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THREETRAN (hex, z) Users' Manual

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by

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ABSTRACT

THREETRAN (hex,z) is a three-dimensional, multigroup, discrete-ordinates neutral particle transport code for use in solving problems in hexagonal,z geometries. An efficient and flexible data management strategy is incorporated and uses three hierarchies of storage: fast core (or small core memory), extended core (or large core memory), and random access disk. Both isotropic (P_0) and linearly anisotropic (P_1) scattering can be treated. This manual is intended to be a guide for the users of THREETRAN (hex,z) in setting up problem input and in interpreting the output. It is not intended to provide a description of code theory or architecture.

I. INTRODUCTION

The THREETRAN (hex,z) computer program was developed at Los Alamos Scientific Laboratory (LASL) in direct response to a request from Hanford Engineering Development Laboratory (HEDL). The program solves the time-independent, three-dimensional, discrete-ordinates approximation to the multigroup neutral particle transport equation in hexagonal, z geometries. Both istropic (P_0) and linearly anisotropic (P_1)scattering processes can be treated.

Although the THREETRAN (hex,z) code followed the development of the THREETRAN code by Lathrop[1] there are significant differences between the two, and the bulk of the THREETRAN (hex,z) development was devoted to these differences. First of all the solution of the transport equation in hexagonal, z geometries

necessitated a research effort in spatial discretization not required in the earlier THREETRAN code which used the customary x,y,z rectangular parallelpiped spatial mesh. To accommodate the hexagons in hexagonal, z geometries a spatial discretization scheme using a uniform mesh of equilateral triangles in the hexagonal, or (x,y), plane was developed and coupled to the z-dimension mesh. The details of this discretization method are not presented in this manual but can be found in Reference 2.

An additional development effort was required to permit the treatment of P_1 scattering (the original THREETRAN was restricted to isotropic scatter). In order to minimize the storage requirements when linearly anisotropic scattering is present, the anisotropic within-group scattering contribution to the source-to-group term is placed in the outer iteration source calculation and appears as a fixed contribution to the source during the inner iterations. This procedure is unique to THREETRAN (hex,z) since other discrete-ordinates codes iterate on the anisotropic within-group scatter term in the inner-iteration process.

The multilevel data management techniques pioneered by Lathrop in THREETRAN were generally followed in THREETRAN (hex,z) but were altered to fully satisfy the standardized procedures as established by the Committee on Computer Code Coordination as set forth in Reference 3.

As a result of the effort involved with the basic development of THREETRAN (hex,z) together with the relatively short time available, the program is by no means a polished, production-type code. As in Lathrop's original code, THREETRAN (hex,z) has only the most rudimentary of convergence acceleration schemes. The code represents only a prototype version - one which provides, simply, a raw capability to perform calculations. Accordingly, this manual is limited to the role of a user's manual only and is not intended to provide the theory and programming details that can be expected with more completely developed production codes. The information provided in this manual includes a brief summary of program options, a section on the data management techniques used in the code, a detailed user's guide to the input required by the code, and a section describing the output provided by the code including error diagnosties. Appendices containing the code output for the sample problem, and the discrete-ordinate quadrature sets used in THREETRAN (hex,z) are provided.

II. PROGRAM OPTIONS

A. Types of Problems

Only three types of problems can be solved by THREETRAN (hex,z), (i) isotropic inhomogeneous source problems without fission, (ii) isotropic inhomogeneous source problems with fission, and (iii) k_{eff} problems. Upscattering is not treated.

B. Geometry

The spatial solution-domain is partitioned into an equilateral triangular mesh lying in the x,y plane. The z-dimension is partitioned into KM coarse-mesh intervals with each coarse-mesh interval containing equally spaced fine-mesh intervals. The code will function as a two-dimensional triangular mesh code if there is only a single z-dimension coarse-mesh interval containing a single fine-mesh interval and if reflective boundary conditions are imposed on both z-boundaries.

C. Flux and Source Inputs

No flux input is required by the code but options are available to provide flux input from RTFLUX standard interface files; either in Version III format[4] or Version IV format[3]. If no flux input is specified, the code begins with a zero flux guess for all three problem types. For k_{eff} calculations with no flux input a spatially constant, normalized fission source in those regions supporting fission is used to begin the problem.

For inhomogeneous source problems the space-energy isotropic inhomogeneous source distribution can be input by use of the standard interface file FIXSRC, Version III format[4] or FIXSRC, Version IV[3]; or it can be directly input by the user. In the latter case the source is created as the product of three shapes; one for energy, one for the triangular mesh x,y plane, and one for the z spatial direction.

D. Cross Sections

Only macroscopic cross sections in Los Alamos format[5] are allowed as input. Both P_0 (isotropic) and P_1 (linearly anisotropic) scattering are permitted.

E. Dumps and Restarts

THREETRAN (hex,z) takes periodic, time limit and final dumps, and problem

restarts can be made from any of these dumps. Periodic and time limit dumps are intermediate dumps, i.e., dumps before problem convergence. Periodic dumps are taken every 20 minutes.

F. Edits and Output

No edits are performed by THREETRAN (hex,z). Optional output from the code are scalar fluxes (for selected planes if printed output is desired; all fluxes if microfiche output is requested), pointwise fission source rate densities (printed output only), and pointwise power densities (printed output only). Scalar fluxes are always output as an RTFLUX, Version IV standard interface file.

III. DATA MANAGEMENT

THREETRAN (hex,z) is designed with rather sophisticated data management techniques in order to accommodate, as efficiently as possible, the transfer of the large amounts of data inherent in a three-dimensional discrete-ordinates code. The data management in the code involves the reading and writing of sequential data files, an extremely flexible capability to block data, and extensive use of multilevel data management/transfer using random access file handling. In all cases the data management in THREETRAN (hex,z) is consistent with the standardized procedures set forth in Reference 3.

A. Sequential Data Files in THREETRAN (hex,z)

There are two types of sequential files used in THREETRAN (hex,z) for the transfer of data between peripheral storage devices and central memory, or fast core. The first type of sequential file is the Binary Coded Decimal (BCD) file and the second type is the binary (BIN) sequential data file.

The BCD files used by the code include the normal INPUT file and the three forms of output files. Each of these files is read/written with formatted FORTRAN READ/WRITE statements and each is identified by the file reference (integer) number. The INPUT file is file number 2 and is internally given the file name NINP. Normal, printed output is provided by the OUTPUT file, file number 3, with internal file name NOUT. On-line, terminal output (for time-sharing systems) is provided by the TERMINAL OUTPUT file, file number 59, with internal

file name NTTY. The assignment of the integer values NINP=2, NOUT=3 and NTTY=59 is made by the code in Subroutine UGONOW. An additional output file for output of FINAL SCALAR FLUXES TO MICROFICHE has a file number of 14 and the internal name NFICHE. The assignment NFICHE=14 is made by the code in Subroutine ASSINE.

A summary of these BCD files, numbers and names is provided in Table I.

The BIN sequential data files used in THREETRAN (hex,z) are limited to standard interface files RTFLUX and FIXSRC, to dumps, and to a single scratch file. All transfers of the binary file data between fast core and peripheral storage are managed and effected by the standardized subroutines SEEK, REED and RITE[3,4].

A binary RTFLUX file of either Version III[4] or Version IV[4] format is optionally allowed for supplying an input scalar flux guess to the code. Upon convergence of a problem a binary RTFLUX, Version IV standard file is always written.

A binary FIXSRC standard file of either Version III[4] or Version IV[3] is optionally allowed for supplying, at input, the inhomogeneous source distribution.

TABLE I

SEQUENTIAL FILE REFERENCE IDENTIFICATION

File	Use	File Reference Identifier	
		LASL Version	Export Version
NINP	CARD Image (BCD)	INPUT	2
NOUT	Printed Output (BCD)	OUTPUT	3
NTTY	User's Terminal Output (BCD)	"terminal"	59
NFICHE	Scalar Flux Microfiche Output (BCD)	TAPE14	14
RTFLUX	Scalar Flux Input (BIN)	RTFLUX	20
RTFLUX	Scalar Flux Output (BIN)	RTFLUX	21
FIXSRC	Inhomogeneous Source Input (BIN)	FIXSRC	22
DMPONE	Restart Dump File Input (BIN)	DMPONE	23
DMPONE	Dump File Output (BIN)	DMPONE	23
DMPTWO	Dump file Output (BIN)	DMPTWO	24
EDITIT	Scratch File (BIN)	EDITIT	25

Periodic, time limit, and final dumps are written sequentially to the binary dump files named DMPONE and DMPTWO alternately. For restart from a dump, the restart is made by reading a file named DMPONE. Section IV.C.1 of this manual describes these dumps and their usage more fully.

A binary sequential scratch file named EDITIT is also created and used to store the planes-for-which-final-scalar-fluxes-are-to-be-printed data (KPRN input array; see Sec. IV.B.). Since the file is a scratch file it only exists during the running of a problem and need not be saved following completion of the problem.

Table I shows the file reference identifications for the various binary sequential files used in THREETRAN (hex,z). With the Los Alamos Scientific Laboratory (LASL) version of the code, the binary sequential files are identified by a file reference name while in the export version the files are identified by a file reference number, as indicated.

B. Multilevel Data Management and Data Blocking

The main data management scheme in THREETRAN (hex,z) uses the multilevel data management and random access file procedures set forth in Reference 3. Three levels of storage are used in the code: fast core or small core memory (SCM), extended core or large core memory (LCM), and random access disk. In the following sections are given a summary of terminology together with a general method overview, a description of fast core (or SCM) data transfers and blocking, and details of extended core (or LCM) and random disk data transfers and blocking.

1. Mutilevel Data Management Terminology and Overview.

To assist the user, the following terminology used in describing the multilevel data management scheme is extracted from Reference 3.

Extended Core:	That portion of a computing system containing storage locations which serve as buffer for random access data. Extended core may be physically separate from central memory as a peripheral large core memory (LCM) on two-hierarchy

memory computers or it may be a portion of central memory which has been designated as extended core on single-hierarchy memory computers.

Fast Core: That portion of a computing system which contains storage for both data and instructions, which is directly coupled to the computations portion of the system, and which is directly coupled to extended core. Fast core may be the entire central memory, i.e., small core memory (SCM) on two-hierarchy memory machines, or it may be that portion of central memory remaining after an extended core portion is designated on single-hierarchy memory machines.

Random Access Data: Data which can be transferred between fast core and extended core in out-of-sequence strings.

Random Access File: (Also called Direct Access File). A named collection of data which is stored on a peripheral storage device. The file data are arranged

	in blocks which can be transferred between extended core and peripheral storage randomly, i.e., out of sequence.
Logical File:	A random access file. The identity of a logical file in a code is established by an integer variable, the (logical) file reference number.
Block:	A subportion of a random access file. The block size is determined by the amount of extended core storage that can be allocated to the random access file. Data transfers between the peripheral device and extended core are block transfers.
String:	A subportion of a random access file block. Data transfers between fast core and extended core are string transfers.
Disk:	A generic name for peripheral storage device used for storing random access files.
Physical Unit:	An identifiable subpart of a disk. One or more physical units comprise a disk.

The standardized method of multilevel data management used in THREETRAN (hex,z) is shown in Fig. 1. Each random access file is composed of blocks and resides on disk, or more correctly, on a physical unit. When needed, the blocks of data are transferred between extended core and the physical unit and strings of data are transferred between extended core and fast core.

