BOUND ON THE NUMBER OF MAT REGIONS LCFW(NRS.)
22 C
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
            IOS2 = SESAME MATERIAL NUMBER
27 C
            TBLS = NAME OF AN ARRAY DESIGNATED FOR THE STORAGE OF TABLES
            LCNT = CRRRENT WORD IN THE ARRAY TBLS
28 C
29 C
            LU41 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SES2CL
            LU42 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SESAME
LU43 = UNIT NUMBER ASSIGNED TO SESAME/8 FILES
30 C
31 C
            LU44 = UNIT NUMBER ASSIGNED TO MIXLIB (MIXTURES)
32 C
33 C
            LU45 = UNIT NUMBER ASSIGNED TO MIXLIB DIRECTORY.
34 C
            KFN = O RATIONAL APPRDXIMATIONS (ACCURATE)
35 C
            KFN = 1 BILINEAR APPROXIMATIONS (FAST)
            ZB (DUTPUT FROM GETINVX) AT. CHARGE, AT. CHG++2, MASS
36 C
37 C
            IOT = DATA TYPE INDICATOR
38 C
            MIO (IO) MATERIAL IO =1 INVERSE TABLES =2 OPACITY
39 C
40 C
         * EXTERNAL FILES TO HANDLE EDS. OPACITIES AND MIXTURES
41 C
         * SES2CL - CLASSIFIED SESAME LIBRARY
         * SESAME - CUCLASSIFIED SESAME LIBRARY
42 C
43 C
            SESAME - OPACITY TABLE FROM T4
44 C
            MIXLIB - PRIVATE (EOS, OPC) TABLES CREATED BY MIXB(OR MIXER)
45 C
            MIXOIR - DIRECTORY OF MIXTURES ON MIXLIB ( NAME, NO (A10.13))
46 C
47 C
         * EXTERNALS AND COMMON BLOCKS-
48 C
            SESAME ROUTINES- S2GET, S2EDS
49 C
            SESAME ROUTINES MATCHKX, TABRANX, INBUFRX, OPACKX, ISRCHKX.
50 C
                T4INTPX.GETINVX.RATFN1X.T40ATIX.INV301X.T4RTPEX
51 C
             SESAME COMMON BLOCKS-S20IRX, RTBLK2X, SESOATX, SESINX, SESOUTX, INTORDX
52 C
            EOSMOO COMMON BLOCKS- EOSC1, -7
53 C
            EDSMOD COMMON (ALSO INSERTED INTO GETINVX) EDSCCE, EDSCCD
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
                       EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
61 C
                       EQUATIONS-OF-STATE AND OPACITIES
62 C
                       LOS ALAMOS SCIENTIFIC LABORATORY RPT..LA-8502-M.1980
```

```
63 C
           + DATE- MARCH 6, 1980
64 C
65 C
66 C
67 C
           COMMON BLOCKS FOR THE SESAME EDS ROUTINES
68 C
69 C
           DIMS TBLS, LCMX, NLBUF, LCFW(,), ZZ()
70 C
           MUST BE WATCHED IF CHANGING DIMENSIONS
71 C
           APPEAR IN RTBLK2X, SESDATX, S20IRX, DATA LCMX...
           LEVEL 2, TBLS
COMMON /S20IRX/ LCMX, NRS, LCFW(10,3)
72
73
           COMMON /SESDATX/ TBLS(11000)
74
75
           COMMON /SESINX/ DUM(4), KBR, DUM1
           COMMON /INTOROX/ KFN
76
77 C
78 C
           COMMON BLOCKS FOR THE EOSMOD ROUTINES
79
           COMMON /EDSCZ/ LOUT
           COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
COMMON /EOSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
80
81
82
           COMMON /EDSC4/ NTABLE, NTABLO, IFLP, LCNT
83
           COMMON /EDSC5/ NMAT, LABMAT(60), IDMAT(60), IMATEL COMMON /EDSC6/ NMCL, LABMCL(60), IDMCL(60)
84
85
           COMMON /EOSC7/ NMATO, LABMO(60), IOMATO(60), IMATOL
86
87 C
88 C
           EOSMOD COMMON BLOCKS USED BY THE MODIFIED SESAME ROUTINES
89
           COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
           COMMON /EDSCCO/ TFACO, RFACO, OFACO, KREPO
90
91 C
92 C
           DESIGNATE THE OUTPUT FILE FOR THE ERROR MESSAGES
           DATA LOUT/"OUTPUT"/
93
94 C
           DATA LCMX /11000/, NRS /10/, LCNT /1/, LCFW /30+0/,
95
96
           1 IR/180+0/.NTABLE/1/.NTABLD/0/.INIT/0/.IRDIM/60/.KUP/180+(-1)/
97 C
           DATA LU41 /41/, LU42 /42/, LU43 /42/, LU44 /44/, LU45 /45/
98
           DATA LF41/6HSES2CL/,LF42/6HSESAME/,LF43/6HSESAME/,LF44/6HMIXLIB/
99
           1 ,LF45/6HMIXDIR/
100
101 C
            INITIALIZE THE CONTENTS OF THE EOS TABLE SESAME
102 C
            DATA NMAT /32/
103
104
            DATA LABMAT/
           1 "ALLUVIUM", "ALUMINUM", "AL203", "BERYLLIUM", "BORON C",
105
          1 "BRASS"."COPPER", "DEUTERIUM"."GOLD", "GRANITE",
2 "HELIUM", "HE", "IRON", "IRON2", "LEAD", "GLID", "GLIH",
3 "MOLY", "NEON", "NICKEL", "PLATINUM", "POLYE", "POLYS", "SIO2",
4 "SOOIUM", "SS", "STEAM", "UO2", "URANIUM", "URETHANE", "VERMICULIT",
106
107
108
109
           6 "WATER"/
110
            DATA IDMAT/7111,3710,7410,2020,7081,
111
112
           1 4100,3330,5263,2700,7390,
113
           2 5760,8180,2140,2145,3200,7240,7370,
114
           3 2980,5410,3100,3730,7170,7590,
115
           4 7380,2448,4270,7151,7432,1540,7560,7520,
116
117 C
118 C
            INITIALIZE THE CONTENTS OF THE CLASSIFIED EOS TABLE SES2CL
            DATA NMCL/O/
119
120
            DATA LABMCL/40+(1H )/
            DATA IDMCL/40+0/
121
122 C
            INITIALIZE THE CONTENTS OF THE OPACITY TABLE SESAME
123 C
            DATA NMATO /27/
124
```

```
DATA LABMO/"ALUMINUM", "ARGON", "BERYLLIUM", "BORON", "CALCIUM"

1 , "CARBON", "CHLORINE", "CHROMIUM", "DEUTERIUM", "HELIUM"

2 , "IRON", "LITHIUM", "MAGNESIUM", "NITROGEN"
125
126
127
              3 ,"OXYGEN","PBX-9502","PHOSPHORUS","POTASSIUM","SID2"
4 ,"SILICON","SODIUM","SS","STAINLESS","SULPHUR"
5 ,"TITANIUM","TITANIUM N","WATER"/
128
129
130
131 C
132
               DATA IDMATD/13710, 15170, 12020, 12330, 12030
              1 , 12180, 15020, 13070, 15263, 15760
133
134
              2 , 12140, 12290, 13080, 15000
135
              3 ,15010,18200,13910,12460,17380
              4 ,13810,12448,14270,14270,14010
5 ,12960,16000,17150/
136
137
138 C
                IMATEL=NMAT
139
140
                IMATOL=NMATO
141 C
142
                INIT=1
                RETURN
143
144
                ENO
```

```
SUBROUTINE EOSCON(KUNIT, KREP, LMAT)
2 C
 3 C
 4 C
         * PURPOSE-
 5 C
             .TO PROVIDE THE APPROPRIATE EOS SCALE FACTORS FOR THE
6 C
7 C
                 SYSTEM OF UNITS CHOSEN BY KUNIT (SEE BELOW)
8 C
9 C
         . INPUT VARIABLES-
10 C
              KUNIT = KIND OF UNITS
               O (SESAMEE) R-G/CC,T-DEG.K,D-CM++2/G,P-GPA,E-MJ/KG
11 C
               1 (CGS) R-G/CC, T-DEG.K, D-CM++2/GM, P-MUBR, E-ERGS/GM
12 C
               2 (SIU) R-KG/M**3,T-DEG.K,P-PA,E-J/KG,D-M**2/KG
13 C
               3 (HYDROXE) R-G/CC,T-DEG.K,P=MBR,E-MBR*CC/GM,D-CM**2/G
14 C
               4 (HYDRDXD) R-G/CC,T-KEV,P-MBR,E-MBR+CC/G,D-CM++2/G
15 C
16 C
               5 (SESAMED) R-G/CC,T-EV,D-CM++2/G,P-GPA,E-MJ/KG
               6 (LASNEX) R-G/CC,T-KEV,O-CM++2/GM,P-JRKS/CC,ED-JRKS/CC
17 C
18 C
19 C
                LEGEND-
                       R = DENSITY
20 C
                       T = TEMPERATURE
21 C
22 C
                       0 = OPACITY
23 C
                       P = PRESSURE
                       E = INTERNAL ENERGY
24 C
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
                       KG = KILDGRAM
35 C
                       M = METER
36 C
37 C
                       MBR = MEGABAR
                       MUBR = MICROBAR
38 C
39 C
                       PA = PASCAL
40 C
41 C
42 C
         * DUTPUT VARIABLES- IN THE COMMON BLOCKS EDSCCE AND EDSCCD
43 C
            TFACE = TEMPERATURE EDS SCALING FACTOR
44 C
            RFACE = DENSITY EDS SCALING FACTOR
45 C
            PFACE = PRESSURE EDS SCALING FACTOR
46 C
            EFACE = ENERGY EDS SCALING FACTOR
47 C
48 C
            TFACD = TEMPERATURE OPACITY SCALING FACTOR
49 C
            RFACO = DENSITY OPACITY SCALING FACTOR
            DFACD = DPACITY SCALING FACTOR
50 C
51 C
52 C
         + LOCAL VARIABLES-
53 C
         * NONE
54 C
55 C
         * EXTERNALS AND COMMON BLOCKS-
56 C
         * EDSMOD COMMON BLOCKS- EDSCCE, EDSCCD
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
         * REFERENCE- J. M. HYMAN. M. M. KLEIN
62 C
```

```
63 C
                       EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
64 C
                       EQUATIONS-OF-STATE AND OPACITIES
65 C
                       LDS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
66 C
67 C
          + DATE- MARCH 6, 1980
68 C
69 C
          *******************************
70 C
         COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
71
         COMMON /EDSCCO/ TFACO, RFACO, DFACO, KREPO
72
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.
          EFACE=1.
82
83 C
          FFACD=4.0646423
84
85
         RFACD=O.
         DFACD=O.
86
87 C
88 C
          RESET THE SCALE FACTORS THAT ARE DIFFERENT FROM THE DEFAULT
89
         KP1=KUNIT+1
          GD TD (45,40,30,20,15,10,25), KP1
90
91 C
92 C
          LASNEX UNITS
93
       25 PFACE=1.E-6
          EFACE=1.E-6
94
95
          TFACE=8_617346719E-8
96
          TFACED=-3.
          GD TD 50
97
98 C
99 C
          SESAME OPACITY UNITS
100
       10 TFACE=8.61703E-5
          TFACD=0.0
101
102
          GD TD 50
103 C
104 C
          HYDROX OPACITY UNITS
105
       15 PFACE=.01
106
          EFACE=.01
          TFACE=8.61703E-8
107
108
          TFACD=-3.
          GD TD 50
109
110 C
111 C
          HYDROX EDS UNITS
112
       20 PFACE=.01
          EFACE=.01
113
          GD TD 50
114
115 C
116 C
          STANDARD INTERNATIONAL UNITS (SIU)
117
       30 RFACE=1.E+3
          PFACE=1.E+9
118
119
          EFACE=1.E+6
120
          RFACD=3.0
121
          DFACD=-1.0
122
          GD TD 50
123 C
124 C
          CGS UNITS
```

```
125
       40 PFACE=1.E+10
126
          EFACE=1_E+10
          GD TD 50
127
128 C
129 C
          SESAME EDS UNITS
       45 DFACD=2.0
130
       50 CONTINUE
131
132 C
          RESCALE THE TABLES IN THE USER PRESCRIBED SCALE FACTORS
133 C
134
          DSFAC=1.0
135
          CALL EDSDSL(LMAT, DSFAC)
          EFACE=EFACE+OSFAC
136
137
          RFACE=RFACE/DSFAC
          RFACD=RFACD/DSFAC
138
139 C
          RETURN
140
141
          ENO
```

SUBROUTINE EDSOSL(LMAT, DSFAC) 2 C 3 C 4 C 5 C * PURPOSE-6 C * TO ALLOW A USER TO RESCALE THE MASS DENSITY IN 7 C * THE EOS TABLES. THIS IS A USEFUL ROUTINE TO APPROXIMATE THE * EDS AND OPACITIES OF DIFFERENT ISOTOBES AND ISOTOPIC MIXTURES 8 C * OF THE MATERIALS IN THE SESAME LIBRARY 9 C 10 C * AN ALTERNATE PURPOSE IS TO ALLOW A USER TO DEFINE NEW 11 C * SCALE FACTORS FOR THE UNITS THE TABLE IS TO BE WRITTEN IN 12 C 13 C 14 C * INPUT VARIABLE-15 C LMAT = MATERIAL IN AN A10 FIELD, FDR 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 * OUTPUT VARIABLE-* DSFAC = DENSITY SCALE FACTOR EQUAL TO THE RATIO OF THE 21 C 22 C ATOMIC MASSES OF THE MATERIALS. THAT IS. 23 C OSFAC=ATOMIC MASS DENSITY OF THE SESAME MATERIAL)/ 24 C (ATOMIC MASS DENSITY OF THE DESIRED MATERIAL) 25 C 26 C * FOR EXAMPLE- THE EOS OF A 60-40 MIXTURE OF DEUTERIUM-TRIDIUM * CAN BE APPROXIMATED BY DEFINING DSFAC=2/(0_6*2+0.4*3)=0.833 27 C 28 C * AND CALLING EDSMOD WITH LMAT="DEUTERIUM" 29 C 30 C * INPUT-OUTPUT VARIABLES IN THE COMMON BLOCKS EDSCC2 AND EDSCCD 31 C TFACE = TEMPERATURE EDS SCALING FACTOR RFACE = DENSITY EDS SCALING FACTOR 32 C 33 C PFACE = PRESSURE EDS SCALING FACTOR 34 C EFACE = ENERGY EOS SCALING FACTOR 35 C 36 C TFACO = TEMPERATURE OPACITY SCALING FACTOR RFACO = DENSITY OPACITY SCALING FACTOR 37 C 38 C OFACO = OPACITY SCALING FACTOR 39 C 40 C * FOR FURTHER INFORMATION ON THESE FACTORS SEE SUBROUTINE EDSCON 41 C 42 C * EXTERNALS AND COMMON BLOCKS-* EOSMOO COMMON BLOCKS- EOSCCE, EOSCCO 43 C 44 C 45 C * REMARKS- THIS SUBROUTINE IS PART OF THE EDSMOD 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 EDSMOD- 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 COMMON /EDSCCE/ TFACE, RFACE, PFACE, EFACE. KREPE 59 COMMON /EOSCCO/ TFACO, RFACO, OFACO, KREPO 60 C DUMMY SUBROUTINE FOR THE PACKAGE. 61 C 62 C IF A USER SUPPLIES THIS ROUTINE THEN THE FACTORS CAN BE

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