2. Fast Core Data Blocking and Data Transfers. The solution-mesh used in THREETRAN (hex,z) is characterized in the x,y plane by JT bands of triangles with each band containing IT equilateral triangles. Since the storage in fast core, or SCM, may be insufficient to accommodate the data for an entire x,y plane, the code automatically divides the range of JT into NJBLOC strings, each of which contains no more than JBLOC bands. Then, the dimension of arrays associated with bands of triangles and stored in fast core is limited to JBLOC bands-worth of data rather than JT bands-worth. Since JT may not be evenly divisible by NJBLOC, an array JINDEX (NJBLOC) is used to indicate the number of bands contained in

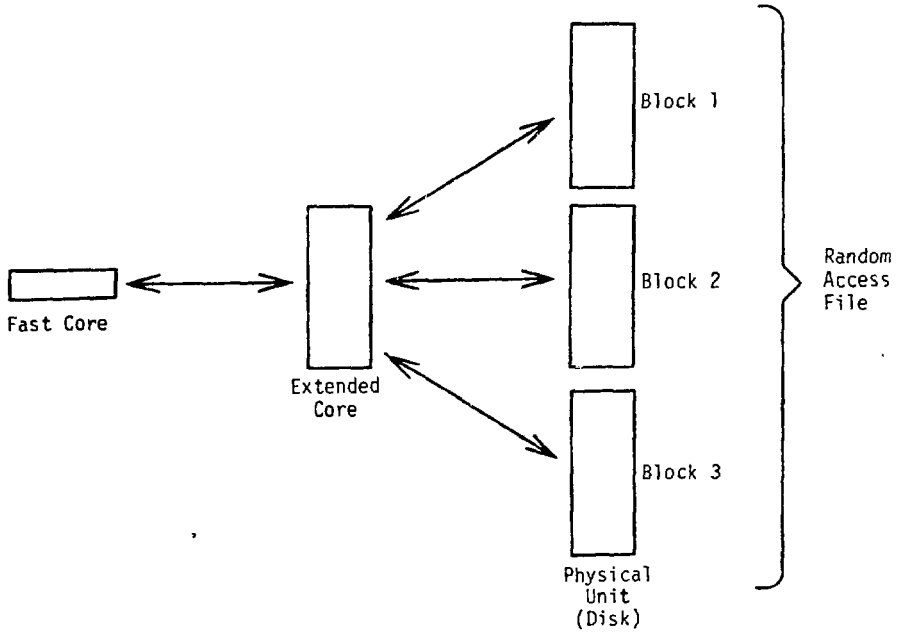


Fig. 1. Scheme for multilevel, random access data transfers.

each string. The first NJBLOC-1 of these strings contain JBLOC bands and the last string contains no more then JBLOC bands. For example, suppose JT = 50 and JBLOC = 17. Then NJBLOC = 3 and the JINDEX array consists of the 3 entries 17, 17, and 16. The FORTRAN programming to sweep all bands in a plane, then, is simply

```
      DO 200 J1 = 1, NJBLOC
      JMAX = JINDEX (J1)
      DO 100 J2 = 1, JMAX
         .
         .
         .
  100 CONTINUE
  200 CONTINUE
```

It is to be noted that the maximum fast core storage is obtained when JBLOC = JT, i.e., NJBLOC = 1. No more than a single plane's worth of data is stored in fast core at any time. If JBLOC is less then JT, i.e., if NJBLOC > 1, the excess data for other strings in the plane resides in extended core. Except for the few sequential file operations described in Section III.A., all data transfers to and from fast core memory are string transfers between fast core and extended core.

The minimum fast core storage occurs when JBLOC = 1, i.e., when each string contains data for only one band of triangles. The code will not execute if the data for one band will not fit into fast core memory.

3. Extended Core Data Blocking and Data Transfers to/from Random Disk. The total solution-mesh used in THREETRAN (hex,z) is characterized by KT planes for each of the IGM number of energy groups. It is desirable to store all of the data for the total solution-mesh in extended core, since fast core-extended core data string transfers are extremely fast. However, because, the storage in extended core may be insufficient to accommodate the data for the entire problem, the code automatically provides the capability to divide both the range of KT and of IGM into blocks small enough to fit into available storage. The blocking of KT and/or IGM is accomplished in a manner analogous to the manner in which JT is divided for fast core storage. IGM can be blocked into NGBLOC group-blocks each

of which contains no more than IGBLOC groups. Similarly KT can be divided into NKBLOC plane-blocks each of which contains no more than KBLOC planes for a single group. Since neither IGM nor KT may be evenly divisible by NGBLOC or NKBLOC, respectively, the arrays IGNDEX (NGBLOC) and KINDEX (NKBLOC) are used to indicate the number of groups and planes contained in each block.

TABLE II

EXTENDED CORE/RANDOM DISK STORAGE MODES

Value of Mode Indicator, NREAD	Description of Storage Mode
0	All problem data contained in extended core. No random disk files used.
1	Data for all planes for at least one, but not all, groups contained in extended core. Groups are blocked and random disk used for group-dependent data.
2	Data for all planes for single group cannot be contained in extended core. Planes are blocked in addition to full group blocking with random disk used to store both group-independent and group-dependent data.

The FORTRAN programming instructions, then, to sweep through all planes for all groups is simply of the form:

```
      DO 400 IG1 = 1, NGBLOC
      IGMAX = IGNDEX (IG1)
      DO 300 IG2 = 1, IGMAX
      DO 200 K1 = 1, NKBLOC
      KMAX = KINDEX (K1)
      DO 100 K2 = 1, KMAX
       .
       .
       .
  100 CONTINUE
  200 CONTINUE
  300 CONTINUE
  400 CONTINUE .
```

With respect to the availability of extended core storage relative to the need for blocking the data for a given problem, there are three possible storage modes characterized by the parameters NREAD as shown in Table II. The appropriate value of NREAD is determined by the code and is printed as part of the output.

In the first, and simplest, storage mode the mode indicator NREAD equals zero. In this case the data for all planes and all groups can be contained in extended core and no random disk storage is required. Thus, for NREAD = 0:

```
NGBLOC = 1
IGBLOC = IGM
NKBLOC = 1
KBLOC  = KT
```

The second storage mode, indicated by NREAD = 1, occurs when extended core cannot accommodate the storage required for all planes and groups but can accommodate the storage for all planes for at least one (but not all) group. In this case

$$2 \leq \text{NGBLOC} \leq \text{IGM}$$

$$\text{IGM} > \text{IGBLOC} \geq 1$$

and the planes are not blocked, i.e.,

$$NKBLOC = 1$$
$$KBLOC = KT.$$

Note that, for NREAD = 1, maximum extended core storage requirements occur when NGBLOC = 2 while the minimum extended core storage requirements occur when IGBLOC = 1 (NGBLOC = IGM).

Under the NREAD = 1 mode the angular hemishpere fluxes (and the directional currents, if anisotropic scattering is treated) are written to a random access file which is blocked as described above. The random file is designated NPHI and block transfers of data are made between extended core and NPHI. In addition to the random flux file NPHI, if the problem contains inhomogeneous sources, these sources are written to a random access file designated NQ and blocked in the same manner as the fluxes. The random files NPHI and NQ (if required) are the only random access files used under NREAD = 1.

The third and final storage mode, NREAD = 2, occurs when the data for all planes for a single group will not fit into extended core. In this case the planes must be blocked such that data for at least one but not all planes for a single group can fit into extended core. Thus, for NREAD = 2

$$NGBLOC = IGM$$
$$IGBLOC = 1$$
$$2 \leq NKBLOC \leq KT$$
$$KT > KBLOC \geq 1 .$$

For NREAD = 2, maximum extended core storage occurs when NKBLOC = 2 while minimum extended core storage occurs when NKBLOC = KT (KBLOC =1). The latter case, in fact, represents the extended core storage limit for problem execution, i.e., if the data required for one plane for one group will not fit into extended core the problem can not be executed in THREETRAN (hex,z).

Under NREAD = 2 a total of five random access files may be used. The source-to-group data is stored on the random file NSOUR; the fluxes (and currents, if P_1 scatter is present) are stored on random file NPHI; if fission exists in the problem, two fission source random files, NF and NFN, are required; if the problem contains inhomogeneous sources they are stored on random access file NQ.

A summary of the random access files required is given in Table III.

TABLE III

RANDOM ACCESS FILE USAGE AND FILE NUMBERS

File Name	Logical File Reference Number	Use	NREAD modes for which required
NSOUR	1	Source-to-group data	2
NQ	2	Inhomogeneous source (if req'd)	1,2
NF	3	Fission source (if req'd)	2
NFN	4	New fission source (if req'd)	2
NPHI	5	Fluxes (and currents, if req'd)	1,2

IV. DESCRIPTION OF PROBLEM INPUT

A. Input Formats

The input single-word control parameters and macroscopic cross section data are read into THREETRAN (hex,z) as fixed format card-images as described in Sec. IV.B. All other input data blocks, consisting of one or more data strings, are read into the code in special LASL card-image formats. These special formats are (6(I1,I2,I9)) for integer data and (6(I1,I2,E9)) for floating point data. Each of the six card-image input entries consists of three fields. The first integer field, I1, is the option field and designates the option described in Table IV below. The second integer field, I2, of each input entry is the execution field and controls the execution of the option. The third field, I9 or E9, is the numeric field and contains the input data word, or for certain options, other information as described in Table IV. With the above special formats, data are input and loaded as a continuous string until terminated with the terminator, 3, in the I1 option field following the last numeric field entry in the string.

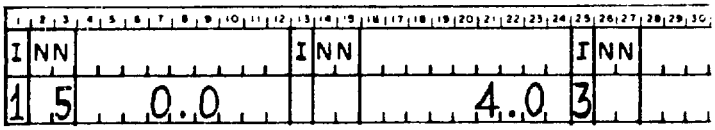
TABLE IV

DESCRIPTION OF OPTIONS FOR SPECIAL LASL FORMATS

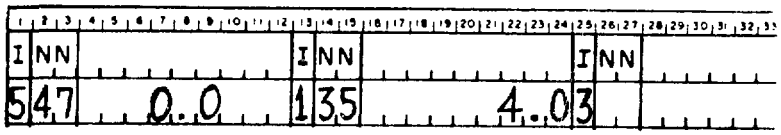
Value of Integer in I1 Field	Value of Integer in I2 Field	Numeric Field Entry	Remarks
0 or blank	Ignored	X	Loads X into current data string.
1	NN	X	Multiple Entry Option 1: Enters the value X NN successive times in the current data string.
2	NN	X	Interpolate Option: Enters the value X into the data string followed by NN Interpolant values. The NN interpolant values are equally spaced between X and the next numeric field entry. Allowed for both integer and floating point data.
3	Ignored	Ignored	Terminate Option: Terminates the data string. All data strings input with special format must be terminated with a 3 in the option field following the last numeric field entry.
4	Ignored	X	String Fill Option: Fills the remainder of string with the value X. (This option must be followed by a Termination Option, 3.).
5	NN	X	Multiple Entry Option 2: Enters the value X into the data string 10·NN times.
6	NN	NX	Set Repeat Option: Repeats the preceding set of NX data entries NN times in the data string. NX is a right-adjusted integer.
7	NN	Ignored	String Repeat Option: The next NN data strings in this data block are made identical to the previously defined data string. A 3 terminator must follow in the next option field. ONLY CERTAIN DATA BLOCKS IN THE CODE PERMIT THIS OPTION.
8	-	-	Not used
9	Ignored	Ignored	Skip Option: Skip to the next card-image and continue.

Several examples of the use of the LASL special formats are given below.

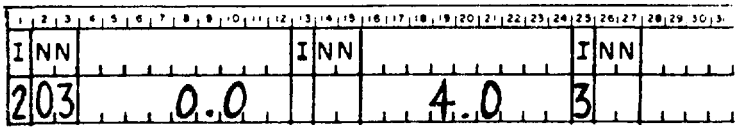
Example 1: Produce a data string consisting of five entries of 0.0 followed by an entry of 4.0.



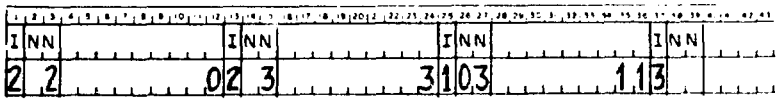
Example 2: Produce a data string consisting of 470 entries of 0.0 followed by 35 entries of 4.0.



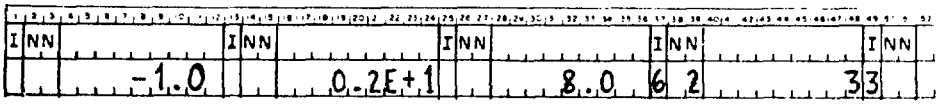
Example 3: Produce the data string 0.0 1.0 2.0 3.0 4.0. (use interpolate option).



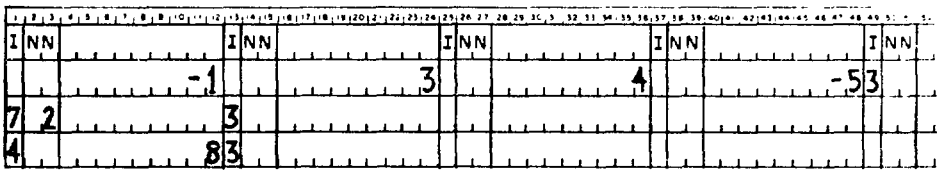
Example 4: Produce the data string 0 1 2 3 5 7 9 11 11 11. (Place two interpolants between 0 and 3, three interpolants between 3 and 11, enter 11 three times and terminate the string).



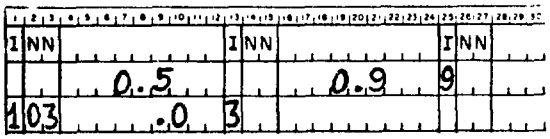
Example 5: Produce the data string -1.0 2.0 8.0 -1.0 2.0 8.0 -1.0 2.0 8.0. (Use the Set Repeat Option).



Example 6: Produce a data block containing four data strings. The first three strings are identical, containing the values -1 3 4 -5. The fourth data string consists entirely of the value 8. (Assume the String Fill Option is allowed for this data block; additionally, use the String Fill option.)



Example 7: Produce a data string containing entries 0.5 0.9 and three successive values of 0.0. (Use the Skip Option).



B. Description of Input Data

On the following pages are listed the problem data required for input to THREETRAN (hex,z). The card-image formats for the input are given. The special LASL formats described in the preceding section are denoted S(I) for integer data blocks and S(E) for floating point data blocks. Descriptive comments are included to assist the user.

Card-Image Entry Number	Name of Variable	Comments
TITLE CARD CONTROL .....(2I12)		
1	ITCARD	Number of Title Cards to follow (may be zero).
2	MAXLRD	LCM adjustment control. -1/0/N = No effect/ Adjust to code value/Adjust to N (USED AT LASL ONLY!)
TITLE CARDS .....(18A4)		
All	TITLE(18)	ITCARD cards containing title, descriptive comments, etc.
CARD 1 CONTROL INTEGERS .....(6I12)		
1	IEVT	Problem type. 0/1/2 Inhomogeneous source without fission/K-effective/Inhomogeneous source with fission.
2	ISTART	Problem starting option. 0/1/2 New problem/ restart from periodic dump or time limit dump/ restart from final dump.
3	ISN	S_N order (Limited to 2,4,6 or 8). Total number of directions ISN*(ISN+2). See Appendix C.
4	IT	Number of triangles per band in x-y plane.
5	JT	Number of bands of triangles in x-y plane.
6	KN	Number of z-direction coarse mesh zones.
CARD 2 CONTROL INTEGERS .....(6I12)		
1	IGEO	Problem x-y plane shape. 0/1 = parallelogram/ sawtooth rectangle.

Card-Image Entry Number	Name of Variable	Comments
2	IQT	Problem termination option. 0/1/2 (See Section IV.C.)
3	IBB	Bottom y-dimension boundary condition. 0/1/2 = vacuum/reflecting/180° rotational.
4	IBT	Top y-dimension boundary condition. 0 = vacuum only.
5	IBA	Back z-dimension boundary conditon. 0/1 = vacuum/reflecting.
6	IBF	Front z-dimension boundary condition. 0/1 = vacuum/reflecting.

CARD 3 CONTROL INTEGERS.....(6I12)

1	IGM	Number of energy groups.
2	ISCT	Legendre order of scatter. 0/1 = P_0/P_1.
3	MT	Total number of materials, i.e., macroscopic cross section sets.
4	IHT	Row, or position, of the total cross section in the cross section table.
5	IHM	Last row, i.e., length, of cross section table for each group.
6	LIMIT	Maximum number of inner iterations allowed per group during initial stages of solution.

Card-Image Entry Number	Name of Variable	Comments
CARDS 4 CONTROL INTEGERS.....(6I12)		
1	IFIX	Negative flux fixup option. 0/1 = no/yes
2	IBAL	Inner iteration rebalance acceleration option. 0/1 = yes/no.
3	IQOPT	Inhomogeneous source input option. 0/1/2/3 = none/ card input/FIXSRC-III/FIXSRC-IV. (If IEVT = 0 or 2, IQOPT must be 1, 2, or 3.)
4	IFOPT	Scalar flux input option. 0/1/2 = none/RTFLUX-III/ RTFLUX-IV. (If IEVT = 0 only IFOPT = 0 is allowed).
5	IOUT	Form of scalar flux output. 0/1 = printed listing/microfiche.
6	KPRINT	Final scalar flux print option (used only if IOUT = 0). -1/0/N = print all planes/none/ print N planes for all groups.
CARD 5 CONTROL INTEGERS.....(4I12)		
1	KFSR	Final fission source rate print option (printed listing output). 0/1 = no/yes.
2	ISTOP	Problem execution option. 0/1/2 = execute problem/process all input and stop/ determine storage option requirements only.
3	NPRT	Printed output detail option. 0/1 = mini/maxi. With mini print all input except coarse mesh-cross section identification numbers and cross

Card-Image Entry Number	Name of Variable	Comments
		sections is printed together with problem storage information and iteration monitor print. With maxi print macroscopic cross sections and a picture-map of the problem are added to the mini print output.
4	KPWD	Final power density print option (printed listing output). 0/1 = no/yes.

CARD 6 CONTROL FLOATING-POINT NUMBERS.....(6E12.4)

1	EPS	Overall convergence precision used on inner and outer iterations.
2	NORM	Normalization amplitude. -NORM/0/NORM = normalize to a system power level of NORM Megawatts (IEVT = 1 only)/no normalization/normalize to a total system neutron source rate of NORM neuts/sec. (For NORM > 0 and IEVT = 1 volume integral of fission source rate is made equal to NORM. For NORM > 0 and IEVT = 0 or 2, volume integral of inhomogeneous source is made equal to NORM.)
3	DTIME	Problem time limit (seconds) for this job submittal. After DTIME seconds a restart dump is taken and execution is halted.
4	XBASE	Overall problem x-length in cm. The side of the triangular mesh is 2.0*XBASE/IT for IGEO = 0 and 2.0*XBASE/(IT-1) for IGEO = 1.
5	EPF	Energy release per fission (MeV). Default = 215.0.

REMAINING DATA IN ORDER OF INPUT

Data Block Name	Format	Number of Data Strings in Block	Number of Entries per String	Comments
KZ	S(I)	1	KM	Number of equally-spaced fine-mesh intervals per z-dimension coarse zone.
KPRN	S(I)	1	KPRINT	Numbers of planes for which the final scalar fluxes by triangle and group are to be printed. ENTER ONLY IF KPRINT>0.
NDSCAT	S(I)	1	IGM*IGM	Matrix indicating whether or not downscatter is possible from one group to another. Used to avoid calculation of scattering source when no scattering is possible. Entered as ((NDSCAT(I,J), I=1, IGM), J=1, IGM). Element NDSCAT (I,J) indicates whether (entry = 1) or not (entry = 0) scatter is possible from group I to group J. Self-scatter is a 1 entry. Thus, for a two-group problem the NDSCAT array entries would be 1, 0, 1, 1.
CHI	S(E)	1	IGM	Fission spectrum.
IDCS	S(I)*	KM*JT	IT	Integers indicating which material (cross section) is assigned to each triangle in each z-dimension coarse zone. Entered as KM sets with each set entered one band at a time, i.e., each of the

Data Block Name	Format	Number of Data Strings in Block	Number of Entries per String	Comments
				KM sets consists of JT data strings each of which contains IT entries. *This data block allows the use of the String Repeat Option, i.e., 7 Option in the special LASL format.
C	6E12.0	MT	IHM*IGM	Macroscopic, material-ordered cross sections. Each cross section data string is preceded by a header title card in 184A format. The string of IHM*IGM cross sections is read as ((C(I,IG), I=1, IHM), IG=1,IGM). Materials are identified by the order in which they are entered and are given identification numbers ranging from 1 to MT. THIS BLOCK OF DATA IS NOT IN SPECIAL LASL FORMAT.
SG	S(E)	1	IGM	Inhomogeneous source energy spectrum. ENTER ONLY IF IEVT = 0 or 2 and IQOPT = 1.
SX	S(E)*	JT	IT	Inhomogeneous source spatial distribution in x,y plane. Enter JT data strings (one for each band of triangles) with each string having IT entries. ENTER ONLY IF IEVT = 0 or 2 AND

Data Block Name	Format	Data Strings in Block	Entries per String	Comments
				IQOPT = 1. *This data block allows the use of the String Repeat Option, i.e., 7 Option, in the special LASL format.
SZ	S(E)	1	KT	Inhomogeneous source spatial distribution in z-direction. NOTE: KT = number of fine mesh intervals in z-direction = $\sum_{k=1}^{KM} KZ(k)$. ENTER ONLY IF IEVT = 0 or 2 AND IQOPT = 1.

C. Details of Input

This section provides a more detailed description of some of the input parameters and data blocks required in THREETRAN (hex,z).

1. ISTART and Starting Problems from Dumps. The value ISTART = 0 is used for the initial run of a problem. Many problems are too large to be executed to completion in this initial run, however. Accordingly, THREETRAN (hex,z) takes frequent dumps and the code can be restarted from these dumps. Periodic dumps are taken by the code every 20 minutes of computation time. A time limit dump is taken after the problem has run DTIME seconds during the current job submittal, provided DTIME is input as a nonzero entry. The time limit dump is identical in form to a periodic dump and the term periodic dump generally is used to denote either type. These dumps are intermediate in nature in the sense that they are taken before the problem has converged. A final dump is taken after the iterative procedure has converged.

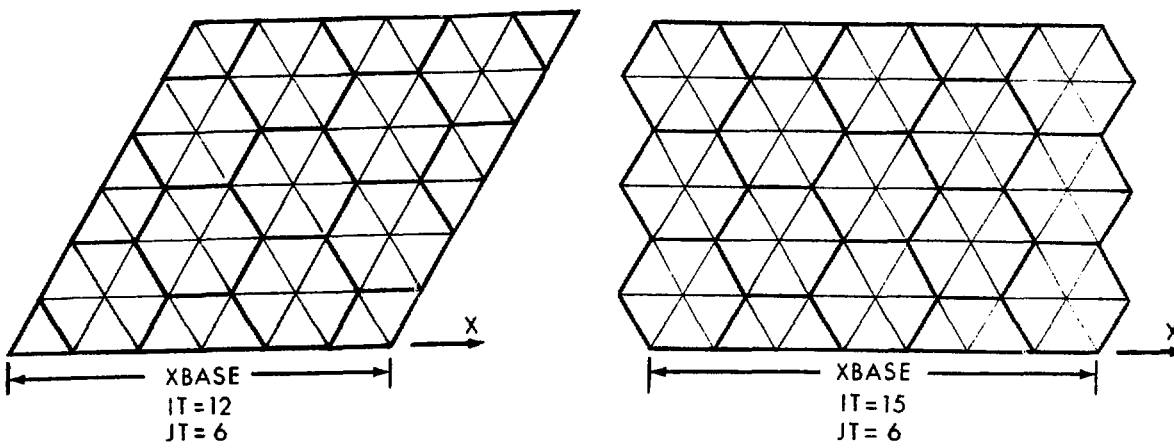
During a run dumps are alternated between files named DMPONE and DMPTWO In restarting the code from a dump, however, the restart dump file named DMPONE is always used. Thus, if the actual dump from which a restart is to be made was on DMPTWO, the LASL user must change the file name to DMPONE before restarting.

To restart a problem (with the appropriate dump on file DMPONE) the user need merely resubmit the original input deck (or file) with the ISTART parameter set to 1 (periodic or time limit dump) or to 2 (final dump). In actuality, if

ISTART > 0, the code will not read the entire input file but, instead, will read only the input through the KPRN data block (if the KPRN data block is required). Such a procedure enables the user to change certain parameters with any restart. These parameters are:

ISTART	KPRINT
IQT	KFSR
LIMIT	KPWD
IFIX	EPS
IBAL	DTIME
IOUT	EPF

2. IGEO. The geometric solution domain for each problem solved by THREE-TRAN (hex,z) must be capable of being represented with an equilateral triangular mesh in the x,y plane. All triangles in each plane must be the same size. Planes are successively stacked to create the three-dimensional domain. The x,y plane shape can take either of two forms. For IGEO = 0 the plane shape is a 60°-120° parallelogram with its base along the x-axis and with the bottom left-most mesh triangle upward pointing as shown in Figure 2a. There are JT bands (rows) of triangles in each plane with IT triangles per band.



a. IGEO = 0 b. IGEO = 1

Fig. 2. Domain-of-solution (x,y) shape options.

For IGEO = 1 the plane shape is a "sawtooth" rectangle. Each of the four corners of this rectangle must be formed by a complete hexagon with its top and bottom sides parallel to the x-axis as shown in Fig. 2b. Within the rectangular domain there are JT bands (rows) of triangles with IT triangles per band. To ensure that THREETRAN (hex,z) properly treats the reentrant surfaces formed by the "sawtooth" shape of the y-boundaries, the code internally inserts additional void, or dummy, triangular cells along the "sawtooth" surfaces for computational purposes. Three of these dummy triangular cells are required for each band (row) of triangles. These dummy cells are used for computational purposes only and neither appear in the input specifications nor in the output results from the code, i.e., these dummy cells are totally invisible to the user.

3. IQT: Iteration Termination option. The input value of IQT determines the manner in which the iterative procedure used to solve a problem will be terminated. For an eigenvalue, or K_{eff}, problem (IEVT = 1) there are three possibilities for termination (IQT = 0, 1, or 2); for an inhomogeneous source with fission problem (IEVT = 2) there are two termination options (IQT = 1 or 2); for a pure inhomogeneous source problem with no fissionable material present (IEVT = 0) the only termination option available is IQT = 2.

a. IQT = 0. This termination option is available only for K_{eff} calculations (IEVT = 1). Under this option the outer iterations are terminated when either two successive pairs of linearly extrapolated values of K_{eff} between outer iterations agree to within 0.1 * EPS or when the pointwise fission source error becomes less than the input value EPS. The pointwise fission source error is defined as the maximum pointwise fractional change in fission source rate from one outer iteration to the next.

The extrapolated values of K_{eff} are obtained by linearly extrapolating the K_{eff} versus ALA "graph" to a value of ALA = 1.0. The quantity ALA, lambda, is the outer iteration convergence criterion and is defined as

$$ALA = TF/TFP,$$

where TF is the energy-volume integral of the fission source rate for the just completed outer iteration and TFP is the value of TF from the previous outer iteration.