```
SUBROUTINE EOSEFO (LMAT.IO.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 IO) EDS NUMBERUMBER
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
                  NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
14 C
15 C
         * OUTPUT VARIABLES-
16 C
17 C
            IO = SESAME OR PRIVATE IO NUMBER AS STOREO IN LIBRARY
              SESAME ( EOS LIBRARY)
18 C
19 C
            IMATE = LOCATION OF MATERIAL IN ARRAY LABMAT+ MIXOIR
20 C
                PROVIDED MATERIAL HAS BEEN LOCATED
21 C
                   = O IF MATERIAL HAS NOT BEEN LOCATED BY ROUTINE
                UPPER BOUND ON IMATE IS 60 (DIM IR(,))
22 C
23 C
24 C
         * LOCAL VARIABLES-
25 C
            ICFASE = 1 IF THE PUBLIC EDS FILES HAVE BEEN ASSIGNED
            ICFASCL = 1 IF THE CLASSIFIED EOS FILES HAVE BEEN ASSIGNED
26 C
27 C
            ICFASP = 1 IF THE PRIVATE EOS FILES HAVE BEEN ASSIGNED
28 C
29 C
         * EXTERNALS AND COMMON BLOCKS-
         * EDSMOD COMMON BLOCKS- EDSC1.2,3,5.6
30 C
31 C
         * FTN ROUTINES- ENCODE. EOF
         * LASL T-4 HYOSES ROUTINE- EOSFAS
32 C
33 C
34 C
         * REMARKS- THIS SUBROUTINE IS PART OF THE EDSMOD 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
                      EDSMDD- 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
         COMMON /EDSC1/ LU41, LU42, LU43, LU44, LU45
COMMON /EDSC2/ LF41, LF42, LF43, LF44, LF45
COMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
48
49
50
51
         COMMON /EDSC5/ NMAT, LABMAT(60). IDMAT(60), IMATEL
         COMMON /EDSC6/ NMCL, LABMCL(60), IDMCL(60)
52
53 C
54
         DATA ICFASE/O/, ICFASCL/O/, ICFASP/O/, IDCNT/1/
55 C
         CHECK IF THE MATERIAL IS IN THE STANDARD SESAME LIST
56 C
         DO 10 IMATE=1, IMATEL
57
58
         IF (LMAT.EQ.LABMAT(IMATE)) GD TO 40
59
      10 CONTINUE
60 C
         CHECK IF THE MATERIAL IS IN THE CLASSIFIED EDS SESAME LIST
61 C
         DD 12 IMATE=1,NMCL
```

```
63
          IF (LMAT.EQ.LABMCL(IMATE)) GO TO 45
       12 CONTINUE
64
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. O ) GO TO 15
70
          ICFASP=1
71
          CALL EDSFAS(3)
72
       15 CONTINUE
73 C
          THE CURRENT PRIVATE LIST DIRECTORY (MIXDIR) IS ON UNIT LU45
74 C
75 C
          CHECK IF LF45 EXISTS IN LOCAL FILE SPACE
76
          CALL FEXIST(LF45, IFFLAG)
          IF(IFFLAG .EQ. 0 ) GO TO 30
IFFLAG = O FILE NOT IN LOCAL FILE SPACE
77
78 C
           IFFLAG = 1 FILE LOCAL
79 C
80 C
          REWIND LU45
81
       20 READ (LU45,80) LABEL, ID
82
          IMATE=IMATE+1
83
          IF (LMAT.EQ.LABEL) GO TO 5Q
84
85
          IF (EDF(LU45)) 30,20
       30 CONTINUE
86
87
       31 CONTINUE
88 C
89 C
          CHECK IF THE LMAT IS A SESAME NUMBER
          IMAT 1=AND(SHIFT(LMAT,6),77B)
90
91 CRAY CODE IMATI=AND(SHIFT(LMAT,8),377B)
92 C
93
          IF(IMAT1.LT.20B) GO TO 35
          IF(IMAT1.GT.31B) GO TO 35
94
95 C
96
          DECODE(10,32,LMAT) ID
97
       32 FORMAT(14)
98 C
99
          DD 33 IMATE=1, IMATEL
100
          IF(ID.EQ.IDMAT(IMATE)) GO TO 40
101
       33 CONTINUE
102 C
          IMATEL=IMATEL+1
103
104
          IMATE=IMATEL
105
          LABMAT(IMATE)=LMAT
106
          IOMAT(IMATE)=IO
107 C
108 C
          ASSUME THE MATERIAL IS IN THE STANDARD SESAME LIST
          IF IT IS NOT, A NONFATAL ERROR WILL OCCUR AT A LATER STEP
109 C
110
          GD TD 40
111 C
          THE MATERIAL WAS NOT FOUND. PRINT AN ERROR MESSAGE
112 C
       35 IMATE=0
113
          WRITE(LOUT, 75) LMAT
114
          GD TD 999
115
116 C
       40 ID=IDMAT(IMATE)
117
118 C
          *** ASSIGN EDS FILES TO PROGRAM
119 C
120
          IF(ICFASE .GT. O ) GO TO 44
121
          ICFASE=1
122
          CALL EDSFAS(1)
       44 CONTINUE
123
124 C
```

```
125
           GD TO 999
126 C
127
        45 IO=IOMCL(IMATE)
128 C
            *** ASSIGN CLASSIFIED EOS FILES TO PROGRAM
129 C
           IF(ICFASCL .GT. 0 ) GO TO 46
130
           ICFASCL=1
131
            CALL EOSFAS(4)
132
133
        46 CONTINUE
134 C
        50 CONTINUE
135
            IF (IMATE.LE.IROIM) GO TO 60
136
137
            IMATE=0
           WRITE(LOUT, 90) LMAT
138
139
        60 CONTINUE
140 C
141
       999 CONTINUE
142
            RETURN
143 C
        75 FORMAT (" MATERIAL LMAT = ".A10," NOT FOUND")
80 FORMAT (A10,13)
90 FORMAT (" IMATE EXCEEDS UPPER BOUND IN SUBROUTINE EOSEFD "
144
145
146
          1 ./." FOR MATERIAL LMAT=".A10)
END
147
148
```

```
SUBROUTINE EOSFAS(KTABLE)
 1
 2 C
 3
  C
 4
   C
 5
  C
         * PURPOSE-
         * TO ASSIGN FILE NAMES TO THE EDS AND OPACITY DATA FILES
 6
   C
 7
   C
         * INPUT VARIABLES-
 8
   C
 9
   C
         * KTABLE = 1 EOS TABLE
                    2 OPACITY TABLE
10
   C
                     3 PRIVATE TABLES
11 C
12 C
                     4 SES2CL TABLES
13 C
         * OUTPUT VARIABLES-
14
  С
15 C
           NONE
16 C
17 C
         * LOCAL VARIABLES-
         . INITE, INITECL, INITO AND INITP ARE SET TO 1 AFTER THE EOS, OPACITY
18 C
19 C
         * AND PRIVATE FILES HAVE BEEN INITIALIZED
20 C
21 C
         * EXTERNALS AND COMMON BLOCKS-
22 C
         * EDSMOD COMMON BLOCKS- EDSC1, EDSC2
         * FTN SUBROUTINES- QASSIGN, ASSIGN
23 C
24
   С
25 C
         * REMARKS- THIS SUBROUTINE IS PART OF THE EDSMOD 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
                       EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
31 C
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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
         CDMMON /EDSC1/ LU41, LU42, LU43, LU44, LU45
         COMMON /EDSC2/ LF41, LF42, LF43, LF44, LF45
40
41
         DATA INITE/O/, INITO/O/, INITP/O/, INITECL/O/
42 C
43
         GD TD (10,20,30,40), KTABLE
44 C
         EDS TABLE ASSIGNMENT CODING
45 C
46
      10 CONTINUE
47
         IF(INITE.NE.O) GD TO 999
48
         IF((INITO.NE.O).AND.(LF42.EQ.LF43)) GO TO 999
49
         INITE=1
50
         CALL QASSIGN (LU42, LF42, 0, 0)
51
         GD TD 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, 0, 0)
         GD TD 999
59
60 C
61 C
         PRIVATE TABLES
      30 CONTINUE
62
```

```
IF(INITP.NE.O) GO TO 999 INITP=1
63
64
          CALL QASSIGN (LU44, LF44,0,0)
CALL ASSIGN (LU45, LF45, 4000B)
65
66
67
          GD TD 999
68 C
69 C
          CLASSIFIED EOS TABLE ASSIGNMENT CODING
       40 CONTINUE
70
71
          IF(INITECL.NE_O) GO TO 999
72
          INITECL=1
73
          CALL QASSIGN (LU41, LF41, 0, 0)
74
          GD TO 999
75 C
     999 RETURN
76
77
          END
```

```
SUBROUTINE EOSGET(LMAT, KUNIT, KREP, IMAT, IOT, IERR)
2 C
3 C
 4 C
         * PURPOSE-
5 C
         * LOAD THE SESAME EOS DATA FILES
6 C
7 C
         * INPUT VARIABLES-
8 C
            LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
9 C
                  THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
10 C
                  THE MATERIAL BY SETTING LMAT TO THE SESAME
11 C
                  NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
12 C
13 C
            KUNIT= KIND OF UNITS
14 C
               O (SESAMEE) R-G/CC,T-DEG.K.D-CM++2/G,P-GPA,E-MJ/KG
15 C
               1 (CGS) R-G/CC, T-DEG_K, D-CM++2/GM, P-MUBR, E-ERGS/GM
16 C
               2 (SIU) R-KG/M++3,T-DEG.K,P-PA,E-J/KG,D-M++2/KG
17 C
18 C
               3 (HYDROXE) R-G/CC,T-DEG.K,P=MBR,E-MBR+CC/GM,D-CM++2/G
               4 (HYDROXO) R-G/CC,T-KEV,P-MBR,E-MBR+CC/G,D-CM++2/G
19 C
               5 (SESAMED) R-G/CC,T-EV,D-CM++2/G,P-GPA,E-MJ/KG
20 C
               6 (LASNEX) R-G/CC.T-KEV.D-CM**2/GM.P-JRKS/CC.ED-JRKS/CC
21 C
22 C
23 C
         * IMAT = INDICATES WHETHER TO LOAD THE DATA FILE IF
                  IT DOES NOT EXIST FOR LMAT OR GO DIRECTLY TO A
24 C
                  PREVIOUSLY LOADED'FILE.
25 C
             =O CHECK IF THE DATA FILE FOR LMAT HAS BEEN LOADED.
26 C
                IF NOT, SEARCH FOR THE FILE, COMVERT IT TO THE PROPER UNITS
27 C
28 C
                AND COPY IT INTO LCM .
             >O EQUAL TO THE LMAT TABLE NUMBER. THIS NUMBER WAS RETURNED
29 C
30 C
                BY THE PACKAGE ON A PREVIOUS CALL TO SUBROUTINE EOSORE,
                EDSIPT OR EDSIRT. THIS OPTION IS FASTER THAN IMAT = O
31 C
                BECAUSE IT SKIPS SEARCH IN THE DIRECTOR OF THE
32 C
33 C
34 C
         * DUTPUT VARIABLES-
         * IERR = O SUCCESSFULL
35 C
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 BLDCKS-
           EDSMOD COMMON BLOCKS- EDSC1, EDSC3
43 C
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
           REFERENCE- J. M. HYMAN, M. M. KLEIN
49 C
50 C
                       EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
51 C
                       EQUATIONS-DF-STATE AND OPACITIES
                       LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M. 1980
52 C
53 C
54 C
         * DATE- MARCH 6, 1980
55 C
56 C
57 C
         LOAD THE SESAME EOS TABLES IN THE INVERTED FORMAT
58 C
59 C
60 C
         COMMON BLOCKS FOR THE SESAME EDS ROUTINES
         LEVEL 2, TBLS
61
62
         CDMMON /S2DIRX/ LCMX, NRS, LCFW(10,3)
```

```
COMMON /SESDATX/ TBLS(11000)
COMMON /SESINX/ DUM(4), KBR, DUM1
63
64
          COMMON /INTOROX/ KFN
65
66 C
67 C
          COMMON BLOCKS FOR THE EOSMOD ROUTINES
          COMMON /EDSCZ/ LOUT
68
          COMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
69
70
          COMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
71
          COMMON /EOSC4/ NTABLE, NTABLD, IFLP, LCNT
72 C
73
          DIMENSION ZB(3)
74 C
75
          IERR*O
76 C
77 C
          CALL THE FILE ASSIGNMENT ROUTINE TO ASSIGN READ AND WRITE
78 C
          UNIT NUMBERS TO THE INPUT DATA FILES
           IF(IOT.NE.2) CALL EDSEFD (LMAT, ID, IMAT)
79
           IF(IDT.EQ.2) CALL EOSOFD (LMAT, ID, IMAT)
80
81 C
          IF (IMAT.LE_O) IERR=-1
82
83
           IF (IMAT.LE.O) GO TO 75
84 C
85 C
          CHECK IF THE TABLES HAVE BEEN INITIALIZED
86
          IF (IR(IMAT, IDT).GT.O) GD TD 70
87 C
          CONVERT TABLES TO APPROPRIATE UNITS
BB C
          CALL EDSCON(KUNIT, KREP, LMAT)
89
90 C
91
          MIXTST=ID/1000
92 C
93
          GD TD (10,20,30), IDT
94 C
95 C
           LOAD THE EOS TABLES IN THE INVERTED FORMAT (IOT=1)
96
       10 CONTINUE
97
           IF(MIXTST.NE.O)CALL GETINVX (NTABLE, IO, IOT, TBLS, LCNT, LU42, IERR, ZB)
98
           IF(MIXTST.EQ.O)CALL GETINVX (NTABLE, IO, IOT, TBLS, LCNT, LU44, IERR, ZB)
99
           GD TD 40
100 C
101 C
          LOAD THE OPACITY TABLES (IOT=2)
102
       20 CONTINUE
103 C
104
           IF (MIXTST.EQ.O) CALL GETRPOX (NTABLO, IO, IOT, TBLS, LCNT, LU44, IERR)
105
           IF (MIXTST.NE.O) CALL GETRPOX (NTABLO,ID,IOT,TBLS,LCNT,LU43,IERR)
106
           GD TD 40
107 C
108 C
          LOAD THE EOS TABLES IN THE STANDARD FORMAT (IDT=3)
109
       30 CONTINUE
           IF(MIXTST.NE.O)CALL GETEDSX (NTABLE, IO, IOT, TBLS, LCNT, LU42, IERR, ZB)
IF(MIXTST.EQ.O)CALL GETEOSX (NTABLE, IO, IOT, TBLS, LCNT, LU44, IERR, ZB)
110
111
112
       40 CONTINUE
113 C
           IERR RETURNS NEGATIVE IF THERE IS AN INITIALIZATION ERROR
114 C
           IF (IERR.GT_O) GD TO 60
115
           IF(IERR.LT.O) WRITE(LOUT,90) IERR
116
           IF(IERR_EQ_O) WRITE(LOUT. 100)LMAT
117
118
           IF(IERR.EQ.O) IERR=-2
           GD TØ 75
119
120 C
121 C
           THE TABLES HAS BEEN LOADED, SET THE EDSMOD VARIABLES
122
       60 | IERR=0
           IF(IDT.NE.2) GD TD 65
123
124 C
```

```
OPACITY TABLE UPDATE
125 C
126
           IR(IMAT, IOT)=NTABLO
           KUP(IMAT, IDT) = 10+KUNIT+KREP
127
           NTABLO=NTABLO+1
128
           GD TD 70
129
130 C
           EOS TABLE UPOATE
131 C
132
        65 CONTINUE
           IR(IMAT, IOT)=NTABLE
133
134
            KUP(IMAT, IDT) = 10+KUNIT+KREP
           NTABLE=NTABLE+1
135
136
        70 CONTINUE
137 C
            CHECK IF THE UNITS ARE VALID
138 C
            IF(10*KUNIT+KREP.NE.KUP(IMAT, IOT)) IERR=-6
139
140 C
            IF(IERR.EQ.-6) WRITE(LOUT,80)KUNIT,KREP,KUP(IMAT,3)
141
        80 FORMAT(" THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE" 2,/." THE CURRENT VALUES OF KUNIT AND KREP ARE ".214 3,/." THE PREVIOUS VALUES OF KUNIT AND KREP WERE",15)
142
143
144
145 C
146
        75 CONTINUE
            IF(IERR.LT.O) IMAT=IERR
147
148 C
149
            RETURN
150 C
151
        90 FORMAT(" INSUFFICIANT STORAGE IN LCM"
          1 ./." LACK", I 10, " WORDS")
152
        100 FORMAT(" UNABLE TO LOCATE MATERIAL ".A10./.
153
           1 " IN SUBROUTINE EOSGET")
154
            ENO
155
```

1 SUBRDUTINE EOSKUT(KPARM.KBR.KUNIT.KREP.KFN,KEOSS.KBRS.KFNS.IMAT. 2 2 IOT. 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 KPARM = 1000*KBR + 100*KUNIT + 10*KREP + KFN WHERE 14 C 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 O (SESAMEE) R-G/CC.T-DEG_K.D-CM++2/G.P-GPA.E-MJ/KG 22 C 23 C 1 (CGS) R-G/CC.T-DEG_K,D-CM++2/GM.P-MUBR.E-ERGS/GM 2 (SIU) R-KG/M++3,T-DEG.K,P-PA,E-J/KG,D-M++2/KG 24 C 25 C 3 (HYDROXE) R-G/CC'T-DEG.K.P=MBR.E-MBR*CC/GM.D-CM**2/G 26 C 4 (HYDRDXD) R-G/CC, T-KEV, P-MBR, E-MBR+CC/G, D-CM++2/G 27 C 5 (SESAMED) R-G/CC, T-EV, D-CM++2/G, P-GPA, E-MJ/KG 28 C 6 (LASNEX) R-G/CC,T-KEV,D-CM++2/GM,P-JRKS/CC,ED-JRKS/CC 29 C 30 C * IF KREP REFERS TO EOS TABLE UNITS KREP = CDMPUTATION FLAG TO INDICATE WHETHER E IS 31 C 32 C IS TO BE REPRESENTED AS ENERGY PER UNIT MASS OR ENERGY 33 C PER UNIT VOLUME O ENERGY IN UNITS OF ENERGY PER UNIT MASS. FOR EXAMPLE-34 C 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 O OPACITY REPRESENTED AS KAPPA IN DIMENSIONAL 45 C UNITS OF LENGTH ++ 2/MASS 46 C 1 DPACITY REPRESENTED AS A MEAN-FREE PATH. 47 C LAMBOA = 1/(KAPPA*RHO), IN DIMENSIONAL 48 C UNITS OF LENGTH. 49 C 50 C KFN = KIND OF FUNTION INTERPOLATION IN THE TABLES 51 C = O RATIONAL APPROXIMATIONS (ACCURATE) - 1 BILINEAR APPROXIMATIONS (FAST) 52 C 53 C 54 C * LOCAL VARIABLES-55 C * EXTERNALS AND COMMON BLDCKS-56 C 57 C * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE 58 C 59 C * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL 60 C 61 C * REFERENCE- J. M. HYMAN, M. M. KLEIN 62 C

```
EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
63 C
                         EQUATIONS-OF-STATE AND OPACITIES
64 C
                         LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
65 C
66 C
67 C
          + DATE- MARCH 6, 1980
68 C
69 C
70 C
          COMMON /EOSCZ/ LOUT COMMON /EOSC3/ INIT, IROIM, IR(60,3), KUP(60,3)
71
72
73 C
74
          IERR=0
75 C
          IF(INIT.EQ.O) CALL EOSBEG
76
77 C
78 C
          UNSCRAMBLE MULTIPLE FLAG KPARM
79 C
          KBR=KPARM/1000
80
81
          ITEMP=KPARM-KBR+1000
82 C
83
          KUNIT=ITEMP/100
          ITEMP=ITEMP-KUNIT+100
84
85 C
86
          KREP=ITEMP/10
87
          KFN=ITEMP-10*KREP
88 C
89
          KEOSS=KPARM
          KFNS=KFN
90
91
          KBRS=KBR
92 C
93 C
          CHECK IF KPARM IS A VALID INPUT PARAMATER
          IF(KPARM.LT.O) IERR=-2
94
95
          IF(KBR.GT.2) IERR=-2
96
          IF(KUNIT.GT.6) IERR=-2
97
          IF(KREP.GT.1) IERR=-2
          IF(KFN.GT.1) IERR=-2
98
99 C
100 C
          PRINT AN ERROR MESSAGE IF KUNIT IS NOT VALIO
101
          IF(IERR_LT.O) WRITE(LDUT, 10)KPARM, KBR, KUNIT, KREP, KFN
       10 FORMAT(" ERROR DETECTED IN KPARM VALUE IN SUBROUTINE EDSKUT"
1 ,/," KPARM=",15," KBR=",15," KUNIT=",15," KREP=",15," KFN=",15)
102
103
104 C
105 C
          CHECK IF THE UNITS HAVE CHANGED
          IF(IMAT.LE.O) GO TO 90
106
107
          IF(10*KUNIT+KREP.NE.KUP(IMAT, IOT)) IERR=-6
          IF (IERR.GE.O) GO TO 90
108
109 C
          WRITE(LOUT, 30)KUNIT, KREP.KUP(IMAT, IOT)
110
111
       30 FORMAT(" THE UNITS HAVE CHANGED SINCE THE LAST USE OF THE TABLE"
         2./." THE CURRENT VALUES OF KUNIT AND KREP ARE ",212
112
          3,/," THE PREVIOUS VALUES OF KUNIT AND KREP WERE", 15)
113
114 C
115
       90 CONTINUE
116 C
117
          RETURN
118
           ENO
```

```
SUBROUTINE EGSOFD (LMAT, 10, IMATO)
 1
2 C
3 C
 4 C
5 C
         * PURPOSE-
           TO OBTAIN MATERIAL NUMBERS FOR OPACITY TABLES
6 C
         *
7 C
         * INPUT VARIABLES-
8 C
            LMAT = MATERIAL IN AN A10 FIELD, FOR EXAMPLE- LMAT = "HELIUM"
9 C
                  THE MATERIAL SESAME NUMBER CAN ALSO BE USED TO SPECIFY
10 C
                   THE MATERIAL BY SETTING LMAT TO THE SESAME
11 C
                  NUMBER, FDR EXAMPLE- LMAT = "5760" FOR HELIUM
12 C
13 C
         * OUTPUT VARIABLES-
14 C
15 C
           IO= SESAME OR MIXTUREID NUMBER AS STORED
                 IN SESAME OR MIXOIR(MIXLIB)
16 C
            IMATO = LOCATION OF MATERIAL IN ARRAY LABMO + MIXDIR
17 C
                 PROVIDED MATERIAL HAS BEEN LOCATED
18 C
19 C
                   . O IF MATERIAL HAS NOT BEEN LOCATED
20 C
21 C
           LOCAL VARIABLES-
            EDSMOD COMMON BLOCKS- EOSC1, EOSC3
22 C
23 C
         * EXTERNALS AND COMMON BLOCKS-
24 C
25 C
         * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GROUP T-7, LASL
26 C
27 C
         * REFERENCE- J. M. HYMAN, M. M. KLEIN
28 C
                       EDSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
29 C
                       EQUATIONS-OF-STATE AND OPACITIES
30 C
                       LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
31 C
32 C
         * DATE- MARCH 6, 1980
33 C
34 C
          35 C
36 C
         COMMON /EOSCZ/ LOUT
37
         COMMON /EDSC1/ LU41, LU42, LU43, LU44, LU45
38
         CDMMON /EDSC2/ LF41, LF42, LF43, LF44, LF45
CDMMON /EDSC3/ INIT, IRDIM, IR(60,3), KUP(60,3)
CDMMON /EDSC7/ NMATO, LABMO(60), IDMATD(60), IMATOL
39
40
41
42 C
         DATA ICFASD, ICFASP/2+0/
43
           **** ASSIGN OPACITY FILES TO PROGRAM
44 C
          IF(ICFASO _GT. O) GO TO 5
45
46
          ICFASO=1
         CALL EOSFAS(2)
47
48
       5 CONTINUE
49 C
          CHECK IF THE MATERIAL IS IN THE STANDARD SESAME TABLES
50 C
          DO 10 IMATO=1, IMATOL
51
          IF (LMAT_EQ_LABMO(IMATO)) GO TO 40
52
       10 CONTINUE
53
          IMATO=IMATOL
54
55 C
          *** ASSIGN PRIVATE OPACITY FILES TO PROGRAM
56 C
57
          IF(ICFASP .GT. O) GO TO 15
58
          ICFASP=1
59
          CALL EDSFAS(3)
60
       15 CONTINUE
61 C
          THE CURRENT PRIVATE LIST DIRECTORY (MIXOIR) IS ON UNIT LU45
62 C
```

```
CHECK IF LF45 EXISTS IN LOCAL FILE SPACE
63 C
64
         CALL FEXIST(LF45, IFFLAG)
         IF(IFFLAG .EQ. Q ) GO TO 30
65
          IFFLAG = O FILE NOT IN LOCAL FILE SPACE
66 C
67 C
          IFFLAG = 1 FILE LOCAL
68
         REWINO LU45
69
      20 READ (LU45.80) LABEL.IO
         IMATO=IMATO+1
70
          IF (LMAT.EQ.LABEL) GO TO 50
71
         IF (EDF(LU45)) 30,20
72
73
       30 CONTINUE
74 C
75 C
          CHECK IF THE LMAT IS A SESAME NUMBER
         IMAT 1=AND(SHIFT(LMAT.6),77B)
76
77 CRAY CODE IMAT1=AND(SHIFT(LMAT,8),377B)
78 C
79
          IF(IMAT1.LT.20B) GD TD 35
          IF(IMAT1.GT.31B) GO TO 35
80
81 C
         DECODE(10,32,LMAT) ID
82
83
       32 FORMAT(15)
84 C
85
          DO 33 IMATO=1, IMATOL
          IF(IO.EQ.IOMATO(IMATO)) GO TO 40
86
87
       33 CONTINUE
88 C
89
          IMATOL=IMATOL+1
90
          IMATD=IMATOL
91
          LABMO(IMATO)=LMAT
          IDMATD(IMATO)=IO
92
93 C
          ASSUME THE MATERIAL IS IN THE STANDARD SESAME LIST
94 C
95 C
          IF IT IS NOT. A NONFATAL ERROR WILL OCCUR AT A LATER STEP
          GD TD 40
96
97 C
98 C
99 C
          THE MATERIAL WAS NOT FOUND. PRINT AN ERROR MESSAGE
       35 CONTINUE
100
101
          IMATO=0
          WRITE(LOUT, 70) LMAT
102
103
          GD TD 999
104 C
105
       40 IO=IOMATO(IMATO)
106
       50 CONTINUE
107 C
108
          IF (IMATO.LE.IRDIM) GO TO 60
109
          IMATO=O
110
          WRITE(LOUT, 90) LMAT
       60 CONTINUE
111
112 C
      999 CONTINUE
113
114
          RETURN
115 C
116 C+++++ IMPROVE THESE DIAGONISTICS++++++++++
       70 FORMAT (" MATERIAL LMAT = ",A10," NOT FOUND")
80 FORMAT (A10,I3)
117
118
       90 FORMAT (" IMATO EXCEEDS UPPER BOUND IN SUBROUTINE EDSOFO "
119
         1 ,/," FOR MATERIAL LMAT=",A10)
120
121
```

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

```
FUNCTION OPACKX(A,B)
2 C---
3 C
4 C
5 C
     FUNCTION OPACKX
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.ABOALLAH, JR.
11 C
               1 MAY 1979
12 C
     DATE
13 C
14 C-----
        EQUIVALENCE (I1,X1),(I2,X2)
15
16
        DATA MASK/7777777770000000000B/
17
        X1=A
18
        X2=B
        I1=I1.AND_MASK
19
20
        12=12.AND.MASK
        I2=SHIFT(I2,30)
21
22 .
        I1=I1.OR.I2
        DPACKX=X1
23
        RETURN
24
25
        END
```