The extrapolated K_{eff} termination option frequently proves to be quite effective in predicting a reliable estimate of K_{eff} long before pointwise quantities are fully converged.

b. IQT = 1. This termination option is available only to problems containing fission (IEVT = 1 or 2). Under this option problem termination occurs when both the pointwise fission source error and the outer iteration criterion | 1.0-ALA | become less than EPS. The pointwise fission source error is defined in the IQT = 0 subsection and the outer iteration convergence criterion, ALA (lambda), is defined as

$$ALA = (TF + TQ)/(TFP + TQ)$$

where TQ is the energy-volume integral of the isotropic inhomogeneous source (if present). TF and TFP are the previously defined total fission sources from the current and preceding outer iterations.

Under this IQT option for K_{eff} calculations (IEVT = 1), extrapolated values of K_{eff} are computed and printed but are not used to terminate the problem.

c. IQT = 2. For all types of problems, when IQT = 2, iteration termination occurs when both the pointwise inner iteration error and the outer iteration criterion | 1.0 - ALA | become less than EPS. The pointwise inner iteration error is defined as the maximum (for each energy group) fractional difference in pointwise scalar fluxes from one inner iteration to the next. The outer iteration convergence criterion ALA is a within-code parameter described below.

If IEVT = 0 (inhomogeneous source without fission) the outer iteration convergence criterion ALA (or lambda) is

$$ALA = (TQ + TM)/(TQ + TMP)$$

where TQ is the volume-energy integral of the isotropic inhomogeneous source (constant); TM is the volume-energy integral of $| J_x | + | J_y | + | J_z |$ for the just completed outer iteration and TMP is the value of TM from the previous outer iteration. TM and TMP are only computed if the problem contains linearly anisotropic scatter, i.e., if ISCT = 1. The J_x, J_y, and J_z are the neutron currents (first angular moments) in the x-, y-, and z-directions, respectively. The use of TM and TMP in the definition of ALA for linearly anisotropic scatter inhomogenous source problems provides a degree of assurance that the anisotropic scatter source is converged at problem termination.

If IEVT = 1 or 2 the outer iteration convergence criterion ALA is defined as described under the IQT = 1 option. In addition to the general requirements that both pointwise inner iteration errors and | 1.0 -ALA | be less the EPS, IQT = 2 requires that the pointwise fission source error be converged as described in the IQT = 0 subsection.

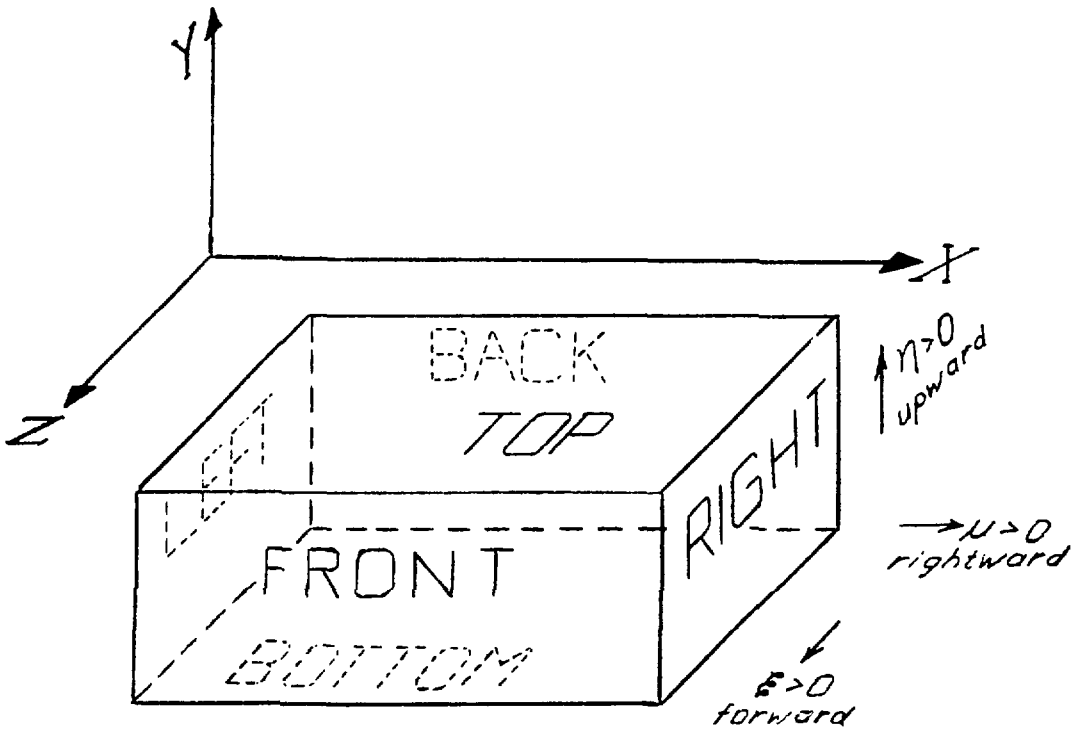


Fig. 3. Orientation of the three-dimensional domain of solution.

4. Boundary Conditions. The THREETRAN (hex,z) code allows only vacuum boundary conditions for the two x-dimension boundaries and, therefore, these boundary conditions are not under user input control. For the first, or bottom, y-dimension boundary the user may select vacuum (IBB=0), reflecting (IBB=1) or 180° rotational (IBB=2) boundary conditions. For the top y-dimension boundary the only allowable boundary condition at the present time is the vacuum condition (IBT=0). For the first, or back, z-dimension boundary both vacuum (IBA=0) and reflecting (IBA=1) conditions are available. The same conditions are available for the second, or front, z-dimension boundary (IBF=0 or 1). Figure 3 indicates the locations of left, right, bottom, top, back and front surfaces relative to the coordinate axes.

5. Cross Sections and Related Input. THREETRAN (hex,z) accepts only macroscopic cross sections and no upscatter is allowed. The number of energy groups is specified by the input parameter IGM and the order of scatter is limited to isotropic, or P_o, (ISCT=0) or linearly anisotropic, or P_1 (ISCT=1). The cross section format for the macroscopic cross sections is in the traditional Los Alamos format. The block of macroscopic cross sections for each of the materials is described by a block of data containing IHM rows and IGM columns. The row position of a given cross section reaction-type is specified relative to the row position of the total cross section, Σ_t (row IHT). The row order of the cross section reaction-types is as follows:

	Row	Group g Reaction-type	Comments
↑	·		Arbitrary reaction-types (not used by code)
	·		Arbitrary reaction-types (not used by code)
	·		Arbitrary reaction-types (not used by code)
	IHT-3	Σ_f	Required only if NORM<0 or KPWD=1
IHM	IHT-2	Σ_a	Always required
	IHT-1	$\nu\Sigma_f$	Always required
	IHT	Σ_t	$\Sigma_t = \Sigma_a + \sum_{h=g}^{IGM} \Sigma_s(g\to h)$ (Always required)
	IHT+1	$\Sigma_s(g\to g)$	Always required
	IHT+2	$\Sigma_s(g-1\to g)$	" "
	IHT+3	$\Sigma_s(g-2\to g)$	" "
	·	·	
↓	·	·	

As is shown above, the total number of rows in the cross section block, or the cross section table length, is IHM. All cross section blocks have the same values of IGM, IHT, and IHM. The fission cross section Σ_f must be present in position IHT-3 if the thermal power normalization is used or if the pointwise power density is desired as output.

When ISCT=1, indicating P_1 anisotropic scattering, an additional block of cross section data is required for each physical material in which P_1 scatter

is present. Since only the anisotropic scatter data (rows IHT+1 through IHM) from the P_1 cross section block are needed by the code, the data in rows 1 through IHT is arbitrary and is usually input as zero. It is required that each block of anisotropic cross sections be located immediately after the corresponding block of isotropic cross sections. For example if material 1 (the first cross section block in the cross section input data) is the macroscopic cross section block for the isotropic cross sections for, say, the mixture called CORE, then material 2 must be the anisotropic cross section block for CORE (provided CORE exhibits anisotropic scattering). The total number of materials, MT, must therefore be equal to the total number of isotropic plus anisotropic cross section blocks in the input.

6. LIMIT and the Allowable Number of Inner Iterations per Group. The input value of LIMIT is the inner iteration count limit. It is used to terminate the inner iteration process for each group if the pointwise fractional flux difference, or error, is greater than EPS after LIMIT inner iterations have been completed. If the pointwise flux error becomes less than EPS before LIMIT iterations have been performed, the inner iterations are terminated at once.

There are several deviations from the above procedure for K_{eff} calculations (IEVT=1). For IQT=0 or 1, i.e., when extrapolated values of K_{eff} are being computed, a variable inner iteration limit, IITL(G), is used for each group G. The variable limit is upper-bounded by LIMIT, i.e., IITL(G)$\leq$ LIMIT, for all G and is further constrained to be nonincreasing from outer iteration to outer iteration. This latter constraint tends to provide a smooth K_{eff} versus lambda (ALA) "graph" for extrapolation purposes. The nonincreasing limit is maintained so long as the pointwise inner iteration flux error at the current variable limit remains less than 5* EPS. If the error equals or exceeds 5*EPS then IITL(G) is reset to LIMIT for that group and the variable limit procedure is started again on the next outer iteration.

For IEVT = 1 and IQT =2 the variable inner iteration limit procedure described above is followed until both the maximum pointwise fission source error between outer iterations and the value of lambda, ALA, fall below 3*EPS. At this point the input value of LIMIT is automatically changed to 100, all variable inner iteration limits are reset to 100, and the code proceeds but does not calculate any further values of extrapolated K_{eff}. The above procedure is adopted to speed the convergence of local pointwise fluxes when the sources are nearing convergence.

7. IFIX and Negative Flux Fixup. Negative angular fluxes can occur with the difference scheme used in THREETRAN (hex,z). With the IFIX input parameter the user can choose whether (IFIX=1) or not (IFIX=0) a negative flux fixup is to be used by the code. Normally it is recommended that IFIX=0, i.e., no negative flux fix-up should be used. Even when negative fluxes appear the difference scheme has been found to be extremely stable and yields better integral quantities than when fixup is involved The use of negative flux fixup is recommended primarily as a check-calculation for comparison with a nonfixed calculation.

8. IBAL and Inner Iteration Rebalance. THREETRAN (hex,z) contains an inner iteration acceleration scheme called hemisphere-plane rebalance. The use of this rebalance is achieved by setting IBAL=0, and this value is recommended. The rebalance scheme invokes a plane-by-plane balance equation obtained by integrating the angular fluxes over all values of the direction cosines μ and η for either of the angular hemispheres $\xi > 0$ or $\xi < 0$ (see Figure 3). In some problems the use of this rebalance may produce iterative instabilities in which case the rebalance can be turned off (IBAL=1). There is no outer iteration acceleration currently in THREETRAN (hex,z).

9. ISTOP. Through the use of the ISTOP input parameter the user may execute the problem in normal fashion (ISTOP=0), may have the code only process the input data and halt (ISTOP=1) in order that problem setup can be verified, or may have the code process the input only through the KZ(KM) input array, determine the large core memory (LCM), i.e., extended core, storage requirements for the various storage modes available, and then halt (ISTOP=2). The various LCM storage modes are explained in Section III of this manual and a discussion of code output when ISTOP=2 is provided in Section V.

10. EPS: Overall Convergence Criterion. The value of EPS is used to control the degree of precision of results obtained through the iterative procedures used in the code. Various ways in which EPS is used as convergence criteria are given in subsection IV.C.3. in the IQT discussion and in subsection IV.C.6. in the LIMIT discussion.

11. NORM and Problem Normalizations Through the input quantity NORM the user can determine the normalization to which system-integral quantities are set. For inhomogeneous source problems either with or without fission (IEVT = 0 or 2) the code will accept either a NORM of 0.0 (default) or a positive value of NORM. If NORM is zero then no normalization is made and the energy-space integral of the inhomogeneous source, TQ, is simply the value obtained from the input source distribution. If NORM > 0.0, the value of TQ is set to NORM and the inhomogeneous distributed source is normalized to produce this value when integrated over space and energy.

For K_{eff} calculations (IEVT = 1) NORM may be negative, zero, or positive. Let us define TF as the space-energy integral of $\nu\Sigma_f\phi$, where ϕ is the local group scalar flux, and K_{in} as the input value of K_{eff}. The latter is unity if the input flux-type option, IFOPT, is zero and is the value taken from the RTFLUX file if IFOPT=1 or 2. If NORM = 0.0 no normalization is effected and the value of TF/K_{in} is set to NORM and all scalar fluxes are normalized to produce TF/K_{eff} when integrated over space and energy. Note that NORM > 0.0 defines the total effective fission source rate in the system (TF is the total fission source rate; TF/K_{eff} is the total effective fission source rate). If NORM is input as negative (NORM < 0.0), the problem is executed as if NORM = 0.0 until converged. Upon convergence the scalar fluxes, fission source rate densities, and thermal power densities are normalized such that the space-energy integral of the thermal power densities yields the value |NORM| Megawatts-thermal, i.e., EPF*1.6021x10^{-19}*TFR= |NORM| in MWth where EPF is the (input) energy-release (MeV) per fission and TFR is the space-energy integral of $\Sigma_f\ \phi$.

12. XBASE. In Figure 2 the dimension XBASE is indicated for each (x,y) plane shape option. In Fig. 2a. the length of each side of the equilateral triangle comprising the (x,y) mesh is 2*XBASE/IT. In Fig. 2b. (IGEO=1) the length of each side of a mesh triangle is 2*XBASE/(IT-1). Recall that IT is the number of triangles per band.

13. IDCS: Mesh Point to Cross Section Identifier. The integer values in the IDCS array indicate which material macroscopic cross section block (numbered in the order they are input) is assigned to each triangular prism in each z-dimension coarse mesh zone. If the integer value is positive, the scattering is assumed to be isotropic for that triangular prism. If the integer value is negative

(N) then the scatter is assumed to be linearly anisotropic and cross section block N+1 is assumed to contain the P_1 scatter data for material N (whose P_0 cross sections reside in block, N). For example, if the first cross section block contains macroscopic P_0 cross sections for the material CORE (Material 1) and the second cross section block contains the P_1 scatter data for CORE, the IDCS entry for a triangular prism consisting of CORE material and for which anisotropic scatter is to be considered would be -1. The value 2 would never appear in the IDCS array. The next larger value permitted would be 3 (or -3). The existence of P_1 scatter data in the cross section blocks does not require their use. In the preceding example, changing the IDCS value form -1 to 1 will remove the P_1 scatter calculation from all cells whose IDCS values are 1. If anisotropic scatter is to be turned off throughout the problem one need merely set the ISCT input control word to zero; any IDCS array negative entries will then be ignored.

V. DESCRIPTION OF OUTPUT

A. Normal Output

Appendix A contains a listing of the THREETRAN (hex,z) output from a sample problem. The problem is designed to illustrate most of the code options and capabilities. Each page of output is numbered and these numbers will be referred to in the following discussion.

The sample problem is an eigenvalue (K_{eff}) calculation of the simple hexagonal system shown in Figure 4. The central hexagon is fueled and is surrounded by an "annulus" of structural (nonfissionable) material. In the z-dimension the system is uniform, 16.0 cm. tall and has a z-mesh spacing of 4.0 cm. Anisotropic scattering is assumed in the fuel (Material 1) and the structure (Material 3). Material 5 is void. Figure 5 shows the x,y solution plane using the IGEO=1 (sawtooth rectangle) geometry. Three energy groups are used.

On page one of the output the control integers and control floating point numbers are listed as they were input along with a brief description of each control word. Each of these is described more fully in Section IV of this manual. Also shown on the first page are the number of equally-spaced fine-mesh intervals per z-dimension coarse-mesh zone. At the bottom of the page is the storage information for this problem. The amount of small core memory (SCM) required and the maximum allowed large core memory (LCM), i.e., extended core, storage are given. Next is given the number of bands of triangles that can be

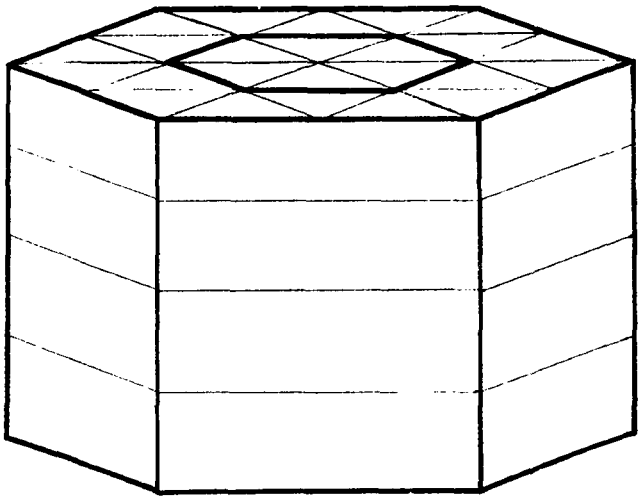


Fig. 4. Sample Problem.

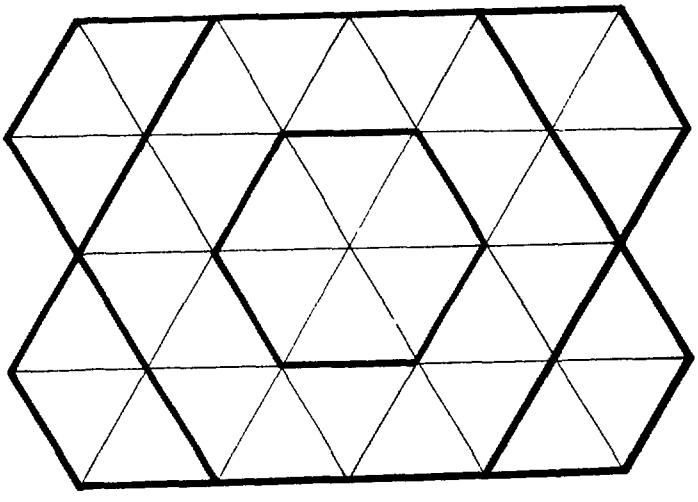


Fig. 5. IGEO=1 plane of sample problem.

stored in SCM. In the sample all 4 bands per plane can be accommodated. The next two entries indicate that LCM storage is sufficient to accommodate data for all 4 planes for all 3 groups. The SCM and LCM required amount of storage are next given followed by the NREAD storage mode used for the problem (see Section II of this report for details of the NREAD storage modes).

On page two of the output are listed the planes for which final scalar fluxes are to be printed as input through the KPRN input data string, the location of the two z-dimension boundaries, the input data entries for the NSDCAT array described in Section IV.B. and the input fission spectrum CHI. Next are printed messages indicating that the code began and successfully completed the processing of the IDCS array (mesh point to cross section identifiers). The full contents of this array are not printed because of the magnitude of the resulting printout and because a more usable check of mesh-to-cross section assignment is provided on the picture plot, or map, optionally available later in the output. Next on page two, and extending onto page three are printed the input macroscopic cross sections for the five cross section blocks (P_o CORE, P_1 CORE, P_o STRUCTURE, P_1 STRUCTURE, and VOID). The printing of the cross sections is optional and is part of the maxi print requested (NPRT=1) on input. Following the cross sections is a list of the z-direction fine-mesh interval spacings. Next is shown the optional picture plot of the x,y plane characteristic of each coarse z-mesh interval or zone (on the sample problem there is only one plot). The picture plot is included in the maxi print requested with NPRT=1. The picture plot is a direct computer-printed representation of Figure 5. Also included with the picture plot are y-dimension boundary conditions (indicated along the bottom and top of the plot), the y-coordinate boundaries of each band, the material (cross section) numbers (IDCS array entries) for each triangle, the z-coordinate boundaries for the coarse z-mesh interval associated with the plot, and the z-direction boundary conditon(s) (if the coarse z-mesh interval is the first or last such interval). Note that the material numbers for fuel and structures are negative to indicate anisotropic scatter is to be considered. For the dummy void cells (material 5) needed to fill out the x,y rectangular domain there is no need to consider anisotropic scatter.

On pages four and five the iteration monitor print for the outer-inner iterations is given. The number of inner iterations required for each group is given along with the maximum hemisphere flux error at the last inner iteration. When all groups have completed their inner iterations the eigenvalue (K_{eff} for this

problem) and lambda (the quantity denoted ALA in Section IV.C.3.) are listed. The eigenvalue for any given outer iteration is simply the product of the lambdas for the current and all previous outers. The extrapolated eigenvalue (for K_{eff} problems only and discussed in Section IV.C.3.) is listed as is the maximum pointwise fission source rate error. The latter error is the fractional difference between the pointwise fission source rate for the current outer iteration and the previous outer. The final print of K_{eff} for the problem is shown following the final outer iteration monitor print. In the sample problem the value printed is just the eigenvalue from the last outer iteration. Had the extrapolated eigenvalues satisfied their convergence criterion (two successive pairs of extrapolated eigenvalues agree to within 0.1*EPS) the last extrapolated eigenvalue would have been printed as the K-effective for the problem.

Immediately following the print of the problem K_{eff} is the execution time in minutes and a message indicating that a Final Dump was successfully made (see Section IV.C.1.). Next is listed the final scalar fluxes for each group for each plane requested with the problem input. For this problem the print for three planes (KPRINT=3), specifically, planes 1,3, and 4, (as input through the KPRN array) was requested. Following the scalar flux print is the optional print of the pointwise cell-average fission source rate density (requested by setting KFSR=1 in the input). The optional pointwise power densities are also printed (requested by setting KPWD=1 in the input). Since NORM was input as -1.0 the fluxes, fission source and power densities are all normalized to a thermal power level of 1.0 Megawatt.

B. ISTOP=2 Output

Appendix B contains a listing of the special output obtained when the ISTOP=2 option is used to obtain storage requirement information for a problem. The reader should refer to Section III of this manual for further information on storage and data management.

The listing in Appendix B is for the same sample problem shown in Appendix A and discussed in the preceding section. The first page of the Normal and ISTOP=2 listings are identical in form. For ISTOP=2, however, under the heading Storage Information five possible large core memory (LCM), i.e., extended core, storage modes are detailed. The first storage information summary is the LCM storage requirement for the data for the entire problem to be contained in LCM, i.e., the NREAD=0 storage mode. Notice that the problem contains 4 bands of triangle

per plane, 4 planes in the problem (for each group), and 3 energy groups. The storage required to fit the data for all 4 planes for all 3 groups into LCM is 5503 words of LCM. This number is the maximum LCM storage required to execute the desired problem (no use of random access disk).

Next the LCM storage for two cases under the NREAD=1 storage mode are given. Under this mode the data for all 4 planes for at least one group but not all three groups can be stored in LCM. The remaining data is stored on random disk. The first case listed is always for the maximum number of groups that will reside in LCM if there are two group-blocks of data. This represents the maximum LCM storage requirement for the NREAD=1 mode. In the sample problem listed this case yields 2 groups (one group-block containing groups 1 and 2, the second block containing group 3). To obtain this storage mode 4351 words of LCM are required. The second case under the NREAD=1 mode is always for the case of IGM group-blocks of data with all planes for one group residing in LCM. This gives the minumum LCM storage required for the NREAD=1 mode. For the sample problem 3199 words of LCM are required.

The fourth and fifth sets of storage information represent the two extremes of LCM storage under the NREAD=2 mode. In this mode the LCM data storage required for at least one but not all planes for one group is given. The first case under NREAD=2 always represents the LCM storage for the maximum number of planes that will reside in LCM if there are two plane-blocks of data. The LCM storage for this case is the maximum LCM storage required for the NREAD=2 mode. In the sample for 2 planes of data (corresponding to 2 blocks each containing 2 planes) the LCM storage required is 2047 words. The second case under NREAD=2, the last of the five cases listed, is always for the case of KT plane-blocks each containing only 1 plane of data. The LCM storage required (1471 words for the sample problem) is the absolute minimum LCM storage needed to execute the problem.

Since the user may be free to select the amount of LCM he wishes to use to execute a problem the storage information supplied under the ISTOP=2 option can prove quite valuable. The selection depends on the amount of LCM available, the charging algorithms for use of LCM and random disk during execution, or other factors. If the user has no random disk capability he is constrained to operate under the NREAD=0 mode. If random disk is available, under most conditions any of the group-blockings under the NREAD=1 mode will execute about as rapidly as under the NREAD=0 mode. Using the NREAD=2 mode, even with the minimum number

of plane-blocks, 2, the random disk -LCM data transfers are frequent (at least twice per inner iteration). Since such transfers are usually slow, problem execution efficiency is reduced (I/O times go up significantly). The exact effect of executing under the various LCM storage modes, of course, is dependent on the local computing environment.

C. Error Diagnostics

THREETRAN (hex,z) contains a large number of error checks in an attempt to ensure that the input data are correct, insofar as the code can determine, before execution of the problem commences. Much of the checking is done on input control integers to ensure that their values are consistent with those available in the code. Other checks are performed on the input data blocks to (i) ensure that the correct number of data entries are made and (ii) to ensure that the options allowed under the special LASL formats (Sec. IV.A) are correct. Attempts have been made to provide error messages that are self explanatory (at least to the extent that they identify the offending input word or data block). Three examples typifying the error diagnostics are provided below.