```
SUBROUTINE GETEOSX(IR, MID, IDT, TBLS, LCNT, LU, IFL, ZB)
2 C****
3 C
     SUBROUTINE GETEOSX(IR, MIO, IOT, TBLS.LCNT, LU, IFL, ZB)
4 C
5 C
     PURPDSE
                  TO LOAD THE TOTAL EDS TABLES
6 C
7 C
     ARGUMENTS
                  IR
                            (INPUT)
8 C
                                      REGION NO.
9 C
                  MID
                            (INPUT)
                                      MATERIAL ID.
                                      DATA TYPE INDICATOR
10 C
                            (INPUT)
                  IOT
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
                            (DUTPUT)
                                      ERROR FLAG
15 C
                                       = 2 FOR MATERIAL ALREADY LOADED
16 C
                                      = 1 FOR SUCCESSFUL LDADING
17 C
                                      - O FOR DATA NOT FOUND
                                          NO. OF EXTRA WORDS NEEDED FOR
18 C
19 C
                                           STDRAGE
20 C
                  ZB
                            (DUTPUT) 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
                  THIS IS THE LASNEX VERSION OF GETEOS
      REMARKS
26 C
27 C
28 C
                  PRESSURES AND ENERGIES ARE DOUBLE PACKED
29 C
                  ENERGY DENSITIES ARE PER UNIT VOLUME (NOT MASS)
30 C
31 C
32 C
      EXTERNALS
                  MATCHKX, TABRANX, DPACKX
33 C
34 C
      PROGRAMMER
                  R.C. ALBERS, T-4
35 C
36 C
                  25 APRIL 79
      DATE
37 C
39
         LEVEL 2, TBLS
         DIMENSION TBLS(1), ZB(3)
40
41 C
         REPLACE FOLLOWING LINE BY USER COMMON BLOCKS
         COMMON/S20IRX/LCMX,NRS,LCFW(10,3)
42
43
         COMMON /EOSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
44 C
45 C
         CHECK TO SEE IF TABLE HAS BEEN LOADED
         CALL MATCHKX(MID, NRS, LCFW(1, IOT), TBLS(1), IFLG)
46
47
         IF(IFLG.EQ.O) GD TD 10
         LCFW(IR, IOT) = IFLG
48
49
         IFL=2
50
         RETURN
51
      10 NLEFT = LCMX - LCNT - 1
52 C
53 C
         FETCH THE 201 TABLE
54
         CALL TABRANX(MIO, 201., LU, TBLS(LCNT+2), NLEFT, IFL)
55
         IF(IFL.LE.O) RETURN
56
         ZB(1) = TBLS(LCNT+2)
57
         ZB(2) = ZB(1)*ZB(1)
         ZB(3) = TBLS(LCNT+3)
58
59
         RHOO=TBLS(LCNT+4)
60 C
61 C
         FETCH THE 301 TABLE
62
         CALL TABRANX(MID,301_,LU.TBLS(LCNT+2),NLEFT,IFL)
```

```
IF(IFL.LE.O) RETURN
63
64 C
          CONVERT TO LASNEX UNITS AND DOUBLE PACK
65 C
66
          NR = TBLS(LCNT+2)
          NT = TBLS(LCN7+3)
67
68
          00 20 I=1,NT
          LOCT = I + (LCNT + NR + 3)
69
      20 TBLS(LOCT)=TFACE+TBLS(LOCT)
70
          NWDS = NR+NT
71
         00 30 J=1,NR
RHD = TBLS(J + LCNT + 3)*RFACE
72
73
          TBLS(J+LCNT+3)=RHO
74
75
          00 40 I=1,NT
          LOCP = (I-1)*NR + J + (NT + NR + LCNT + 3)
LOCE = LOCP + NWOS
76
77
78
          PTEM=TBLS(LOCP) *PFACE
          ETEM=TBLS(LOCE) * EFACE
79
80
          IF(KREPE.EQ.1)ETEM=ETEM+RHO
          TBLS(LOCP) = DPACKX(PTEM, ETEM)
81
82
      40 CONTINUE
83
      30 CONTINUE
84 C
          RESET INPUT PARAMETERS AND END
85 C
          TBLS(LCNT)=FLOAT(MIO)
86
          TBLS(LCNT+1)=RHOO
87
          LCFW(IR, IOT)=LCNT
88
          LCNT = LCNT + 2 + IFL - NWOS
IFL = 1
89
90
          RETURN
91
92
          ENO
```

```
SUBROUTINE GETINVX(IR, MIO, IOT, TBLS, LCNT, LU, IFL, ZB)
2 C---
3 C
 4 C
      SUBROUTINE GETINVX(IR.MID.IDT.TBLS.LCNT.LU.IFL.ZB)
5 C
6 C
                   TO LOAD INVERTED (ENERGY BASED) SESAME II
      PURPOSE
 7 C
                   EOS TABLES
8 C
      ARGUMENTS
9 C
                   IR
                              (INPUT)
                                        REGIDN NO.
                                        SESAME MATERIAL ID
10 C
                   MID
                              (INPUT)
                                        DATA TYPE INDICATOR
                              (INPUT)
11 C
                   IOT
12 C
                   TBLS
                              (INPUT)
                                        TABLE STORAGE ARRAY
13 C
                   LCNT
                              (IN/OUT)
                                        POSITION IN ARRAY FOR STORING TABLES
14 C
                              (INPUT)
                                        SESAME LIBRARY UNIT NO.
                   LU
15 C
                   IFL
                              (OUTPUT)
                                        ERROR FLAG
16 C
                                        2=MATERIAL ALREADY LOADED
                                        1=SUCCESSFUL LOADING
17 C
18 C
                                        O=DATA NOT FOUND
19 C
                                        LT.O FOR - THE NO. OF EXTRA WORDS
                                        NEEDEO FOR LDADING
20 C
                              (OUTPUT)
21 C
                   ZΒ
                                        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
                   UNITS - ENERGY
                                       MBAR+CC/GM
      REMARKS
                                       DEGREES KELVIN
27 C
                           TEMP
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 EDSMOD
33 C
34 C
      EXTERNALS
                   MATCHKX, TABRANX, INV301X
35 C
      PROGRAMMER
36 C
                   J. ABOALLAH, JR.
37 C
38 C
      DATE
                   13 JUNE 1979
39 C
40 C-----
41 C
42
         LEVEL 2, TBLS
          COMMON/S2DIRX/LCMX,NRS,LCFW(10.3)
43
         DIMENSION ZB(3), TBLS(1)
44
45 C
          OBTAIN THE UNIT CONVERSION FACTORS FROM THE EDSMOD ROUTINES
46 C
          COMMON/EDSCCE/TFACE.RFACE, PFACE, EFACE, KREPE
47
48 C
          CALL MATCHKX(MID, NRS, LCFW(1, IOT), TBLS(1), IFL)
49
50
          IF(IFL.EQ.O) GD TO 10
51
          LCFW(IR, IOT)=IFL
52
          IFL=2
53
          RETURN
54
    10
         NL=LCMX-LCNT-1
55 C . . FETCH EOS TABLES
          CALL TABRANX(MID, 201., LU, TBLS(LCNT+2), NL, IFL)
56
57
          IF(IFL.LE.O) RETURN
58
          ZB(1)=TBLS(LCNT+2)
59
          ZB(2)=ZB(1)+ZB(1)
60
          ZB(3)=TBLS(LCNT+3)
61
          TBLS(LCNT+1)=TBLS(LCNT+4)
          CALL TABRANX(MID.301., LU, TBLS(LCNT+2), NL, IFL)
62
```

```
63
          IF(IFL.LE.O) RETURN
          TBLS(LCNT)=FLGAT(MID)
64
65 C
          CALL PERTCB(IR. TBLS(LCNT), ZB(1), ZB(3))
          NR=TBLS(LCNT+2)
66
67
          NT=TBLS(LCNT+3)
68
          NRT=NR+NT
69
          LOCP=LCNT+3+NR+NT
70 C
71 C
     . . CONVERT TO DESIRED UNITS
72
          DD 30 I=1,NT
73 C
74
          TBLS(3+I+LCNT+NR)=TFACE+TBLS(3+I+LCNT+NR)
75 C
          DD 30 J=1,NR
76
77 C
          IF(I.GT.1) GD TD 20
78
          TBLS(3+J+LCNT)=TBLS(3+J+LCNT)+RFACE
79
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
     . . INVERT TABLES
90 C
     . . CHECK TO SEE IF THERE IS ENOUGH ROOM TO INVERT THE TABLES
91 C
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
          CALL INV301X(TBLS,LDC,RO,LDS)
99
100 C . . DOUBLE PACK DEPENDENT VARIABLES
          LOCP=LCNT+3+NR+NT+NR
101
102
          00 50 I=1.NRT
103
          LOCP=LOCP+1
104
          PTEM=TBLS(LOCP)
105
          TTEM=TBLS(LOCP+NRT)
106
          TBLS(LOCP) = OPACKX(PTEM.TTEM)
    50
107
          CONTINUE
108 C . . WRAP UP
109
          LCFW(IR, IDT)=LCNT
110
          LCNT=LCNT+2+LOS-NRT
111
          IFL=1
112
          RETURN
          ENO
113
```

```
SUBROUTINE GETRPOX(IR, MID, IDT, TBLS, LCNT, LU. IFL)
 2 C-
 3 C
 4 C
      SUBROUTINE GETRPOX(IR, MIO, IDT, TBLS, LCNT, LU, IFL)
 5 C
      PURPOSE
 6 C
                   TD LOAD THE ROSSELAND/PLANCK OPACITY TABLE
 7 C
 8 C
                   IR
                             (INPUT)
      ARGUMENTS
                                        REGION NO.
 9 C
                             (INPUT)
                   MIO
                                        SESAME MATERIAL ID
10 C
                   IDT
                             (INPUT)
                                        DATA TYPE INDICATOR
11 C
                   TBLS
                             (OUTPUT)
                                        ARRAY FOR TABLE STORAGE
                  LCNT
12 C
                             (I/O)
                                        POSITION IN ARRAY FOR
13 C
                                        STORING TABLES
14 C
                             (INPUT)
                                        SESAME LIBRARY UNIT NO.
                  LU
15 C
                   IFL
                             (OUTPUT)
                                        ERROR FLAG
                                        =1 FOR SUCCESSFUL LOADING
16 C
17 C
                                        =O FDR 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 DN 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 EDSMOD
28 C
29 C
      EXTERNALS
                  MATCHKX, TABRANX, DPACKX
30 C
                   COMMON/EDSCCO/ FROM THE EDSMOD 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
                      24 APRIL 1979
37 C
38 C--
39
         LEVEL 2.TBLS
40
         DIMENSION TBLS(1)
41
         CDMMON/S2DIRX/LCMX,NRS,LCFW(10,3)
42 C
43 C
         THE COMMON BLOCK EDSCCO PROVIDES THE UNIT CONVERSION FACTORS
44 C
         FROM THE EOSMOO PACKAGE
45
         COMMON/EOSCCO/ TFACO.RFACD.OFACO.KREPD
46 C
47 C
         UNITS..TEMP..DEG.K,RHO IN G/CC,DPACITY IN CM++2/G
48 C
         CHECK TO SEE IF TABLE HAS BEEN LOADED ALREADY
         CALL MATCHKX(MID, NRS, LCFW(1, IOT), TBLS(1), IFL)
49
         IF(IFL.EQ_O) GD TD 10
50
51
         LCFW(IR, IOT) = IFL
52
         IFL=2
53
         RETURN
         NLEFT=LCMX-LCNT-1
   10
54
55 C . . FETCH THE 502 TABLE
         CALL TABRANX(MID,502.,LU,TBLS(LCNT+2),NLEFT,IFL)
56
57
         IF(IFL.LE.O) RETURN
58 C . _ CONVERT TO DESIREO UNITS
59 C . . LINES THROUGH STATEMENT 60 MAY BE DELETED IF NO CONVERSION IS
60 C . . REQUIRED
61
         NR=TBLS(LCNT+2)
62
         NT=TBLS(LCNT+3)
```

```
63
         IPT=LCNT+3+NR+NT
64
         00 60 K=1,NT
         TBLS(LCNT+3+NR+K)=TBLS(LCNT+3+NR+K) + TFACO
65
66
         00 60 J=1,NR
         IF(K.GT.1) GO TO 50
TBLS(LCNT+3+J)=TBLS(LCNT+3+J)+RFACO
67
68
69
    50
         IPT=IPT+1
70
         ROP=TBLS(IPT)
71
         POP=SHIFT(ROP,30)
         ROP=ROP+TBLS(LCNT+3+J)+KREPO+DFACO
72
73
         POP=POP+TBLS(LCNT+3+J)+KREPO+OFACO
         ROP=DPACKX(ROP,POP)
74
75
         TBLS(IPT)=ROP
         CONTINUE
    60
76
77
          TBLS(LCNT)=FLOAT(MIO)
78
         TBLS(LCNT+1)=FLOAT(IOT)
79
         LCFW(IR, IDT)=LCNT
80
         LCNT=LCNT+IFL+2
81
          IFL=1
         RETURN
82
83
          END
```

```
SUBROUTINE INBUFRX(LU,Z,NW,IAO,IFLG)
1
2 C-
3 C
     SUBROUTINE INBUFRX(LU,Z.NW,IAD,IFLG)
4 C
5 C
     PURPOSE
                 RANDOM I/O READ
6 C
7 C
                      (INPUT) UNIT NO.
(DUTPUT) STORAGE AREA WHERE DAT IS RETURNED
     ARGUMENTS
8 C
                 LU
9 C
                 Z
                       (INPUT) NO. OF WORDS TO BE READ
10 C
                 NW
                 IAD (INPUT) STARTING DISK ADDRESS OF DATA IFLG (DUTPUT) O=NORMAL
11 C
12 C
13 C
                               1=EOF ENCOUNTERED
                              -1=ERROR
14 C
15 C
16 C
      REMARKS
                  NDNE
17 C
                  ROISK
18 C
     EXTERNALS
19 C
      PROGRAMMER J.ABOALLAH, JR.
20 C
21 C
22 C
      DATE
                  1 MAY 1979
23 C 24 C-----
25
        LEVEL 2,Z
        CALL ROISK(LU,Z,NW,IAD)
26
        IF(UNIT(LU)) 10,20,30
27
28
        IFLG=1
   10
         RETURN
29
   20
         IFLG=0
30
31
         RETURN
         IFLG=-1
    30
32
33
         RETURN
34
         END
```

```
SUBROUTINE INV301X(OSTR, LOC, RO, LDS)
 1
 2 C--
 3 C
      SUBROUTINE: INV301X(DSTR,LOC,RO,LDS)
 4 C
 5 C
                   INVERT DATA STRING OF TYPE 301 TO TYPE 302.
 6 C
      PURPOSE:
 7 C
                   OSTR (INPUT) - TABLE STORAGE ARRAY
 8 C
      ARGUMENTS:
 9 C
                   LOC (INPUT) - STARTING LOCATION OF DATA STRING
10 C
                                   IN OSTR
   C
                    RO
                         (INPUT) - APPROXIMATE DENSITY OF SOLIO
11
                   LOS (OUTPUT) - LENGTH OF NEW DATA STRING
12 C
13
                   OSTR CAN BE DECLARED LCM ON THE CDC 7600.
14 C
      REMARKS:
15 C
                    THIS ROUTINE OVERWRITES LOCATIONS FOLLOWING THE
                   DATA STRING. IT EXPANDS THE STRING BY NR WORDS,
16 C
17 C
                    WHERE NR IS THE NUMBER OF DENSITIES. IT ALSO
                    USES 3+NT WORDS AS TEMPORARY STORAGE, WHERE NT
18 C
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 2,0STR
29
         DIMENSION DSTR(1)
30
         COMMON/INTOROX/IFN
31
         COMMON/RTBLK1X/LOCX,NR,LQCY,KY,JX,NT,INT,ET,Z(2)
32
         INT=1
         IFNS=IFN
33
34
         IFN=0
         NR = OSTR(LOC)
35
         NT = OSTR(LOC+1)
36
37
         LOCT = 2+NR+LOC
38
         LCEC = LOCT+NT
         LOCP = LCEC+NR
39
40
         LOCE = LOCP+NR+NT
         LOCN = LOCE+NR+NT
41
42
         IMAX = 2*NR*NT
         DO 1 I=1, IMAX
43
44
         OSTR(LOCN-I) = DSTR(LOCN-I-NR)
45
         00 2 I=1,NR
46
         JJ = LOCE+I-1
         Q = 1_E-12*ABS(DSTR(JJ))
47
48
         DSTR(LCEC+I-1) = DSTR(JJ)
         DSTR(JJ) = 0.
49
50
         DO 2 J=2,NT
         JJ = JJ+NR
51
52
         OSTR(JJ) = OSTR(JJ) - OSTR(LCEC + I - 1)
53
         IF(OSTR(JJ)-OSTR(JJ-NR).LT.Q) DSTR(JJ)=DSTR(JJ-NR)+Q
54
         CONTINUE
         I = ISRCHKX(RO,DSTR(LOC+3),NR-2,1,0)+1
55
56
         00 3 J=1,NT
57
         DSTR(LOCN+J-1) = DSTR(LOCT+J-1)
58
         DSTR(LOCT+J-1) = DSTR(LOCE+I-1+NR+(J-1))
         DO 5 I=1,NR
59
         LOCX = LOCE+I-1
60
         DO 4 J=1,NT
61
62
         ET = OSTR(LOCT+J-1)
```