In example 1, the sample problem listed in Appendix A was attempted using an S_{16} quadrature set, i.e., ISN=16 was placed on the Control Integer Card 1. Since only S_2, S_4, S_6 and S_8 are allowed a fatal error was encountered as shown.

```
********************************************** F A T A L   E R R O R **************************************
     ISN ERROR
*****************************************************************************************************************
 FILE    I/O TIME (MICROSEC)    READS    WRITES

OUTPUT            78664            1         0
INPUT             64279            2         0

TOTALS           142943            3         0

**DOPC**NOT INITIALIZED FOR IOP/NREF/NGREF/MXLEN/MXBLOK      4     0     0     0     0
```

In example 2, the sample problem listed in Appendix A was attempted with an incorrect number of entries in the NDSCAT array (Sec. IV.B.) The correct entries for NDSCAT (9 in number) should be 1,0,0,1,1,0,1,1,1. For this example, however, only the first 8 entries were supplied. The resulting error message was printed and execution was halted.

```
********************************************** F A T A L   E R R O R **********************************************
**LOAD ERROR** BLOCK=NDSCAT ARRAY     COUNT=     9 CARD=     1 ACTUAL COUNT=     8

    TOO FEW DATA ENTRIES

*****************************************************************************************************************
          1         0         0         1         1         0         1         1
```

As can be seen, a highly visible FATAL ERROR message is first printed. This is followed by the words LOAD ERROR indicating that the subroutine LOAD (which reads the input data and loads it into the proper arrays) encountered the error. Next come the words BLOCK=NDSCAT ARRAY indicating that NDSCAT was the input data block being processed when the error occurred. COUNT=9 indicates that the correct length of the data string being processed should have been 9 words. CARD=1 indicates that the error occurred on the first card image of input data and ACTUAL COUNT=8 indicates that only 8 words of data were provided in the string (instead of 9). The message TOO FEW DATA ENTRIES is self-explanatory. Just below the second line of asterisks is listed the contents of the NDSCAT string processed up to the point where the error was located. As can be seen the last entry of 1 in the string is not present.

In example 3 the sample problem of Appendix A was attempted with an error in the IDCS block. As described in Sec. IV.B this block consists of KM sets with each set consisting of JT data strings each of which contains IT entries. For this problem KM=1, JT=4 and IT=9. Thus, the problem expects 1 set of 4 data strings each of which contains 9 words and each of which must be terminated by the "3" terminator of the LASL special format (Sec. IV.A). In the example the "3" terminator on the second string (corresponding to the second band) was replaced by a "9" (skip to the next card). As a result, the LOAD Subroutine read the card for band 2 (with 9 words), skipped to the card for band 3 and read 9 more words before encountering the "3" terminator. It thus appeared to LOAD that 18 words were being input for the string and a FATAL ERROR resulted with the error message shown below. The highly visible message FATAL ERROR is printed. The message **LOAD ERROR** indicates that Subroutine LOAD found the error;

```
**********************************************F A T A L   E R R O R **********************************************
**LOAD ERROR** BLOCK=IDCS BLOCK        K-PLANE= 1 J-BAND= 2 COUNT=     9 CARD=     2 ACTUAL COUNT=    18

     TOO MANY DATA ENTRIES

**********************************************************************************************************************
          5         -3         -3         -1         -1         -1         -3         -3          5
```

BLOCK = IDCS BLOCK indicates that the error occurred in the input for the IDCS block. K-PLANE = 1, J-BAND=2 tells us that the error occurred in the input for the first coarse z-dimension set and, specifically, for the second band in that set. COUNT=9 indicates that 9 words were expected; CARD=2 indicates that LOAD discovered the error in reading the second card for the string. ACTUAL COUNT=18 gives the number of words erroneously input for the string. The message TOO MANY DATA ENTRIES is self evident. Just below the asterisks, the contents of the offending IDCS string (the first COUNT entries) is printed.

The above examples give the typical types of prints that may be encountered as error messages. Through these the user should be able to quickly discover his error (with, perhaps, referral to this User's Manual).

REFERENCES

1. K.D. Lathrop, "THREETRAN: A Program to Solve the Multigroup Discrete Ordinates Transport Equation in (x,y,z) Geometry," Los Alamos Scientific Laboratory report LA-6333-MS (May 1976).

2. W. F. Walters and R. D. O'Dell, "A Three-Dimensional Hexagonal-Z Difference Scheme for Discrete-Ordinates Codes," Proc. Amer. Nucl. Soc. Top. Meeting on Computational Methods in Nuclear Engineering, Williamsburg, VA, April 23-25, 1979, Vol. 2, pp. 4-49 through 4-63.

3. R. D. O'Dell, "Standard Interface Files and Procedures for Reactor Physics Codes, Version IV," Los Alamos Scientific Laboratory report LA-6941-MS (Sept. 1977).

4. B. M. Carmichael, "Standard Interface Files and Procedures for Reactor Physics Codes, Version III," Los Alamos Scientific Laboratory report LA-5486-MS (Feb. 1974).

5. K. D. Lathrop and F. W. Brinkley, Jr., "TWOTRAN-II: An Interfaced, Exportable Version of the TWOTRAN Code for Two-Dimensional Transport," Los Alamos Scientific Laboratory report LA-4848-MS (July 1973).

APPENDIX A

SAMPLE PROBLEM OUTPUT

On the following pages is a complete printed output from the THREETRAN (hex, z) code for the sample problem described in Sec. V.A.

```
CASE PROCESSED BY THREETRAN(HEX,Z) CODE OF 07/06/79 ON  07/19/79
        5600 MAXLCM LCM ADJUSTMENT (-1/0/N NONE/CURRENT/USE VALUE)


   TEST PROBLEM FOR MANUAL K-EFFECTIVE CALCULATION
   THIS IS P1 SCATTER WITH POWER & FISSION SOURCE RATE PRINT
   SAWTOOTH RECTANGLE INPUT GEOMETRY

         1 IEVT    PROBLEM TYPE 0/1/2=SOURCE/K EFFECTIVE/SOURCE PLUS FISSION
         0 ISTART  0/1/2=INITIAL PROBLEM/RESTART FROM PERIODIC DUMP/RESTART FROM FINAL DUMP
         4 ISN     SN ORDER (LIMITED TO 2,4,6, OR 8)
         9 IT      NUMBER OF TRIANGLES PER BAND
         4 JT      NUMBER OF BANDS PER PLANE
         1 KM      NUMBER OF Z-DIRECTION COARSE MESH ZONES

         1 IGEO    X-Y PLANE SHAPE   0/1 = PARALLELOGRAM/RECTANGLE
         1 IQT     TERMINATION OPTION 0/1/2 EXTRAPOLATED K/ FISSION SOURCE RATE/ FISSION SOURCE RATE AND FLUXES
         0 IBB     BOTTOM Y-DIMENSION BOUNDARY CONDITION  0/1/2=VACUUM/REFLECTING/180-DEG. ROTATIONAL
         0 IBT     TOP Y-DIMENSION BOUNDARY CONDITION  0 (VACUUM) ONLY
         0 IBA     BACK Z-DIMENSION BOUNDARY CONDITION  0/1=VACUUM/REFLECTING
         0 IBF     FRONT Z-DIMENSION BOUNDARY CONDITION  0/1=VACUUM/REFLECTING

         3 IGM     NUMBER OF ENERGY GROUPS
         1 ISCT    LEGENDRE ORDER OF SCATTERING  0/1
         5 MT      TOTAL NUMBER OF MACRO CROSS SECTION SETS
         4 IHT     ROW OF TOTAL CROSS SECTION IN CROSS SECTION TABLE
         7 IHM     LAST ROW OF CROSS SECTION TABLE
        10 LIMIT   MAX NUMBER OF INNER ITERATIONS ALLOWED PER GROUP

         0 IFIX    NEGATIVE FLUX FIXUP  0/1=NO/YES  STRONGLY RECOMMEND NO FIXUP
         0 IBAL    REBALANCE INNER ITERATION ACCELERATION  0/1=YES/NO
         0 IQOPT   FIXED SOURCE INPUT OPTION (IEVT=0 OR 2 ONLY)  0/1/2/3 =NONE/CARDS/FIXSRC VERS III/FIXSRC VERS IV
         0 IFOPT   SCALAR FLUX INPUT OPTION  0/1/2 = NONE/RTFLUX VERS III/RTFLUX VERS IV
         0 IOUT    OUTPUT FORM  0/1=PRINT/FICHE
        -1 KPRINT  FINAL SCALAR FLUX PRINT OPTION  -1/0/N=ALL/NONE/NO. OF PLANES

         1 KFSR    FINAL FISSION SOURCE RATE PRINT BY MESH POINT OPTION  0/1=NO/YES
         0 ISTOP   0/1/2 = EXECUTE PROBLEM/PROCESS INPUT ONLY/DETERMINE STORAGE REQUIREMENTS ONLY
         1 NPRT    PRINT OPTION 0/1=MINI/MAXI
         1 KPWD    FINAL POWER DENSITY PRINT BY MESH POINT OPTION  0/1 = NO/YES


  1.000E-03 EPS     OUTER ITERATION (OVERALL PROBLEM) CONVERGENCE CRITERION
 -1.000E+00 NORM    NORMALIZATION FACTOR (IN MEGAWATTS IF ,LT.0., NOT USED IF 0.0 , IN NEUTS/SEC IF .GT.0.)
  6.000E+01 DTIME   RESTART DUMP TAKEN AFTER DTIME SECONDS AND PROBLEM HALTED
  2.771E+01 XBASE   OVERALL PROBLEM X-LENGTH IN CM. (LENGTH OF SIDE OF TRIANGLE MESH-CELL = 2*XBASE/(IT-IGEO) )
  0.        EPF     ENERGY (MEV) PER FISSION (DEFAULT=215.0)

INPUT INT. PER Z MESH      1
ALL ENTRIES =              4

************************************** S T O R A G E   I N F O R M A T I O N ***************************************


SMALL CORE (SCM) REQUIRED =  1879    MAXIMUM LCM ALLOWED =  5600

      JBLOC                  KBLOC                  IGBLOC              SCM        LCM                NREAD
BANDS IN SCM (MAX)   PLANES IN LCM (MAX)   GROUPS IN LCM (MAX)   STORAGE    STORAGE   STORAGE MODE (SEE MANUAL)

         4                     4                     3              1879       5503              0
```

```
PLANES FOR WHICH FINAL SCALAR FLUXES ARE TO BE PRINTED
 ALL

INPUT  Z BOUNDARIES        2
  0.          1.6000E+01

INPUT NDSCAT ARRAY         9
          1            0           0           1           1           0           1           1           1

INPUT FISSION SPECTRUM     3
  7.6000E-01  2.3000E-01  1.0000E-02


BEGIN PROCESSING X-SECTION ID NUMBERS



X-SECTION ID NUMBERS SUCCESSFULLY PROCESSED

  1   LOADED FROM CARDS          CORE        P0     3 GROUP SIMPLIFIED LCCBR SET

      GROUP     1    GROUP     2    GROUP     3
1   .500000E-02    .250000E-02    .900000E-02
2   .600000E-02    .300000E-02    .100000E-01
3   .120000E+00    .500000E-02    .180000E-01
4   .180000E+00    .250000E+00    .400000E+00
5   .140000E+00    .242000E+00    .390000E+00
6  0.              .330000E-01    .550000E-01
7  0.             0.              .100000E-02

  2   LOADED FROM CARDS          CORE        P1     3 GROUP SIMPLIFIED LCCBR SET

      GROUP     1    GROUP     2    GROUP     3
1  0.             0.             0.
2  0.             0.             0.
3  0.             0.             0.
4   .490000E-01    .240000E-01    .100000E-01
5   .500000E-01    .250000E-01    .100000E-01
6  0.             -.200000E-02   -.100000E-02
7  0.             0.             0.

  3   LOADED FROM CARDS          STRUCTURE   P0     3 GROUP SIMPLIFIED LCCBR SET

      GROUP     1    GROUP     2    GROUP     3
1  0.             0.             0.
2   .300000E-02    .100000E-02    .400000E-02
3  0.             0.             0.
4   .275000E+00    .400000E+00    .160000E+01
5   .225000E+00    .390000E+00    .996000E+00
6  0.              .460000E-01    .900000E-02
7  0.             0.              .100000E-02

  4   LOADED FROM CARDS          STRUCTURE   P1     3 GROUP SIMPLIFIED LCCBR SET
```

	GROUP 1	GROUP 2	GROUP 3
1	0.	0.	0.
2	0.	0.	0.
3	0.	0.	0.
4	.7000000E-01	.4300000E-01	.2000000E-01
5	.7960000E-01	.4100000E-01	.2000000E-01
6	0.	-.9000000E-02	-.1000000E-02
7	0.	0.	0.

5 LOADED FROM CARDS VOID PO

ALL ENTRIES OF THIS ARRAY EQUAL 0.

	Z ZONE	DELTA Z
1	1	4.0000E+00
2	1	4.0000E+00
3	1	4.0000E+00
4	1	4.0000E+00

********** F I N E M E S H M A T E R I A L M A P F O R C O A R S E Z - I N T E R V A L 1 **********
BETWEEN Z= 0.00 AND Z= 16.00 THERE ARE 4 PLANES. AT Z= 0.00 BOUND. COND. IBA= 0. AT Z= 16.00 BC IBF= 0.
BOUNDARY CONDITION CHARACTERS (-=VAC, *=REFL, +=180 ROTATE). LEFT NUMBER INDICATES Y-COORDINATE.

```
   24.00      1-----2-----3-----4-----5
BAND             5    -3    -3     5
  4            5    -3    -3    -3     5
   18.00   1-----2-----3-----4-----5-----6
BAND             5    -3    -1    -3     5
  3             -3    -1    -1    -3
   12.00      1-----2-----3-----4-----5
BAND            -3    -1    -1    -3
  2            5    -3    -1    -3     5
    6.00   1-----2-----3-----4-----5-----6
BAND             5    -3    -3    -3     5
  1               5    -3    -3     5
    -.00       1-----2-----3-----4-----5
```

********** I T E R A T I O N M O N I T O R P R I N T **********

GROUP	ITERATIONS	MAX. FLUX ERROR
1	10	1.0310E-03
2	10	2.1583E-02
3	10	1.0681E+00

OUTER ITERATION 1 EIGENVALUE= 6.8619501E-01 LAMBDA= 6.8619501E-01

EXTRAPOLATED EIGENVALUE= 1.0700000E+00
FISSION SOURCE RATE ERROR= 7.2897994E-01

****

GROUP	ITERATIONS	MAX. FLUX ERROR
1	5	7.5290E-04
2	6	6.2129E-04
3	10	4.5327E-02

OUTER ITERATION 2 EIGENVALUE= 6.6259062E-01 LAMBDA= 9.6560105E-01

EXTRAPOLATED EIGENVALUE= 6.5968457E-01
FISSION SOURCE RATE ERROR= 9.5238457E-02

****

GROUP	ITERATIONS	MAX. FLUX ERROR
1	4	5.0097E-04
2	3	8.1059E-04
3	10	2.4859E-03

OUTER ITERATION 3 EIGENVALUE= 6.5984356E-01 LAMBDA= 9.9586161E-01

EXTRAPOLATED EIGENVALUE= 6.5947356E-01
FISSION SOURCE RATE ERROR= 2.0596900E-02

****

GROUP	ITERATIONS	MAX. FLUX ERROR
1	3	6.5044E-04
2	2	6.3434E-04
3	3	7.5318E-04

OUTER ITERATION 4 EIGENVALUE= 6.5984113E-01 LAMBDA= 9.9996873E-01

EXTRAPOLATED EIGENVALUE= 6.5984111E-01
FISSION SOURCE RATE ERROR= 4.5544917E-03

****

GROUP	ITERATIONS	MAX. FLUX ERROR
1	2	6.4461E-04
2	1	8.2075E-04
3	1	5.4029E-04

OUTER ITERATION 5 EIGENVALUE= 6.5989316E-01 LAMBDA= 1.0000789E+00

EXTRAPOLATED EIGENVALUE= 6.5984763E-01
FISSION SOURCE RATE ERROR= 1.1659527E-03

****

GROUP	ITERATIONS	MAX. FLUX ERROR
1	1	9.2520E-04
2	1	5.1039E-04
3	1	3.7588E-04

OUTER ITERATION 6 EIGENVALUE= 6.5992607E-01 LAMBDA= 1.0000499E+00

EXTRAPOLATED EIGENVALUE= 6.5998267E-01
FISSION SOURCE RATE ERROR= 2.9763042E-04

****

****

K-EFFECTIVE FOR THIS PROBLEM = 6.5992607E-01

****

EXECUTION TIME (MINUTES) = 2.34563E-01

* * FINAL DUMP TAKEN * * DMPONE

SCALAR FLUX FOR GROUP 1, PLANE 1

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	3.0239E+13	1.8266E+13	1.2545E+14	1.2904E+14	2.7271E+14	1.2904E+14	1.2545E+14	1.8266E+13
2	3.4947E+13	1.2681E+14	2.6387E+14	6.6338E+14	6.6969E+14	6.6338E+14	2.6387E+14	1.2681E+14
3	3.4947E+13	1.2681E+14	2.6387E+14	6.6338E+14	6.6969E+14	6.6338E+14	2.6387E+14	1.2681E+14
4	3.0239E+13	1.8266E+13	1.2545E+14	1.2904E+14	2.7271E+14	1.2904E+14	1.2545E+14	1.8266E+13

BAND	TRIANG 9	TRIANG
1	3.0239E+13	
2	3.4947E+13	

4	3.0289E+13

SCALAR FLUX FOR GROUP 1, PLANE 2

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	4.5263E+13	2.7931E+13	1.9009E+14	1.9985E+14	4.1672E+14	1.9985E+14	1.9009E+14	2.7931E+13
2	5.4253E+13	2.0311E+14	4.0368E+14	1.0146E+15	1.0224E+15	1.0146E+15	4.0368E+14	2.0311E+14
3	5.4253E+13	2.0311E+14	4.0368E+14	1.0146E+15	1.0224E+15	1.0146E+15	4.0368E+14	2.0311E+14
4	4.5263E+13	2.7931E+13	1.9009E+14	1.9985E+14	4.1672E+14	1.9985E+14	1.9009E+14	2.7931E+13

BAND	TRIANG 9	TRIANG
1	4.5263E+13	
2	5.4253E+13	
3	5.4253E+13	
4	4.5263E+13	

SCALAR FLUX FOR GROUP 1, PLANE 3

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	4.5264E+13	2.7930E+13	1.9009E+14	1.9985E+14	4.1672E+14	1.9985E+14	1.9009E+14	2.7930E+13
2	5.4254E+13	2.0311E+14	4.0368E+14	1.0146E+15	1.0224E+15	1.0146E+15	4.0368E+14	2.0311E+14
3	5.4254E+13	2.0311E+14	4.0368E+14	1.0146E+15	1.0224E+15	1.0146E+15	4.0368E+14	2.0311E+14
4	4.5264E+13	2.7930E+13	1.9009E+14	1.9985E+14	4.1672E+14	1.9985E+14	1.9009E+14	2.7930E+13

BAND	TRIANG 9	TRIANG
1	4.5264E+13	
2	5.4254E+13	
3	5.4254E+13	
4	4.5264E+13	

SCALAR FLUX FOR GROUP 1, PLANE 4

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	3.0289E+13	1.8265E+13	1.2544E+14	1.2904E+14	2.7270E+14	1.2904E+14	1.2544E+14	1.8265E+13
2	3.4947E+13	1.2680E+14	2.6386E+14	6.6338E+14	6.6969E+14	6.6338E+14	2.6386E+14	1.2680E+14
3	3.4947E+13	1.2680E+14	2.6386E+14	6.6338E+14	6.6969E+14	6.6338E+14	2.6386E+14	1.2680E+14
4	3.0289E+13	1.8265E+13	1.2544E+14	1.2904E+14	2.7270E+14	1.2904E+14	1.2544E+14	1.8265E+13

BAND	TRIANG 9	TRIANG
1	3.0289E+13	
2	3.4947E+13	
3	3.4947E+13	
4	3.0289E+13	

SCALAR FLUX FOR GROUP 2, PLANE 1

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8

1	4.2228E+13	4.5139E+13	1.9465E+14	1.9487E+14	3.6732E+14	1.9487E+14	1.9465E+14	4.5139E+13
2	4.8742E+13	1.9786E+14	3.6770E+14	6.6128E+14	6.6264E+14	6.6128E+14	3.6770E+14	1.9786E+14
3	4.8742E+13	1.9786E+14	3.6770E+14	6.6128E+14	6.6264E+14	6.6128E+14	3.6770E+14	1.9786E+14
4	4.2228E+13	4.5139E+13	1.9466E+14	1.9487E+14	3.6732E+14	1.9487E+14	1.9465E+14	4.5139E+13

BAND	TRIANG 9	TRIANG
1	4.2228E+13	
2	4.8742E+13	
3	4.8742E+13	
4	4.2228E+13	

SCALAR FLUX FOR GROUP 2, PLANE 2

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	6.4738E+13	7.3692E+13	3.2629E+14	3.2712E+14	6.0831E+14	3.2712E+14	3.2629E+14	7.3692E+13
2	7.8364E+13	3.3541E+14	6.1225E+14	1.0682E+15	1.0680E+15	1.0682E+15	6.1225E+14	3.3541E+14
3	7.8364E+13	3.3541E+14	6.1225E+14	1.0682E+15	1.0680E+15	1.0682E+15	6.1225E+14	3.3541E+14
4	6.4738E+13	7.3692E+13	3.2629E+14	3.2712E+14	6.0831E+14	3.2712E+14	3.2629E+14	7.3692E+13

BAND	TRIANG 9	TRIANG
1	6.4738E+13	
2	7.8364E+13	
3	7.8364E+13	
4	6.4738E+13	

SCALAR FLUX FOR GROUP 2, PLANE 3

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	6.4738E+13	7.3691E+13	3.2628E+14	3.2711E+14	6.0831E+14	3.2711E+14	3.2628E+14	7.3691E+13
2	7.8363E+13	3.3540E+14	6.1224E+14	1.0682E+15	1.0680E+15	1.0682E+15	6.1224E+14	3.3540E+14
3	7.8363E+13	3.3540E+14	6.1224E+14	1.0682E+15	1.0680E+15	1.0682E+15	6.1224E+14	3.3540E+14
4	6.4738E+13	7.3691E+13	3.2628E+14	3.2711E+14	6.0831E+14	3.2711E+14	3.2628E+14	7.3691E+13

BAND	TRIANG 9	TRIANG
1	6.4738E+13	
2	7.8363E+13	
3	7.8363E+13	
4	6.4738E+13	

SCALAR FLUX FOR GROUP 2, PLANE 4

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	4.2232E+13	4.5142E+13	1.9465E+14	1.9487E+14	3.6731E+14	1.9487E+14	1.9465E+14	4.5142E+13
2	4.8745E+13	1.9786E+14	3.6769E+14	6.6128E+14	6.6264E+14	6.6128E+14	3.6769E+14	1.9786E+14
3	4.8745E+13	1.9786E+14	3.6769E+14	6.6128E+14	6.6264E+14	6.6128E+14	3.6769E+14	1.9786E+14
4	4.2232E+13	4.5142E+13	1.9465E+14	1.9487E+14	3.6731E+14	1.9487E+14	1.9465E+14	4.5142E+13

BAND	TRIANG 9	TRIANG
1	4.2232E+13	
2	4.8745E+13	

3	4.8745E+13
4	4.2232E+13

SCALAR FLUX FOR GROUP 3, PLANE 1

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	1.8071E+13	1.7124E+13	1.6435E+14	1.6667E+14	3.5121E+14	1.6667E+14	1.6835E+14	1.7124E+13
2	1.8387E+13	1.7502E+14	3.5895E+14	6.6293E+14	6.6064E+14	6.6293E+14	3.5895E+14	1.7502E+14
3	1.8387E+13	1.7502E+14	3.5895E+14	6.6293E+14	6.6064E+14	6.6293E+14	3.5895E+14	1.7502E+14
4	1.8071E+13	1.7124E+13	1.6435E+14	1.6667E+14	3.5121E+14	1.6667E+14	1.6835E+14	1.7124E+13

BAND	TRIANG 9	TRIANG
1	1.8071E+13	
2	1.8387E+13	
3	1.8387E+13	
4	1.8071E+13	

SCALAR FLUX FOR GROUP 3, PLANE 2

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	3.3957E+13	3.5439E+13	3.2220E+14	3.2021E+14	6.5468E+14	3.2021E+14	3.2220E+14	3.5439E+13
2	3.5858E+13	3.3766E+14	6.7102E+14	1.1582E+15	1.1509E+15	1.1582E+15	6.7102E+14	3.3766E+14
3	3.5858E+13	3.3766E+14	6.7102E+14	1.1582E+15	1.1509E+15	1.1582E+15	6.7102E+14	3.3766E+14
4	3.3957E+13	3.5439E+13	3.2220E+14	3.2021E+14	6.5468E+14	3.2021E+14	3.2220E+14	3.5439E+13

BAND	TRIANG 9	TRIANG
1	3.3957E+13	
2	3.5858E+13	
3	3.5858E+13	
4	3.3957E+13	

SCALAR FLUX FOR GROUP 3, PLANE 3

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	3.3957E+13	3.5439E+13	3.2220E+14	3.2021E+14	6.5467E+14	3.2021E+14	3.2220E+14	3.5439E+13
2	3.5858E+13	3.3766E+14	6.7102E+14	1.1582E+15	1.1509E+15	1.1582E+15	6.7102E+14	3.3766E+14
3	3.5858E+13	3.3766E+14	6.7102E+14	1.1582E+15	1.1509E+15	1.1582E+15	6.7102E+14	3.3766E+14
4	3.3957E+13	3.5439E+13	3.2220E+14	3.2021E+14	6.5467E+14	3.2021E+14	3.2220E+14	3.5439E+13

BAND	TRIANG 9	TRIANG
1	3.3957E+13	
2	3.5858E+13	
3	3.5858E+13	
4	3.3957E+13	

SCALAR FLUX FOR GROUP 3, PLANE 4

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8

1	1.4872E+13	1.7125E+13	1.6835E+14	1.6667E+14	3.5121E+14	1.6667E+14	1.6835E+14	1.7125E+13
2	1.4387E+13	1.7501E+14	3.6495E+14	6.6294E+14	6.6055E+14	6.6294E+14	3.6895E+14	1.7501E+14
3	1.4387E+13	1.7501E+14	3.6495E+14	6.6294E+14	6.6055E+14	6.6294E+14	3.6895E+14	1.7501E+14
4	1.8072E+13	1.7125E+13	1.6835E+14	1.6667E+14	3.5121E+14	1.6667E+14	1.6835E+14	1.7125E+13

BAND	TRIANG 9	TRIANG
1	1.8072E+13	
2	1.8387E+13	
3	1.8387E+13	
4	1.8072E+13	

FISSION SOURCE RATE (NEUTS/SEC PER CC) FOR PLANE 1

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	9.4845E+13	9.5568E+13	9.4845E+13	0.	0.
3	0.	0.	0.	9.4845E+13	9.5568E+13	9.4845E+13	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

FISSION SOURCE RATE (NEUTS/SEC PER CC) FOR PLANE 2

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	1.4794E+14	1.4874E+14	1.4794E+14	0.	0.
3	0.	0.	0.	1.4794E+14	1.4874E+14	1.4794E+14	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

FISSION SOURCE RATE (NEUTS/SEC PER CC) FOR PLANE 3

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	1.4794E+14	1.4874E+14	1.4794E+14	0.	0.
3	0.	0.	0.	1.4794E+14	1.4874E+14	1.4794E+14	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	

3	0.
4	0.