```
JX = ISRCHKX(ET,OSTR(LOCX+NR),NT-2,NR,O)+1
LOCY = LOCP+I-1
63
64
                KY = NR
CALL RATFN1X
DSTR(LOCN+NT+J-1) = Z(1)
65
66
67
68
                LOCY = LOCN
                KY = 1
CALL RATFN1X
DSTR(LOCN+NT+NT+J-1) = Z(1)
69
70
71
                DSTR(LOCHNITHITO-1) = Z(1)

DD 5 J=1,NT

DSTR(LOCP+I-1+NR*(J-1)) = DSTR(LOCN+NT+J-1)

DSTR(LOCX+NR*(J-1)) = DSTR(LOCN+NT+NT+J-1)

LDS = LOCN-LOC

IFN=IFNS
72
73
74
75
76
77
                 RETURN
78
                 END
```

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

```
SUBROUTINE MATCHKX(MID, NRS, LOC, TBLS, IFLG)
 2 C---
 3 C
 4 C
      SUBROUTINE MATCHKX(MID, NRS.LOC, TBLS, IFLG)
 5 C
                  TD CHECK IF A MATERIAL HAS BEEN
 6 C
      PURPOSE
 7 C
                  PREVIOUSLY LOADED
 8 C
 9 C
                  MIO
                             (INPUT)
      ARGUMENTS
                                       SESAME MATERIAL ID
10 C
                  NRS
                             (INPUT)
                                       NUMBER OF REGIONS
11 C
                  LOC
                             (INPUT)
                                       ARRAY OF FIRST WORD LOCATIONS
12 C
                                       IN TABLE STDRAGE ARRAY FOR
13 C
                                       FOR EACH REGION
14 C
                  TBLS
                             (INPUT)
                                       TABLE STORAGE ARRAY
15 C
                   IFLG
                             (OUTPUT)
                                       =O MATERIAL NOT PREVIOUSLY LOADED
16 C
                                       GT.O 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
         DIMENSION LOC(1), TBLS(1)
29
30
         IFLG=0
         DD 100 J=1,NRS
LC=LDC(J)
31
32
33
         IF(LC.LE.O) GD TD 100
34
         ITEST=TBLS(LC)
35
         IF(MID.EQ.ITEST) GD TO 200
    100 CONTINUE
36
37
         RETURN
38
    200 IFLG=LC
39
         RETURN
         ENO
40
```

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

```
63
         IF(YY(2)+(YY(2)-YY(4)+YY(6)).LE.O.) YY(6)=YY(2)/YY(4)
         YY(5) = YY(6)
64
65
         GD TD 2
    1
         DM = YY(3)-TBLS(IX-KX)
66
67
         SM = (YY(1)-TBLS(IY-KY))/OM
         YY(5) = (YY(2)-SM)/(YY(4)+DM)
68
         IF(I.EQ.N-1) YY(6)=YY(5)
69
70
         IF(I.GT.2) GO TO 2
         IF(SM*(SM-DM*YY(5)).LE.O.) YY(5)=(YY(2)-SM-SM)/YY(4)
71
         IF(YY(6).NE.O.) YY(5)=YY(5)/YY(6)
72 2
73 C EVALUATE RATIONAL FUNCTION FROM PRECALCULATED COEFFICIENTS
   3
74
         Q = X-YY(3)
75
         R = YY(4)-Q
76
         IF(R.NE.O.) GO TO 4
77
         W = 1.
         GO TO 5
78
79
         W = 1.-1./(1.+ABS(YY(5)+Q/R))
80
    5
         F = YY(6)*(W+YY(5)*(1.-W))
         Y(1) = YY(1)+Q*(YY(2)-R*F)

Y(2) = YY(2)+(Q-R)*F+YY(4)*W*(F-YY(6))
81
82
83
         RETURN
84 C CALCULATE COEFFICIENTS FOR LINEAR INTERPOLATION
85
         IF(IP.EQ.O) GO TO 7
         IX = LOCX+KX+(I-1)
86
         IY = LOCY+KY+(I-1)
87
         YY(3) = TBLS(IX)

YY(1) = TBLS(IY)
88
89
         YY(2) = (TBLS(IY+KY)-YY(1))/(TBLS(IX+KX)-YY(3))
90
91 C CALCULATE LINEAR ESTIMATE FROM PRECALCULATED COEFFICIENTS
         Y(1) = YY(1)+YY(2)+(X-YY(3))
Y(2) = YY(2)
92 7
93
         RETURN
94
95
         ENO
```

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

```
IF(ITEST.NE.MID) GD TO 100
63
64
         NW=A(J+N)
65
         IAO=A(J+N+N)
         GD TD 200
66
67
    100 CONTINUE
         RETURN
68
69 C .
       . GET MATERIAL INDEX
70
    200 IF(LEN.LT.NW) GD TD 999
71
         IADX=IAD
72
         CALL INBUFRX(LIB, A, NW, IAOX, IER)
73
         00 210 J=1,NW
74
         HINDEX(J)=A(J)
75
    210 CONTINUE
76
         IF(TID.EQ.O.O) GO TO 500
    230 N=HINDEX(5)
77
         DD 300 J=1,N
IF(TID.NE.HINDEX(5+J)) GD TD 300
78
79
80
         NW=HINDEX(5+J+N)
81
         IAD=HINDEX(5+J+N+N)
82
         IAO=IADX+IAO
83
         GD TD 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, IAO, IER)
89
    500 IFLAG=NW
90
         RETURN
         IFLAG=LEN-NW
91
    999
         RETURN
92
93
         ENO
```

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

```
63
         KX = 1
          LOCX = LOCR
64
65
          LDCY = LDCX+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 OD NOT NEED TO BE REPEATED
      UNLESS A NEW REGION HAS BEEN ENTERED
73 C
          LOCLST=LOC
74
75
          IXLAST = 0
76
          IYLAST = O
77
          LOCI = LOCX+NX/2-1
78
          LOCJ = LOCY+NY/2-1
79
          LOCNX=LOCX+NX-2
          LOCNY=LOCY+NY-2
80
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
          IF(LOCI.EQ.LOCNX) GO TO 20
84
85
          LOCI=LOCI+1
          GD TD 10
86
87
     15
          IF(LDCI.EQ.LOCX) GO TO 20
88
          LDCI=LOCI-1
89
          IF(R.LT.TBLS(LOCI)) GO TO 15
90
    20
          IX=LOCI-LOCX+1
91 C
       INTERPOLATE FOR ENERGY ON COLO CURVE. IF ISAME = O, DENSITY
     INDEX IS THE SAME AS IN THE LAST CALL TO THIS ROUTINE
92 C
93
          IRX = IX
94
          ISAME = IABS(IX-IXLAST)
95
          RX1=R
96
          CALL RATFN1X
97
          ET = AMAX1(O.,E-PX1(1))
          DECOR = PX1(2)
98
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(LDCJ.EQ.LDCNY) GD TD 40
104
          LOCJ=LOCJ+1
105
          GD TD 30
     35
          IF(LDCJ.EQ.LOCY) GD TD 40
106
107
          LOCJ=LOCJ-1
108
          IF(ET_LT_TBLS(LOCJ)) GO TO 35
109
          IY=LOCJ-LOCY+1
110 C
      IF ISAME = O, DENSITY AND TEMPERATURE INDICES ARE
       THE SAME AS IN THE LAST CALL TO THIS ROUTINE
111 C
          ISAME = ISAME+IABS(IY-IYLAST)
112
113
          IP = MINO(1, IP + ISAME)
          IT = MINO(1, IT+ISAME)
114
115
          IXLAST = IX
116
          IYLAST = IY
117
          IOS=(IOT-1)+32+1
118
          IF(IBR.EQ.2) GO TO 50
119 C
       PRESSURE CALCULATION
120
          NSFT = 0
          INT=IP
121
          CALL T4INTPX
P(1)=PX2(1)
122
123
          P(2)=PX2(2)-DECOR+PX2(3)
124
```

```
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)-DECOR+PX2(3)
135 T(3)=PX2(3)
136 IT = 0
137 RETURN
138 END
```

```
SUBROUTINE T40ATX
 2 C--
 3 C
 4 C
      SUBROUTINE: T40ATX
 5 C
 6 C
                    SEARCH/INTERPOLATE FOR ATOMIC DATA AS
      PURPOSE:
                    FUNCTIONS OF REGION, DENSITY AND TEMPERATURE, USING PACKED SESAME 2 DATA STRING
 7 C
 8 C
 9 C
                    COMMON/SESINX/IR, IOT, AR, AT, IBR, IFL
10 C
11 C
                         (INPUT) - MATERIAL REGION NUMBER
                    IR
                         (INPUT) - DATA TYPE INDICATOR
12 C
                    IDT
13 C
                    AR
                         (INPUT) - DENSITY
                         (INPUT) - TEMPERATURE
14 C
                    AT
15 C
                         (INPUT) - SPECIFIES VARIABLES REQUIRED
                    IBR
16 C
                      IBR = O, BOTH VARIABLES
17 C
                      IBR = 1, FIRST HALF VARIABLE ONLY
                      IBR = 2, SECOND HALF VARIABLE ONLY
18 C
19 C
                    IFL (NOT USEO)
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
                    LA301A. TABLES OF 2 VARIABLES ARE DOUBLE PACKED.
28 C
29 C
                    THE SEARCH INDICES AND INTERPDLATION CONSTANTS
30 C
                    ARE SAVEO AND REUSED. IF POSSIBLE.
31 C
32 C
                    SYSTEM DEPENDENT FEATURE. THE CONSTANT NSFT
                    IN STATEMENT 60 SHOULD BE SET TO 1/2 THE BIT
33 C
             ****
34 C
             ****
                    LENGTH. FOR A COC 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. ABOALLAH, T-4
41 C
42 C
      DATE:
                    11 JULY 1978.REVISEO 27 APRIL 1979
43 C
44 C-
45
         LEVEL 2,TBLS
46
         DIMENSION LOCLST(3), IXLAST(3), IYLAST(3),
47
                    IPLAST(3), IELAST(3)
48
         COMMON/S201RX/LCMX,NRS,LCFW(10,3)
         COMMON/RTBLK2X/LDCX, IX, NX, LOCY, IY, NY, LOCZ, NZ, NSFT,
49
50
         1 R.T.Z(3), INT.IDS.ZZ(96)
         CDMMON/SESDATX/TBLS(10000)
51
52
         COMMON/SESINX/IR, IOT, AR, AT, IBR, IFL
         COMMON/SESOUTX/P(3),E(3)
53
54
         DATA IPLAST/3+0/
         DATA IELAST/3+1/
55
56
         DATA LOCLST/3+0/
57 C
     LOC IS POINTER TO START OF DATA STRING FOR REGION IR
58
         LOC = LCFW(IR, IOT)+2
59
         NZ = 1
60
         NX=TBLS(LOC)
61
         NY=TBLS(LOC+1)
62
         LOCX=LOC+2
```

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

125 RETURN 126 ENO

```
SUBROUTINE T4INTPX
 2 C-
 3 C
   C
      SUBROUTINE: T4INTPX
 5 C
                    INTERPOLATE FOR A FUNCTION Z(X,Y) AND ITS
 6
  C
      PURPOSE:
                    DERIVATIVES FROM TABLES LOCATED IN ARRAY TBLS.
 7 C
 8 C
                    THE ROUTINE REQUIRES COMMON BLOCKS,
   C
                    COMMON/RTBLK2X/LOCX, IX, NX, LOCY, IY, NY, LOCZ, NZ, NSFT,
10 C
11 C
                                  X.Y.Z(3), IP, IOS, ZZ
                      LOCX = LOCATION OF X VECTOR
12 C
13 C
                      ΙX
                          = INDEX OF X VECTOR
                           - LENGTH DF X VECTOR
14 C
                      NX
                      LOCY = LOCATION OF Y VECTOR
15 C
                           - INDEX OF Y VECTOR
16 C
                      ΙY
                           = LENGTH OF Y VECTOR
17 C
                      NY
                      LOCZ = LOCATION DF Z(X,Y) ARRAY
18 C
                           = SPACING OF Z ARRAY
19 C
                      NSFT = BIT SHIFT PARAMETER
20 C
21 C
                    X.Y (INPUT) - INDEPENDENT VARIABLES
                        (OUTPUT) - VECTOR OF LENGTH 3, WHERE
22 C
23 C
                      Z(1) = VALUE OF FUNCTION
24 C
                      Z(2) = X DERIVATIVE DF FUNCTION
                      Z(3) = Y DERIVATIVE OF FUNCTION
25 C
                    ZZ (IN/OUT) - COEFFICIENT VECTOR OF LENGTH 16
26 C
                         (INPUT) - BRANCH PARAMETER
27 C
                      IP.EQ.O, USE INPUT COEFFICIENTS IN ZZ IP.NE.O, CALCULATE ZZ VECTOR FIRST
28 C
29 C
30 C
                    IDS (INPUT) - DISPLACEMENT INTO ZZ FOR COEFFS.
31 C
                                    TO BE USEO
32 C
                    COMMON/INTORDX/IFN.
                    IFN (INPUT) - INTERPOLATION TYPE
33 C
                      IFN.NE_1, RATIONAL FUNCTION
34 C
35 C
                      IFN.EQ.1, BILINEAR
36 C
                    COMMON/SESOATX/TBLS
37 C
                      TBLS IS THE TABLE STORAGE ARRAY
38 C
39 C
                    UNLESS BILINEAR FORM IS SPECIFIED, ROUTINE
40 C
      REMARKS:
                    USES RATIONAL FUNCTION METHOD WITH QUADRATIC
41 C
42 C
                    ESTIMATE OF DERIVATIVES AT THE MESH POINTS.
43 C
                    TBLS CAN BE DECLARED LCM ON THE CDC 7600.
44 C
                    SYSTEM DEPENDENT FEATURE. THE Z-ARRAY CAN BE
45 C
46 C
                    DOUBLE PACKED. PARAMETER NSFT SPECIFIES THE
                    NUMBER OF BITS TO BE SHIFTED WHEN UNPACKING THE
47 C
             ****
48
             ****
                    RIGHT HALF OF THE WORD. THIS ROUTINE USES
                    THE LASL SHIFT FUNCTION
49 C
50 C
                    NONE, BUT A SEARCH ROUTINE MUST BE CALLED
51 C
      EXTERNALS:
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
                    01 AUG 1979
      DATE:
57 C
58 C-
59
          LEVEL 2, TBLS
60
          COMMON/RTBLK2X/LOCX,IX,NX,LOCY,IY,NY.LOCZ,NZ,NSFT,X,Y,Z(3),
         $ IP.IDS,ZZ(96)
61
          COMMON/INTORDX/IFN
62
```