FISSION SOURCE RATE (NEUTS/SEC PER CC) FOR PLANE 4

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	9.4845E+13	9.5568E+13	9.4845E+13	0.	0.
3	0.	0.	0.	9.4845E+13	9.5568E+13	9.4845E+13	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

POWER DENSITY (W/CC) FOR PLANE 1

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	3.7671E+02	3.7720E+02	3.7671E+02	0.	0.
3	0.	0.	0.	3.7671E+02	3.7720E+02	3.7671E+02	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

POWER DENSITY (W/CC) FOR PLANE 2

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	6.2579E+02	6.2483E+02	6.2579E+02	0.	0.
3	0.	0.	0.	6.2579E+02	6.2483E+02	6.2579E+02	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

POWER DENSITY (W/CC) FOR PLANE 3

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8

1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	6.2579E+02	6.2484E+02	6.2579E+02	0.	0.
3	0.	0.	0.	6.2579E+02	6.2484E+02	6.2579E+02	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

POWER DENSITY (W/CC) FOR PLANE 4

BAND	TRIANG 1	TRIANG 2	TRIANG 3	TRIANG 4	TRIANG 5	TRIANG 6	TRIANG 7	TRIANG 8
1	0.	0.	0.	0.	0.	0.	0.	0.
2	0.	0.	0.	3.7671E+02	3.7720E+02	3.7671E+02	0.	0.
3	0.	0.	0.	3.7671E+02	3.7720E+02	3.7671E+02	0.	0.
4	0.	0.	0.	0.	0.	0.	0.	0.

BAND	TRIANG 9	TRIANG
1	0.	
2	0.	
3	0.	
4	0.	

FILE	I/O TIME (MICROSEC)	READS	WRITES
OUTPUT	55430	1	0
INPUT	48875	2	0
DMPDNE	905841	5	8
RTFLUX	95255	1	1
TOTALS	1106401	9	9

APPENDIX B

ISTOP = 2 SAMPLE PROBLEM OUTPUT

On the following pages is a listing of the printed output form the THREETRAN (hex,z) code for the sample problem using the special ISTOP = 2 storage-information-only flag as described in Sec. V.B.

```
CASE PROCESSED BY THREETRAN(HEX,Z) CODE OF 07/06/77 ON  07/17/79
       5600 MAXLRD LCM ADJUSTMENT (-1/0/N NONE/CURRENT/USE VALUE)


   TEST PROBLEM FOR MANUAL K-EFFECTIVE CALCULATION
   THIS IS P1 SCATTER WITH POWER & FISSION SOURCE RATE PRINT
   SAWTOOTH RECTANGLE INPUT GEOMETRY
   ISTOP=2 FOR STORAGE INFORMATION ONLY

         1 IEVT     PROBLEM TYPE 0/1/2=SOURCE/K EFFECTIVE/SOURCE PLUS FISSION
         0 ISTART   0/1/2=INITIAL PROBLEM/RESTART FROM PERIODIC DUMP/RESTART FROM FINAL DUMP
         4 ISN      SN ORDER (LIMITED TO 2,4,6, OR 8)
         9 IT       NUMBER OF TRIANGLES PER BAND
         4 JT       NUMBER OF BANDS PER PLANE
         1 KM       NUMBER OF Z-DIRECTION COARSE MESH ZONES

         1 IGEO     X-Y PLANE SHAPE   0/1 = PARALLELOGRAM/RECTANGLE
         1 IQT      TERMINATION OPTION 0/1/2 EXTRAPOLATED K/ FISSION SOURCE RATE/ FISSION SOURCE RATE AND FLUXES
         0 IBB      BOTTOM Y-DIMENSION BOUNDARY CONDITION  0/1/2=VACUUM/REFLECTING/180-DEG. ROTATIONAL
         0 IBT      TOP Y-DIMENSION BOUNDARY CONDITION  0 (VACUUM) ONLY
         0 IBA      BACK Z-DIMENSION BOUNDARY CONDITION  0/1=VACUUM/REFLECTING
         0 IBF      FRONT Z-DIMENSION BOUNDARY CONDITION  0/1=VACUUM/REFLECTING

         3 IGM      NUMBER OF ENERGY GROUPS
         1 ISCT     LEGENDRE ORDER OF SCATTERING  0/1
         5 MT       TOTAL NUMBER OF MACRO CROSS SECTION SETS
         4 IHT      ROW OF TOTAL CROSS SECTION IN CROSS SECTION TABLE
         7 IHM      LAST ROW OF CROSS SECTION TABLE
        10 LIMIT    MAX NUMBER OF INNER ITERATIONS ALLOWED PER GROUP

         0 IFIX     NEGATIVE FLUX FIXUP  0/1=NO/YES  STRONGLY RECOMMEND NO FIXUP
         0 IBAL     REBALANCE INNER ITERATION ACCELERATION  0/1=YES/NO
         0 IQOPT    FIXED SOURCE INPUT OPTION (IEVT=0 OR 2 ONLY)  0/1/2/3 =NONE/CARDS/FIXSRC VERS III/FIXSRC VERS IV
         0 IFOPT    SCALAR FLUX INPUT OPTION  0/1/2 = NONE/RTFLUX VERS III/RTFLUX VERS IV
         0 IOUT     OUTPUT FORM  0/1=PRINT/FICHE
        -1 KPRINT   FINAL SCALAR FLUX PRINT OPTION  -1/0/N=ALL/NONE/NO. OF PLANES

         1 KFSR     FINAL FISSION SOURCE RATE PRINT BY MESH POINT OPTION  0/1=NO/YES
         2 ISTOP    0/1/2 = EXECUTE PROBLEM/PROCESS INPUT ONLY/DETERMINE STORAGE REQUIREMENTS ONLY
         1 NPRT     PRINT OPTION 0/1=MINI/MAXI
         1 KPWD     FINAL POWER DENSITY PRINT BY MESH POINT OPTION  0/1 = NO/YES


  1.000E-03 EPS     OUTER ITERATION (OVERALL PROBLEM) CONVERGENCE CRITERION
 -1.000E+00 NORM    NORMALIZATION FACTOR (IN MEGAWATTS IF .LT.0., NOT USED IF 0.0 , IN NEUTS/SEC IF .GT.0.)
  6.000E+01 DTIME   RESTART DUMP TAKEN AFTER DTIME SECONDS AND PROBLEM HALTED
  2.771E+01 XBASE   OVERALL PROBLEM X-LENGTH IN CM. (LENGTH OF SIDE OF TRIANGLE MESH-CELL = 2*XBASE/(IT-IGEO) )
  0.        EPF     ENERGY (MEV) PER FISSION (DEFAULT=215.0)

INPUT INT. PER Z MESH      1
ALL ENTRIES =              4

****************************************** S T O R A G E   I N F O R M A T I O N ******************************************


SMALL CORE (SCM) REQUIRED =   1879     MAXIMUM LCM ALLOWED =   5600
```

BANDS	JBLOC IN SCM (MAX)	KBLOC PLANES IN LCM (MAX)	IGBLOC GROUPS IN LCM (MAX)	SCM STORAGE	LCM STORAGE	NREAD STORAGE MODE (SEE MANUAL)
	4	4	3	1879	5503	0

********** S T O R A G E I N F O R M A T I O N **********

SMALL CORE (SCM) REQUIRED = 1879 MAXIMUM LCM ALLOWED = 5600

BANDS	JBLOC IN SCM (MAX)	KBLOC PLANES IN LCM (MAX)	IGBLOC GROUPS IN LCM (MAX)	SCM STORAGE	LCM STORAGE	NREAD STORAGE MODE (SEE MANUAL)
	4	4	2	1879	4351	1

********** S T O R A G E I N F O R M A T I O N **********

SMALL CORE (SCM) REQUIRED = 1879 MAXIMUM LCM ALLOWED = 5600

BANDS	JBLOC IN SCM (MAX)	KBLOC PLANES IN LCM (MAX)	IGBLOC GROUPS IN LCM (MAX)	SCM STORAGE	LCM STORAGE	NREAD STORAGE MODE (SEE MANUAL)
	4	4	1	1879	3199	1

********** S T O R A G E I N F O R M A T I O N **********

SMALL CORE (SCM) REQUIRED = 1879 MAXIMUM LCM ALLOWED = 5600

BANDS	JBLOC IN SCM (MAX)	KBLOC PLANES IN LCM (MAX)	IGBLOC GROUPS IN LCM (MAX)	SCM STORAGE	LCM STORAGE	NREAD STORAGE MODE (SEE MANUAL)
	4	2	1	1879	2047	2

********** S T O R A G E I N F O R M A T I O N **********

SMALL CORE (SCM) REQUIRED = 1879 MAXIMUM LCM ALLOWED = 5600

BANDS	JBLOC IN SCM (MAX)	KBLOC PLANES IN LCM (MAX)	IGBLOC GROUPS IN LCM (MAX)	SCM STORAGE	LCM STORAGE	NREAD STORAGE MODE (SEE MANUAL)
	4	1	1	1879	1471	2

ISTOP=2 PROBLEM HALTED AFTER STORAGE DETERMINATION.

FILE	I/O TIME (MICROSEC)	READS	WRITES
OUTPUT	30976	1	0
INPUT	187029	2	0

APPENDIX C

QUADRATURE SETS USED IN THREETRAN (hex,z)

The quadrature sets used in THREETRAN are the S_N built-in quadrature sets of TWOTRAN-II[5]. The sets possess complete (μ,η,ξ) symmetry with the quadrature ordinates constrained to be on (μ,η,ξ) levels. Here μ,η and ξ are the x,y and z direction cosines, respectively.

The following moments can be defined over a single octant of the unit sphere

$$M_{k\ell} = M_{\ell k} = \frac{2}{\pi} \int_0^1 d\xi \int_0^{\pi/2} d\theta \mu^k \eta^\ell,$$

$$\mu = \sqrt{1-\xi^2} \cdot \cos\theta, \quad \eta = \sqrt{1-\xi^2} \cdot \sin\theta$$

The S_N set integrates the M_{00}, M_{11}, and M_{02} (diffusion condition) moments exactly on an octant.

The number of quadrature points per octant is given by $n(n+2)/8$ where n is the quadrature order. The code contains the S_2, S_4, S_6, and S_8 quadrature sets. Values of μ,η, and ξ for the principle octant along with quadrature weights are indicated below for these four sets.

	Point,m	μ_m	η_m	ξ_m	Weight, W_m
S_2	1	0.577 350 27	μ_1	μ_1	0.125
S_4	1	0.301 638 78	μ_3	μ_1	0.041 666 67
	2	μ_1	μ_1	μ_3	W_1
	3	0.904 449 05	μ_1	μ_1	W_1

	Point, m	μ_m	η_m	ξ_m	Weight, W_m
S_6	1	0.230 091 94	μ_6	μ_1	0.021 180 82
	2	μ_1	μ_4	μ_4	0.020 485 85
	3	μ_1	μ_1	μ_6	W_1
	4	0.688 134 32	μ_4	μ_1	W_2
	5	μ_4	μ_1	μ_4	W_2
	6	0.945 576 76	μ_1	μ_1	W_1
S_8	1	0.192 327 47	μ_{10}	μ_1	0.014 598 56
	2	μ_1	μ_8	μ_5	0.011 656 90
	3	μ_1	μ_5	μ_8	W_2
	4	μ_1	μ_1	μ_{10}	W_1
	5	0.577 350 27	μ_8	μ_1	W_2
	6	μ_5	μ_5	μ_5	0.011 262 90
	7	μ_5	μ_1	μ_8	W_2
	8	0.793 521 78	μ_5	μ_1	W_2
	9	μ_8	μ_1	μ_5	W_2
	10	0.962 299 48	μ_1	μ_1	W_1

Notice that the arrangement of points is such that $\theta_1 > \theta_2 > \ldots . \theta_N$. This ordering is required by the sweeping routines ISWP1 and ISWP2 of the code.

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