```
63
          CDMMDN/SESDATX/TBLS(10000)
64 C
      CALCULATE COEFFICIENTS FOR RATIONAL FUNCTION INTERPOLATION
65
          IF(IFN.EQ.1) GD TO 13
66
          IF(IP.EQ.O) GD TD 8
          I = LOCX+IX-1
67
68
          IZ = LOCZ+NZ*(IX-1+NX*(IY-1))
          KZ = NZ
69
70
          IBR = IX
          NBR = NX-IX
71
          ZZ(IDS+4) = TBLS(I)
72
73
          DD 7 K=1,4
74
          KI=IDS+K-1
75
          IF(K.LT.4) GO TO 1
76
          IZ = IZ+NZ
77
          GD TD 4
          IF(K_LT_3) GO TO 2
78
79
          ZZ(IOS+6) = 0
80
          I = LOCY+IY-1
          KZ = KZ+NX
81
          IZ = IZ-KZ
82
83
          IBR = IY
          NBR = NY-IY
84
85
          ZZ(IOS+5) = TBLS(I)
86
          GO TD 3
87
          IF(K.LT.2) GO TO 3
    2
88
          IZ = IZ+NX+NZ
89
          GD TD 4
90
    3
          D = TBLS(I+1)-TBLS(I)
          ZZ(KI)=SHIFT(TBLS(IZ),NSFT)
91
92
          S=SHIFT(TBLS(IZ+KZ),NSFT)
93
          S = (S-ZZ(KI))/D
94
          IF(NBR.EQ.1) GD TO 5
          SP=SHIFT(TBLS(IZ+KZ+KZ),NSFT)
95
          SP = (SP-D*S-ZZ(KI))/(TBLS(I+2)-TBLS(I+1))
96
          G2 = (SP-S)/(TBLS(I+2)-TBLS(I))
97
98
          IF(IBR.GT.1) GO TO 5
99
          IF(S*(S-D*G2).LE.O.) G2=S/O
100
          G1 = G2
101
          GD TD 6
102
          DM = TBLS(I)-TBLS(I-1)
103
          SM=SHIFT(TBLS(IZ-KZ),NSFT)
104
          SM = (ZZ(KI)-SM)/OM
105
          G1 = (S-SM)/(D+DM)
106
          IF(NBR.EQ.1) G2=G1
107
          IF(IBR.GT.2) GD TO 6
          IF(SM*(SM-DM*G1).LE.O.) G1=(S-SM-SM)/D
108
109
          IF(G2.NE.O.) G1=G1/G2
          ZZ(KI+8) = G1
110
111
          ZZ(KI+12) = G2
112
          ZZ(IOS+7)=0
113
          ZZ8=ZZ(IOS+7)
114
          ZZ7=ZZ(IDS+6)
115
          ZZ(IOS+2)=(ZZ(IOS+1)-ZZ(IOS))/ZZ8
116
          ZZ(IOS+1)=(ZZ(IOS+3)-ZZ(IOS))/ZZ7
          ZZ(IOS+3)=(S-ZZ(IOS+2))/ZZ7
117
118
          ZZ(IDS+12)=ZZ(IOS+12)/ZZ8
119
          ZZ(IOS+13)=ZZ(IOS+13)/ZZ8
120
          ZZ(IDS+14)=ZZ(IOS+14)/ZZ7
          ZZ(IOS+15)=ZZ(IOS+15)/ZZ7
121
122 C EVALUATE RATIONAL FUNCTION FROM PRECALCULATED COEFFICIENTS
          QX = X-ZZ(IOS+4)
123
    8
124
          RX = ZZ(IDS+6)-QX
```

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

```
SUBROUTINE TAPTREX(IR, IOT, TBLS, P.T, R, E, IFL)
2 C-
 3 C
 4 C
      SUBROUTINE: T4PTREX(IR, IDT, TBLS, P, T, R, E, IFL)
5
  С
 6 C
      PURPOSE:
                    FIND DENSITY AND INTERNAL ENERGY AS FUNCTIONS
 7 C
                    OF PRESSURE AND TEMPERATURE FROM A 302
                    SESAME TABLE. USES DOUBLE BINARY SEARCH TO
8 C
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.
                    IOT (INPUT) - DATA TYPE CORRESPONDING TO E BASED EOS
13 C
                    TBLS (INPUT) - TABLE STORAGE ARRAY
14 C
15 C
                          (INPUT) - PRESSURE
16 C
                    T
                          (INPUT) - TEMPERATURE
17 C
                         (DUTPUT) - DENSITY
                    R
18 C
                         (DUTPUT) - ENERGY
                    IFL (DUTPUT) - ERROR FLAG
19 C
                      IFL=1, IF CALCULATION IS SUCCESSFUL IFL=0, IF CALCULATION FAILS
20 C
21 C
22 C
23 C
      REMARKS:
                    TBLS CAN BE DECLARED LCM ON THE COC 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----
         LEVEL 2, TBLS
32
33
         OIMENSION 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
         IOTX=IOT
         LOC=LCFW(IR, IDT)+1
41
42
         NR = TBLS(LOC+1)
         NT = TBLS(LOC+2)
43
44
         ILO = 1
         IHI = NR
45
46
          I = .5*(ILO+IHI)
         LOCT = LOC+2+NR+NR+NT+I+NR
47
48
         J = ISRCHKX(T,TBLS(LOCT),NT-2,NR,30)+1
         LOCP = LOC+2+NR+NT+I+NR*(J)
49
50
          IF(IHI-I_EQ. 1) GD TO 3
51
          IF(P.LT_TBLS(LOCP)) GO TO 2
52
         ILO = I
         GO TD 1
53
54
         IHI = I
55
         GD TD 1
56
          RX = TBLS(LOC+2+I)
         EX = TBLS(LOC+2+NR+J)+TBLS(LOC+2+NR+NT+I)
57
58
         K = 0
59
         IFL = 1
60
         K = K+1
61
         IF(K.EQ.50) GD TD 6
62
          CALL T4DATIX
```

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

```
SUBROUTINE TARTPEX(IR, 10T, TBLS, R, T, P, E, IFL)
 2 C--
 3 C
      SUBROUTINE TARTPEX(IR, IDT, TBLS, R, T, P, E, IFL)
 4 C
 5 C
 6 C
      PURPOSE
                  TO FIND PRESSURE AND ENERGY AS FUNCTIONS
 7 C
                  DF DENSITY AND TEMPERATURE FROM A
                  SESAME TYPE 302 TABLE USING NEWTONS METHOD.
8 C
 9 C
                             (INPUT)
                                        REGION NO.
      ARGUMENTS
10 C
                  IR
                                        DATA TYPE FOR 302 TABLES
11 C
                  IDT
                              (INPUT)
                              (INPUT)
                                        TABLE STORAGE ARRAY
12 C
                  TBLS
13 C
                              (INPUT)
                                         TEMPERATURE
                  T
                              (OUTPUT)
                                        PRESSURE
                  P
14 C
15 C
                   Ε
                              (OUTPUT)
                                        ENERGY
                              (DUTPUT) DUTPUT FLAG
                   IFL
16 C
                                         =1 FOR SUCCESS
17 C
                                         -O FOR FAILURE
18 C
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--
         LEVEL 2, TBLS
28
29
          COMMON/S201RX/LCMX,NRS,LCFW(10,3)
30
          DIMENSION TBLS(1)
         COMMON/SESINX/IRXX, IOTX, RX, EX, IBR, IFLX
31
          COMMON/SESOUTX/ZP(3), ZT(3)
32
          IBR=0
33
34
          IFLX=1
35
          RX=R
36
          IRXX=IR
37
          IDTX=IOT
          LOC=LCFW(IR, IOT)
38
39
          NR=TBLS(LOC+2)
          NE=TBLS(LOC+3)
40
41 C _ GET INITIAL GUESS ON ENERGY
42 C . . FIND CLOSEST DENSITY INDEX
43
          LOCX=LOC+4
          IRX=1
44
45
          DELS=ABS(R-TBLS(LOCX))
          IF(NR.EQ.1) GD TO 20
46
47
          00 10 J=2.NR
          LDCX=LOCX+1
48
49
          DEL = ABS(R-TBLS(LOCX))
          IF(DEL.GT.DELS) GO TO 10
50
51
          IRX=J
52
          OELS=OEL
53
    10
          CONTINUE
54 C . .
          FIND THE ENERGY INDEX ASSOCIATED WITH THE CLOSEST TEMP
55
          LOCX=LOC+3+NR+NE+NR+IRX
          OELS=TBLS(LOCX)
56
          DELS=SHIFT(DELS,30)
57
58
          OELS=ABS(T-DELS)
59
          IEX±1
60
          IF(NE_EQ. 1) GO TO 40
          DD 30 J=2.NE
61
          LOCX=LOCX+NR
62
```

```
DEL=TBLS(LOCX)
63
         DEL=SHIFT(DEL,30)
64
65
          DEL=ABS(T-DEL)
          IF(DEL.GT.DELS) GO TO 30
66
67
          IEX=J
          OELS=OEL
68
69 30
          CONTINUE
70 C . . INITIAL GUESS ON ENERGY
71 40 EX=TBLS(LDC+3+NR+IEX)+TBLS(LDC+3+NR+NE+IRX)
72 C . . ITERATE USING NEWTONS METHOD
73
          K=O
74
          IFL=1
    50
75
          K=K+1
          IF(K.EQ.50) GD TD 90 CALL T40ATIX
76
77
          E=EX
78
          P=ZP(1)
79
          TTEST=ABS(T-ZT(1))-1.0E-05*(ABS(T)+1.0E-02)
80
          IF(TTEST_LT.O.) RETURN
81
          D=-ZT(3)
82
          IF(D.EQ.O.O) GD TO 90
83
84
          EX=EX-(T-ZT(1))/0
          GD TD 50
85
86
          IFL=0
    90
          RETURN
87
88
          ENO
```

APPENDIX B

CROSS-REFERENCE DIRECTORY OF EOSLIB

NO UNUSED SPACE

	ROUTINE	INDEX	RECORD LENGTH	DSKAD	EXTERNAL	SYMBOLS	COMMON 8	LOCKS
1.	DPACKX DPACKX	18	15	017113				
2-	EDSBEG EDSBEG	5	7	002354			S2DIRX SESINX EDSCZ EDSC2 EDSC4 EDSC6 EDSCCE	SESDATX INTOROX EDSC1 EDSC3 EDSC5 EDSC7 EDSCCD
Э.	EDSCON EDSCON	1	81	000000	EOSOSL	GOTOER.	EDSCCE	EDSCCO
4.	EOSORE EOSORE	6	81	005404	T4DATIX Edskut	EDSGET	S2D1RX 1NTOROX SESOUTX EOSC3	SESDATX SESINX EDSCZ EDSC4
5.	EDSDRT EDSDRT	7	80	006173	T4DATX EDSKUT	EDSGET	S2DIRX INTOROX SESOUTX EDSCCE EDSC3	SESDATX SESINX EDSCZ EDSC1 EDSC4
6.	EDSDSL EDSDSL	2	6	000454			EDSCCE	EDSCCD
7.	EOSEFD EOSEFO	4	166	001320	DUTCI. EDF REWIND. EDSFAS	DECODI. INPCI. FEXIST	EDSCZ EDSC2 EDSC5	EDSC1 EDSC3 EDSC6
₽.	EDSFAS EDSFAS	3	74	000644	ASSIGN GOTDER.	QASSIGN	EDSCZ EDSC2	EDSC 1
9.	EDSGET EDSGET	11	231	011374	DUTCI. GETRPDX GDTDER. Ensdfo	GETEDSX GETINVX EDSCON EDSEFD	S2DIRX SESINX EDSCZ EDSC3	SESDATX INTORDX EDSC! EDSC4
10.	EOSIPT EOSIPT	9	128	007722	DUTCI. Edsget	T4PTREX EDSKUT	S2DIRX SES1NX EDSCZ EDSC4	SESDATX INTORDX EDSC3
11.	EDSIRT EDSIRT	•	128	007020	DUTCI.	T4RTPEX	S2D1RX	SESDATX

					EOSGET	EDSKUT	SESINX EDSCZ EDSC4	INTOROX EDSC3
12.	EDSKUT EDSKUT	10	123	010624	putci.	EOSBEG	EDSCZ	EDSC3
13.	EOSOFO EOSOFO	12	145	012524	OUTCI. EDF REWIND. EDSFAS	DECODI INPCI. FEXIST	EDSCZ EDSC2 EDSC7	EDSC3
14.	EOSORT EOSORT	13	106	013464	XTDY\$ QLDG1D EDSKUT	T4DATX EDSGET DUTCI.	S201RX INTOROX SESOUTX EDSCCO EDSC3	SESDATX SESINX EDSCZ EDSC1 EDSC4
15.	GETEDSX GETEDSX	14	171	014330	DPACKX Matchkx	TABRANX	S201RX	EDSCCE
16.	GETINVX GETINVX	21	201	021107	DPACKX Tabranx	INV3D+X Matchkx	S2DIRX	EDSCCE
17_	GETRPDX GETRPDX	26	139	0256 11	DPACKX Matchkx	TABRANX	S201RX	EDSCCO
18.	INBUFRX INBUFRX	17	29	016627	UNIT	ROISK		
19.	INV301X INV301X	24	166	023711	RATFN1X	ISRCHKX	INTOROX	RTBLKIX
20.	ISRCHKX ISRCHKX	19	55	017303				
21.	MATCHKX MATCHKX	16	22	016437				
22.	RATFNIX RATFNIX	22	128	022237			SESDATX RTBLK1X	INTOROX
23.	T4DATIX T4DATIX	23	124	022770	T4 INTPX	RATFN1X	S201RX RTBLK2X SESOUTX	RTBLK IX SESINX SESDATX
24.	T4DATX T4DATX	27	130	026551	T4INTPX		S2DIRX SESDATX SESDUTX	RTBLK2X SESINX
25.	T4INTPX T4INTPX	20	289	017702			RTBLK2X Sesdatx	INTOROX

26.	T4PTREX T4PTREX	15	156	015403	T4DATIX	ISRCHKX	S2DIRX Sesoutx	SESINX
27.	T4RTPEX T4RTPEX	25	128	024613	T4DATIX		S201RX SESDUTX	SESINX
28.	TABRANX Tabranx	28	188	027566	INBUFRX			

1 NO.	ENTRY PT:	CALLED BY:				
1	EDSCON					
		EDSGET				
2	EOSDSL	EOSCON				
3	EOSFAS					
		EOSEFO	EOSOFO			
4	EOSEFO	EDSGET				
5	EOSBEG					
		EOSKUT				
	EOSDRE					
7	EOSDRT					
8	EOSIRT					
9	EOSIPT					
10	EOSKUT	EOSORE	EOSORT	EOSIRT	EOSIPT	EOSORT
11	EDSGET		2000			LUJUKI
	_ •	EOSORE	EOSORT	EOSIRT	EDSIPT	EOSORT
12	EOSOFO	EOSGET				
13	EOSORT					
	GETEDSX					
		EOSGET				
15	T4PTREX	EOSIPT				
16	MATCHKX					
		GETEOSX	GETINVX	GETRPOX		
17	INBUFRX	TABRANX				
18	DPACKX					
		GETEOSX	GETINVX	GETRPOX		
19	ISRCHKX	T4PTREX	INV301X			
20	T4INTPX	141 TREX	INVOVIA			
-0		T40ATIX	T4DATX			
21	GETINVX	EOSGET				
22	RATFN1X					

	T4DATIX	INV301X	
23 T4DATIX	EOSORE	T4PTREX	T4RTPEX
24 INV301X	GETINVX		
25 TARTPEX	EOSIRT		
26 GETRPOX	EOSGET		
27 T40ATX	EOSORT	EOSORT	
28 TABRANX	GETEOSX	GETINVX	GETRPOX

1 COMMON BLOCK	: USEO BY:							
EDSCCE	EDSCON	EDSDSL	EDSBEG	EDSORT	GETEDSX	GETINVX		
EDSCCD	EDSCON	EOSOSL	EDSBEG	EDSORT	GETRPDX			
EOSCZ	EDSFAS EDSGET	EDSEFD EDSOFD	EDSBEG EDSDRT	EDSDRE	EDSORT	EOSIRT	EOSIPT	EDSKUT
EDSC1	EDSFAS	EDSEFD	EDSBEG	EDSORT	EDSGET	EDSOFD	EDSORT	
EDSC2	EDSFAS	EDSEFD	EDSBEG	EDSOFD				
£05C3	EOSEFD EOSOFO	EDSBEG EDSDRT	EOSORE	EOSORT	EOSIRT	EOSIPT	EDSKUT	EDSGET
EDSC5	EOSEFO	EDSBEG						
EDSC6	EOSEFO	EDSBEG						
\$201RX	EDSBEG T4PTREX	EDSORE GET INVX	EDSDRT T4DATIX	EOSIRT TARTPEX	EDSIPT GETRPDX	EDSGET T4DATX	EDSORT	GETEDSX
SESDATX	EDSBEG RATFN1X	EDSDRE T4DATIX	EDSDRT T4DATX	EOSIRT	EOSIPT	EDSGET	EDSORT	T4INTPX
SESINX	EDSBEG T4DATIX	EDSORE T4RTPEX	EDSDRT T4DATX	EDSIRT	EOSIPT	EDSGET	EDSORT	T4PTREX
INTOROX	EDSBEG Ratfn1x	EDSDRE INV301X	EDSDRT	EDSIRT	EOSIPT	EDSGET	EDSORT	T4INTPX
EDSC4	EDSBEG	EDSDRE	EDSORT	EDSIRT	EOSIPT	EDSGET	EOSORT	
EDSC7	EOSBEG	EOSOFO						
SESOUTX	EOSORE	EDSORT	EDSORT	T4PTREX	T4DATIX	T4RTPEX	T4DATX	
MTBLK2X	T41NTPX	T4DATIX	T4DATX					
RTBLK 1X	RATFN1X	T4DATIX	INV301X					

APPENDIX C

TEST PROGRAM

```
PROGRAM SES (INPUT, DUTPUT, TAPE6=DUTPUT, TAPE59=TTY, TAPE3)
 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
                  THE MATERIAL BY SETTING LMAT TO THE SESAME NUMBER, FOR EXAMPLE- LMAT = "5760" FOR HELIUM
13 C
14 C
15 C
16 C
            R = DENSITY (RHD)
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. KEDS HAS FOUR DECIMAL DIGITS.
22 C
            KEDS = 1000*KBR + 100*KUNIT + 10*KREPE + KFN WHERE
23 C
24 C
25 C
             KBR = COMPUTATIONAL MODE FLAG TO INDICATE WHICH
26 C
                  QUANTITIES AND THEIR PARTIAL DERIVATIVES ARE TO
                  BE CALCULATED AND RETURNED BY THE PACKAGE.
27 C
28 C
                   = 0
                         COMPUTE PRESSURE AND TEMPERATURE
29 C
                          COMPUTE PRESSURE ONLY
30 C
                   = 2
                          COMPUTE TEMPERATURE ONLY
31 C
32 C
            KUNIT= KIND OF UNITS
33 C
               O (SESAMEE) R-G/CC.T-DEG.K,D-CM++2/G.P-GPA,E-MJ/KG
34 C
               1 (CGS) R-G/CC.T-DEG.K,D-CM++2/GM,P-MUBR.E-ERGS/GM
35 C
               2 (SIU) R-KG/M++3,T-DEG.K,P-PA,E-J/KG,D-M++2/KG
36 C
               3 (HYDROXE) R-G/CC,T-DEG.K.P=MBR,E-MBR+CC/GM.D-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.D-CM++2/G,P-GPA,E-MJ/KG
39 C
               6 (LASNEX) R-G/CC, T-KEV. D-CM++2/GM, P-JRKS/CC. ED-JRKS/CC
40 C
41 C
                LEGENO-
42 C
                       R = DENSITY
43 C
                        T = TEMPERATURE
44 C
                       D = OPACITY
45 C
                       P = PRESSURE
                       E = INTERNAL EN
46 C
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 = JDULES
55 C
                        JRKS = JERKS
                       KEV = KILO ELECTRON VOLTS
56 C
57 C
                       KG = KILOGRAM
58 C
                       M = METER
59 C
                       MBR = MEGABAR
60 C
                       MUBR = MICROBAR
61 C
                       PA = PASCAL
62 C
```

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

```
125 C
                  IMATE = O
                  CALL EOSORE(LMAT.R.E.P.T.KEOS.IMATE)
126 C
127 C
                  PRINT 10,P(1)
128 C
               10 FORMAT(" PRESSURE = ",E10.2," MICROBARS")
129 C
                  CALL EXIT
130 C
                  ENO
131 C
           * OUTPUT VARIABLES- IN THE COMMON BLOCKS EDSCCE AND EDSCCD
132 C
133 C
              TFACE = TEMPERATURE EDS SCALING FACTOR
134 C
              RFACE = DENSITY EDS SCALING FACTOR
135 C
              PFACE = PRESSURE EOS SCALING FACTOR
136 C
              EFACE = EN EDS SCALING FACTOR
137 C
138 C
              TFACD = TEMPERATURE OPACITY SCALING FACTOR
              RFACO = DENSITY OPACITY SCALING FACTOR
139 C
              DFACD = DPACITY SCALING FACTOR
140 C
141 C
              TBLS = ARRAY FOR STORAGE OF THE EOS TABLES LCMX = LENGTH OF THE TBLS ARRAY
142 C
143 C
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
              IOS2 = SESAME MATERIAL NUMBER
149 C
              TBLS = NAME OF AN ARRAY DESIGNATED FOR THE STORAGE OF TABLES LCNT = CRRRENT WORD IN THE ARRAY TBLS
150 C
151 C
              LU41 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SES2CL
152 C
              LU42 = UNIT NUMBER ASSIGNED TO THE SESAME INPUT FILE SES2L
              LU43 = UNIT NUMBER ASSIGNED TO SES20P/8 FILES
LU44 = UNIT NUMBER ASSIGNED TO MIXLIB (MIXTURES)
153 C
154 C
155 C
              LU45 = UNIT NUMBER ASSIGNED TO MIXLIB DIRECTORY.
              KFN = O RATIONAL APPROXIMATIONS (ACCURATE)
KFN = 1 BILINEAR APPROXIMATIONS (FAST)
156 C
157 C
158 C
              ZB (OUTPUT FROM GETINVX) AT. CHARGE.AT. CHG++2.MASS
159 C
              IOT * DATA TYPE INDICATOR
160 C
              MIO (IO) MATERIAL IO =1 INVERSE TABLES =2 OPACITY
161 C
162 C
           * EXTERNAL FILES TO HANDLE EDS. OPACITIES AND MIXTURES
           * SES2CL - CLASSIFIED SESAME LIBRARY
* SES2L - CUCLASSIFIED SESAME LIBRARY
163 C
164 C
165 C
              SES20P - OPACITY TABLE FROM T4
              MIXLIB - PRIVATE (EOS,OPC) TABLES CREATED BY MIXB(OR MIXER)
MIXOIR - DIRECTORY OF MIXTURES ON MIXLIB ( NAME, ND (A10.13))
166 C
167 C
168 C
169 C
           * EXTERNALS AND COMMON BLOCKS-
              SESAME ROUTINES- S2GET, S2EOS
170 C
171 C
               SESAME ROUTINES MATCHKX, TABFCHX, INBUFRX, DPACKX, ISRCHKX,
                  T4INTPX,GETINVX.RATFN1X.T40ATIX.INV301X,T4RTPEX
172 C
               SESAME COMMON BLOCKS-S20IRX,RTBLK2X,SESDATX.SESINX.SESOUTX.INTO
173 C
               EOSMOO COMMON BLOCKS- EDSC1,-7
174 C
               EDSMOD COMMON (ALSO INSERTED INTO GETINVX) EDSCCE. EDSCCD
175 C
176 C
177 C
           * LOCAL VARIABLES-
178 C
           * NONE
179 C
180 C
           * EXTERNALS AND COMMON BLOCKS-
           * EDSMOD COMMON BLOCKS- EDSCCE.EDSCCD
181 C
182 C
           * REMARKS- THIS SUBROUTINE IS PART OF THE EOSMOD PACKAGE
183 C
184 C
185 C
           * PROGRAMMER- J. M. HYMAN AND M. KLEIN, GRDUP T-7. LASL
186 C
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187 C
             REFERENCE- J. M. HYMAN, M. M. KLEIN
188 C
                          EOSMOD- A SUBROUTINE PACKAGE FOR CALCULATING
189 C
                          EQUATIONS-OF-STATE AND OPACITIES
                          LOS ALAMOS SCIENTIFIC LABORATORY RPT., LA-8502-M, 1980
190 C
191 C
           + DATE- MARCH 6, 1980
192 C
193 C
194 C
195 C
           LEVEL 2, TBLS
COMMON /S20IR/ LCMX, NRS, LCFW(10.3)
196
197
198
           COMMON /SESDAT/ TBLS(11000)
           COMMON /SESIN/ IRC, IDT, DUM(2), KBR, DUM1
199
           COMMON /INTORO/ KFN
200
201 C
           COMMON BLOCKS FOR THE EDSMOD ROUTINES
202 C
           CDMMDN /EDSC1/ LU41, LU42, LU43, LU44. LU45
CDMMDN /EDSC2/ LF41, LF42. LF43, LF44, LF45
203
204
           COMMON /EOSC3/ INIT, IROIM, IR(60.3), KUT(60,3)
205
           COMMON /EOSC4/ NTABLE, NTABLO, IFLP. LCNT
206
           COMMON /EDSC5/ NMAT, LABMAT(60), IDMAT(60)
COMMON /EDSC6/ NMCL, LABMCL(60). IDMCL(60)
207
208
           COMMON /EDSC7/ NMATO, LABMO(60), IDMATD(60)
209
210 C
211 C
           EDSMOD COMMON BLOCKS USED BY THE MODIFIED SESAME ROUTINES
212
           COMMON /EDSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
           COMMON /EDSCCO/ TFACD, RFACD, DFACD, KREPO
213
214 C
           NAMELIST /INP/ KUNIT, KREP, NLMAT, NBR, NFN, IIPT, IIRT, IDRT, IORE, LCMX
215
          1 ,NRS,DUM,KBR,DUM1,KFN.INIT,IRDIM,NTABLE.NTABLO.IFLP,LCNT.NMAT
216
          2 ,NMCL,NMATO,TFACE,RFACE,EFACE,KREPE,TFACO,RFACO.OFACO,KREPO.RHO
217
218
          3 ,TEMP,PR,EN,IRC,IOT,IORT,NGO
           DATA RHO /0.16/, TEMP /5.E4/, PR /19.2/, EN /310./
219
220 C
           DATA KUNIT /O/, KREP /O/, NLMAT /2/, NBR /1/, NFN /1/
DATA IIPT /1/, IDRT /1/, IIRT /1/, IDRE /1/, IDRT /1/, NGD /O/
221
222
223 C
224
           WRITE (3,210)
           OD 10 I=1,NMAT
WRITE (3,220) LABMAT(I),IDMAT(I)
225
226
        10 CONTINUE
227
228 C
229
           WRITE (3.230)
           00 20 I=1,NMATO
230
           WRITE (3,220) LABMO(I), IOMATO(I)
231
232
        20 CONTINUE
233 C
        30 CONTINUE
234
235 C**
           READ (59, INP)
236 C
237
           WRITE (6, 160)
238 C
239
           DD 60 LMATP=1.NLMAT
240
           LMAT=6HHELIUM
           LMATO=LMAT
241
           IF (LMATP.EQ.2) LMAT="5760"
242
           IF (LMATP.EQ.2) LMATD="15760"
243
244 C
           00 50 KBRP=1,NBR
245
           KBR=KBRP-1
246
247 C
248
           DD 40 KFNP=1,NFN
```

```
249
          KFN=KFNP-1
250 C
251
          KEDS = 1000 + KBR + 100 + KUNIT + 10 + KREP + KFN
252 C
253
          CALL ES (LMAT, LMATO, RHO.TEMP, PR.EN, KEOS. IIPT, IORT. IIRT, IORE. IORT. 1
254
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) GD TD 30
263 C
          IF (NGD.GT.O) GD TD (70,80,90,100,110.130), NGD
264
265 C
          CHECK THE ERROR MESSAGES
266.C
267 C
268 C
          CHANGE UNITS
269
       70 CONTINUE
270
          KEDS=KEDS+100
271
          CALL ES (LMAT, LMATO, RHO, TEMP, PR, EN, KEOS, IIPT. IORT, IIRT. IDRE. IORT. 1
272
273
          KEDS=KEDS-100
274 C
          CHANGE TABLE FORMAT FOR THE ENERGY AND OPACITY REPRESENTATION
275 C
276
       80 CONTINUE
277
          KEDS=KEDS+10
278
          CALL ES (LMAT, LMATO. RHO, TEMP, PR.EN, KEOS, IIPT, IORT, IIRT, IORE, IORT, 1
279
          1)
280
          KEDS=KEDS-10
281 C
282 C
          NON MATERIAL TEST
283
       90 CONTINUE
          LMAT="NOMAT"
284
285
          CALL ES (LMAT, LMATO, RHO, TEMP, PR. EN, KEOS, IIPT, IORT. IIRT, IORE. IORT, 1
286
287 C
          LMAT="99999"
288
289
          CALL ES (LMAT,LMATO.RHO.TEMP.PR,EN.KEOS.IIPT.IORT.IIRT,IORE.IORT.1
290
291 C
292 C
          NEGATIVE DENSITY TEST
      100 CONTINUE
293
294
           R=-RHO
295
          CALL ES (LMAT.LMATO,R,TEMP,PR.EN.KEOS.IIPT,IORT,IIRT,IORE.IORT,1)
296
           GD TD 150
297 C
           CHECK IF ALL THE MATERIALS ARE AVAILABLE
298 C
299 C
300 C
           EDS MATERIALS CHECK
301
       110 CONTINUE
          DD 120 I=1,NMAT
302
303 C
304
           LMAT=LABMAT(I)
305
           CALL ES (LMAT.LMATD.RHD.TEMP.PR.EN.KEDS.O.1.O.O.O.O)
306 C
307
           ENCODE (4,190,LMAT) IDMAT(I)
308 C
309
           CALL ES (LMAT.LMATO.RHO.TEMP, PR.EN.KEOS.O.1.0.0.0.0)
310 C
```

```
311
        120 CONTINUE
312 C
313 C
            OPACITY MATERIALS CHECK
314
        130 CONTINUE
            00 140 I=1,NMATO
315
316 C
            LMATO=LABMO(I)
317
318
            CALL ES (LMAT, LMATO, RHD, TEMP, PR.EN. KEDS, O.O.O.O.1.0)
319 C
320
            ENCODE (5,200,LMATD) IDMATO(I)
321 C
            CALL ES (LMAT, LMATO, RHO, TEMP, PR, EN, KEOS, O. 1, O.O.O.O)
322
323
        140 CONTINUE
324
        150 CONTINUE
325 C
            CALL EXITA (1)
326
327 C
       160 FORMAT (" KEDS
170 FORMAT (" CONTINUE?")
180 FORMAT (A1)
328
                                    KEOS IMATE R
                                                             T
                                                                           Р
                                                                                         E")
329
330
331
        190 FORMAT (14)
       200 FORMAT (15)
210 FORMAT (" THE EOS MATERIALS ARE")
220 FORMAT (1X,A10,I10)
230 FORMAT (" THE OPACITY MATERIALS ARE")
332
333
334
335
336
             ENO
```

```
SUBROUTINE ES (LMAT, LMATO, RHO, TEMP, PR.EN, KEOS, IIPT, IORT, IIRT, IORE
        1 , IORT, IWNL)
2
3 C
 4 C
 5 C
 6 C
         * PURPOSE-
7 C
8 C
         * INPUT VARIABLE-
9 C
10 C
           INPUT-DUTPUT VARIABLES IN THE COMMON BLOCKS EDSCC2 AND EDSCCD
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
                       EDSMOD- 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. TBLS
         COMMON /S20IR/ LCMX, NRS. LCFW(10.3)
30
31
         COMMON /SESDAT/ TBLS(11000)
32
         COMMON /SESIN/ IRC. IOT, DUM(2), KBR, DUM1
         COMMON /INTORD/ KFN
33
         COMMON BLOCKS FOR THE EOSMOD ROUTINES
35 C
         CDMMON /EOSC1/ LU41, LU42, LU43, LU44, LU45
COMMON /EOSC2/ LF41, LF42, LF43, LF44, LF45
36
37
         COMMON /EDSC3/ INIT. IROIM. IR(60.3), KUT(60.3)
38
         COMMON /EDSC4/ NTABLE, NTABLO. IFLP. LCNT
COMMON /EDSC5/ NMAT. LABMAT(60). IDMAT(60)
39
40
         COMMON /EDSC6/ NMCL, LABMCL(60), IDMCL(60)
41
42
         COMMON /EDSC7/ NMATO. LABMO(60), IDMATD(60)
43 C
44 C
         EDSMOD COMMON BLOCKS USED BY THE MODIFIED SESAME ROUTINES
45
         COMMON /EDSCCE/ TFACE, RFACE, PFACE, EFACE, KREPE
46
         COMMON /EDSCCO/ TFACD, RFACD, DFACD. KREPD
47 C
48
         NAMELIST /INP/ KUNIT, KREP, NLMAT, NBR, NFN, IIPT, IIRT, IDRT, IORE, LCMX
        1 ,NRS,DUM, KBR,DUM1.KFN,INIT,IRDIM.NTABLE,NTABLO,IFLP.LCNT,NMAT
49
50
        2 .NMCL,NMATO.TFACE,RFACE,EFACE,KREPE.TFACO.RFACO.OFACO.KREPO.RHO
51
        3 ,TEMP,PR,EN,IRC,IOT,IORT
52 C
53
         R(1)=RHO
54
         T(1)=TEMP
         P(1)=PR
55
56
         E(1)=EN
57 C
          58 C
59
         IF (IIPT_EQ.O) GD TO 10
         WRITE (6.70)
WRITE (3,70)
60
61
62
          IMATE=Q
```

```
63
           R(1)=R(2)=R(3)=0.0
           E(1)=E(2)=E(3)=0.0
64
           CALL EDSIPT (LMAT, P.T, R, E, KEOS, IMATE)
65
           WRITE (6,60) LMAT, KEOS, IMATE.(R(I),T(I),P(I),E(I).I=1,3) WRITE (3,60) LMAT, KEOS, IMATE,(R(I),T(I),P(I),E(I).I=1,3)
66
67
68
           IF (IWNL.NE.O) WRITE (3, INP)
69
           IF (IMATE.LE.O) IMATE=O
70 C
71
           R(1)=R(2)=R(3)=0.0
           E(1)=E(2)=E(3)=0.0
72
73
           CALL EDSIPT (LMAT.P.T.R.E.KEDS.IMATE)
74
           WRITE (6,60) LMAT.KEDS,IMATE.(R(I).T(I).P(I),E(I),I=1,3)
75
           WRITE (3,60) LMAT, KEDS, IMATE, (R(I), T(I), P(I), E(I), I=1,3)
           IF (IWNL.NE.O) WRITE (3.INP)
76
77
           IF (IMATE.LE_O) IMATE=O
        10 CONTINUE
78
79 C
80 C
           ******* EOSDRT TEST **********
81 C
82
           IF (IDRT.EQ.O) GD TD 20
          WRITE (6,80)
WRITE (3,80)
83
-84
85
           IMATE=O
           P(1)=P(2)=P(3)=0.0
86
87
           E(1)=E(2)=E(3)=0.0
           CALL EOSDRT (LMAT,R,T,P,E,KEDS,IMATE)
88
           WRITE (6,60) LMAT, KEOS, IMATE, (R(I), T(I), P(I), E(I), I=1,3)
89
90
           WRITE (3,60) LMAT, KEDS, IMATE. (R(I).T(I),P(I),E(I),I=1,3)
           IF (IWNL.NE.O) WRITE (3,INP)
IF (IMATE_LE.O) IMATE=O
91
92
93 C
94
           P(1)=P(2)=P(3)=0.0
95
           E(1)=E(2)=E(3)=0.0
96
           CALL EDSDRT (LMAT,R,T,P,E,KEDS,IMATE)
           WRITE (6,60) LMAT, KEDS, IMATE, (R(I),T(I),P(I),E(I),I=1.3)
97
98
           WRITE (3,60) LMAT, KEDS, IMATE, (R(I), T(I), P(I), E(I), I=1.3)
           IF (IWNL.NE_O) WRITE (3, INP)
99
100
           IF (IMATE.LE.O) IMATE=O
       20 CONTINUE
101
102 C
           103 C
104 C
105
           IF (IIRT.EQ.O) GO TO 30
           WRITE (6,90)
106
           WRITE (3,90)
107
108
           IMATE=0
109
           P(1)=P(2)=P(3)=0_0
110
           E(1)=E(2)=E(3)=O_{-}O
           CALL EDSIRT (LMAT.R.T.P.E.KEDS.IMATE)
WRITE (6,60) LMAT.KEDS.IMATE.(R(I).T(I).P(I).E(I).I=1.3)
111
112
           WRITE (3,60) LMAT, KEOS, IMATE. (R(I).T(I), P(I), E(I). I=1,3)
113
           IF (IWNL.NE.O) WRITE (3.INP)
IF (IMATE.LE.O) IMATE=O
114
115
116 C
117
           P(1)=P(2)=P(3)=0.0
118
           E(1)=E(2)=E(3)=0.0
           CALL EOSIRT (LMAT.R,T,P,E.KEOS,IMATE)
119
120
           WRITE (6.60) LMAT, KEOS. IMATE. (R(I), T(I).P(I).E(I).I=1,3)
           WRITE (3,60) LMAT, KEOS, IMATE, (R(I).T(I).P(I).E(I).I=1,3)
121
122
           IF (IWNL_NE_O) WRITE (3,INP)
123
           IF (IMATE_LE_O) IMATE=O
        30 CONTINUE
124
```

```
125 C
126 C
           ********** EOSORE TEST ***********
127 C
128
           IF (IDRE_EQ.O) GD TD 40
           WRITE (6,110)
WRITE (3,110)
129
130
           IMATE=0
131
           P(1)=P(2)=P(3)=0.0
132
133
           T(1)=T(2)=T(3)=0.0
           CALL EDSORE (LMAT.R.E.P.T.KEDS.IMATE)
134
           WRITE (6,60) LMAT, KEDS, IMATE. (R(I), T(I).P(I), E(I).I=1.3)
135
           WRITE (3.60) LMAT, KEOS. IMATE. (R(I), T(I), P(I), E(I), I=1,3)
136
           IF (IWNL_NE.O) WRITE (3, INP)
137
           IF (IMATE.LE.O) IMATE=O
138
139 C
140
           P(1)=P(2)=P(3)=0.0
141
           T(1)=T(2)=T(3)=0.0
142
           CALL EDSORE (LMAT.R,E,P,T,KEDS.IMATE)
           WRITE (6,60) LMAT, KEOS. IMATE, (R(I), T(I).P(I), E(I).I=1,3) WRITE (3,60) LMAT, KEOS, IMATE, (R(I).T(I).P(I).E(I).I=1,3)
143
144
145
           IF (IWNL.NE.O) WRITE (3, INP.)
           IF (IMATE.LE.O) IMATE=O
146
147
        40 CONTINUE
148 C
149 C
           150 C
151
           IF (IDRT_EQ_O) GO TO 50
152
           KOPC=KEOS
           WRITE (6,100)
WRITE (3,100)
153
154
155
           TMATD=0
156
           DPACITY=0.0
           CALL EDSORT (LMATO.R,T.OPACITY,KOPC,IMATO)
157
           WRITE (6,60) LMAT, KOPC, IMATO.R(1).T(1), DPACITY WRITE (3.60) LMAT, KOPC, IMATO,R(1),T(1).OPACITY
158
159
           IF (IWNL.NE.O) WRITE (3.INP)
160
            IF (IMATO.LE.O) IMATO=O
161
162 C
163
           DPACITY=0.0
           CALL EDSORT (LMATD, R, T, DPACITY, KDPC, IMATD)
164
            WRITE (6,60) LMATD KOPC, IMATO, R(1).T(1), DPACITY
165
166
            WRITE (3.60) LMATO, KOPC. IMATO, R(1).T(1).OPACITY
           IF (IWNL.NE.D) WRITE (3.INP)
IF (IMATO.LE.O) IMATO=O
167
168
        50 CONTINUE
169
170 C
171
           RETURN
172 C
        60 FDRMAT (1X,A10.14,13,12(1PE9.2))
173
        70 FORMAT (" EDSIPT")
80 FORMAT (" EDSORT")
174
175
176
        90 FORMAT (" EDSIRT")
       100 FORMAT (" EDSORT")
177
       110 FORMAT (" EDSDRE")
178
            END
179
```

OUTPUT

110

	EOS	IM	TE	R			T				P			(Ē											
EOSIPT HELIUM)E -U		5.0	ne .	Ω4	• .	92E+	٥.	3.	10	•02	,	n.	0.		0.	0.	0.	0.		0.	0.
HELTUM											92E •							ŏ.		o.	0.	0.	Ö.		O.	O.
EOSOAT																					_					
HELIUM											9 (F+							0.			-1.62E+02		o.			1.13E-02
HELJUM		0 1	11	1.59	9E - C)	5.0	OE+	04	1.	9 1E +	01	Э.	Ю	+02	3 (D.	0.		1.15E+02	- 1 . 62E + O2	0.	0.		4.7JE-04	1.13€-02
EOSIRT HELJUM					¥ - 6		* ^	ne.	^4		92E+	۸,	3	10	••	, (n.	0.		0.	0.	0.	0.		0.	0.
HELIUM											92E •							Ö.		o.	o.	ō.	o.		o.	0.
EOSORE		_																								_
HELIUM											92E+									1.23E+02		0.			3.82E-02	
HELIUM		0 1	1	1.59	Æ ∙ C)1 !	5.0	OE +	04	1.1	92E+	01	Э.	10	+02	3 (o.	1,43E+0	34	1.23E+02	0.	ο.		10F +O1	3.82E-02	0.
EOSORT HELIUM)E - 0		. .	~	^4		27E+	^7														
HELIUM											27E+															
EOSIPT		_	_						_													_				_
5760											92E+									1.23E+02		0.			3.82E-02	- •
5760		0 1	1	1 . 51)E - Q)1 !	5.0	OE+	04	1.	93E+	01	Э.	101	E+02	3 (D.	1,43E+0	04	1.23E+02	0.	Ο.		PF +01	3.82E-02	0.
EDSORT)			~	~4		91E+	^•	2	•	•		n	1 435 44	04	1.15F+02	- 1.62E+02	0.	8.8	16E+01	4.73E-04	1.13E-02
5760 5760											91E+										-1.62E+02				4.73E-04	
EOSIRT		•	•		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	•			•	•••	- ••	••		•		•	•		•							
5760											92E+							1.43E+0			0.	o.		10+33		0.
5760		0 1	11	1 , 51	Æ -0	1	5.0	OE+	04	1.1	92E+	01	Э.	10	+02	5 (D.	1.43E+0	04	0.	0.	Ο.	8.1	I6E+01	0.	0.
EOSDRE												•	•	•			^	4 4254	24	1,23E+02	^	0.	8.5	18F+01	3.82E-07	٥.
5760 5760											92E+ 92E+									1,23E+02		ŏ.			3.82E-02	
EDSORT		0	•	1,9	- U	,,,,	9. U	OE V	•	•••	74 L •	ν.	J.			•	٠.		-		•	••			•	
5760		0 1	10	1.5	9€ -C	1	5.0	ΘE+	04	1.	27E+	07														
15760		0 1	10	1.51	Œ-C	1	6.0	OE+	04	1.	27E+	07														
EOSIPT			. .																							
THE UNITS													1 "			LE										
THE PREVI													٠,	_												
5760		Ö									92E+		ο.			(ο.	1,43E+	04	1.23E+02	0.	Ο.	4.6	10+38E	3.82E-02	0.
THE UNITS																LE										
THE CURRE													١_	_												
THE PREVI					F KU						92E+		٧,				0.	1.43E+	04	1.23E+02	0.	0.	8.5	36E+O1	3.82E-02	0.
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