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Summary Report

CAVEAT: A REVISED VERSION OF THE GENERAL PURPOSE MONTE CARLO PROGRAM, COHORT

Volume II - Users' Manual

by N. R. Byrn

August 1969

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CAVEAT - A REVISED VERSION OF THE GENERAL PURPOSE
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VOLUME II - USERS' MANUAL

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N. R. Byrn

August 1969

SPACE AND MILITARY SYSTEMS DIVISION
SCIENCE AND ENGINEERING GROUP
BROWN ENGINEERING COMPANY, INC.
HUNTSVILLE, ALABAMA

ABSTRACT

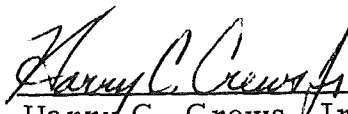
CAVEAT (COHORT with Air Model, Variable Dimensioning, Energy Deposition, And Time Dependence) is a general purpose Monte Carlo computer code for neutron, gamma, and secondary gamma radiation transport calculations. The code is written in the FORTRAN IV language and has been run on the IBM 7094, IBM 360, and UNIVAC 1108 computers. CAVEAT is a revised version of the COHORT program, with additional features such as time dependence, real atmosphere model for air transport, variable dimensioning, and, for third generation machines, a pass option which allows complete execution of a given problem, from source particle generation to fluence calculation.

The Users' Manual describes the input format of each of the CAVEAT routines, data file definition, and proper use of the pass option. Suggestions on the proper use of CAVEAT are included.

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1. INTRODUCTION

CAVEAT is a revised version of the Monte Carlo program, COHORT, and is capable of performing source generation, transport calculations, and analysis for neutrons, gammas, and secondary gammas. In addition to the features of the COHORT program, CAVEAT includes

- Real atmosphere (air) model
- Variable dimensioning
- Time dependence.

These features were included to better handle nuclear weapons problems and to optimize the use of available computer storage. Also included in CAVEAT are several programming and physics improvements and corrections.

Like COHORT, CAVEAT is actually a family of routines, each having a specific purpose in the Monte Carlo procedure. Figure 1-1 illustrates the interrelation of the different routines. The dashed lines used on the J01 block indicate that J01 is not always needed and that under certain conditions H01 data can be used directly in A01 and A02. A complete description of each of the CAVEAT routines is included in Volume I; however, an abbreviated description is given below.

1.1 S01 ROUTINE

The primary source routine S01 generates the primary source particles, either neutrons or gammas, which are to be tracked in the history routine (H01). Each source particle is described by the following parameters:

- Spatial coordinates X, Y, and Z
- Direction cosines A, B, and C
- Energy, E

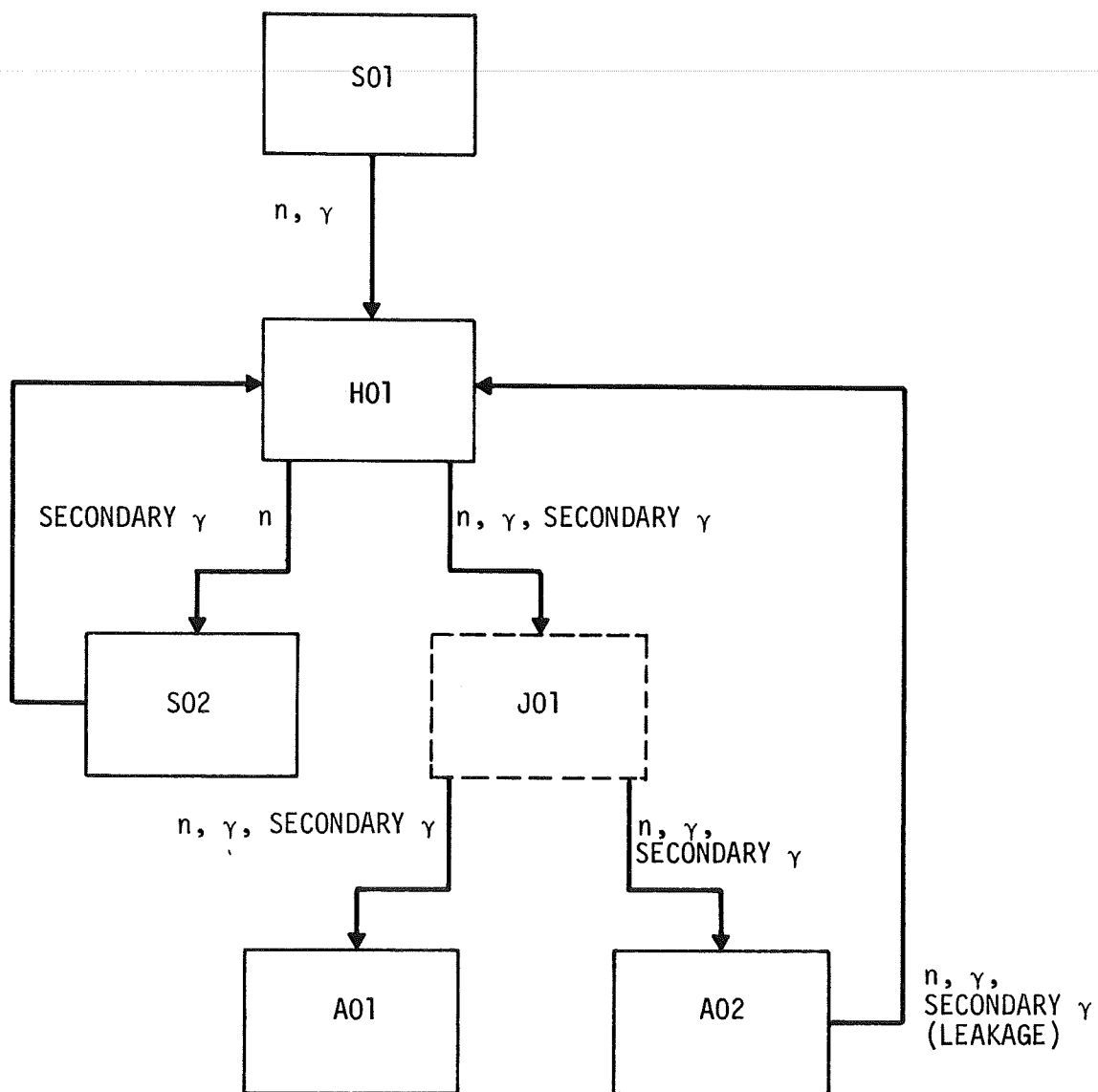


FIGURE 1-1. FLOW DIAGRAM OF CAVEAT ROUTINES

- Initial weight, W
- Time of emission, T
- Source region, NRI.

These parameters are written on a data file* and will be read by the H01 routine.

1.2 H01 ROUTINE

The H01 routine determines the life history of the source particles as they scatter through the input geometry, which is described by regions bounded by quadratic surfaces. Because of its large size, this routine has been written in three exclusive sections which are called by the main routine. These sections are

- Input and setup
- Tracking and computations
- Output.

In this way, it is possible to overlay the routine to reduce core storage requirements. Also, all arrays whose dimensions are problem-dependent have been variably dimensioned to conserve core storage.

The input and setup section of the H01 routine reads necessary data such as cross sections, nuclear data, problem geometry, "real" atmosphere description, importance sampling information, and problem size parameters. These problem size parameters are used to set up core storage for the variably dimensioned arrays.

The most important function of H01 is the tracking of source particles. The distance between source (or collision) and the subsequent collision is randomly selected from an exponential distribution. Absorption of a particle at a collision is not allowed; therefore, the weight of the particle is multiplied by the ratio of the macroscopic

*The term "data file" will refer to data recording media such as magnetic tape, disk, or drums as may be applicable for a given computer system.

total scattering cross section to the total cross section to compensate for the absorption probability at each collision. An option has been provided to allow for transport in a real atmosphere, which is described by 233 layers of air whose density varies exponentially. Time-of-flight computations are made, enabling calculation of time dependent responses; and the energy deposition is calculated for each geometric region. At each collision, the collision parameters are stored and, at regular intervals, the data are written on a data file for processing in the analysis codes. Tracking of individual particles is terminated whenever the particle has reached a state in which it is no longer considered important. The termination conditions include minimum weight, minimum energy, maximum time, and escape from the problem geometry.

1.3 S02 ROUTINE

The output from a neutron H01 run can be used to determine the distribution of a secondary gamma source if additional nuclear data are supplied. This calculation is made by the S02 routine that generates the 10 source parameters as described above for input into the H01 routine. The S02 routine is capable of generating two different sources

- The inelastic secondary gamma source
- The capture secondary gamma source.

However, by proper manipulation of the input data, any secondary gamma source (or even fission gammas) can be generated. Secondary gammas are generated on a material basis, which means that the gammas could be emitted from any nuclide in the collision material and not necessarily the scattering nuclide determined in the S02 routine. Special features have been written into S02 that allow secondaries to be generated at each collision or on a probabilistic basis. The problem-dependent arrays in S02 have been variably dimensioned for more optimum use of core storage.

1.4 J01 ROUTINE

Whenever the amount of nuclear data and cross sections become so great that the core storage required is greater than that available, an option has been provided in H01 and the analysis codes to break these data into energy supergroups, each containing a portion of the data. In this manner, it is possible to reduce the core storage required by the program at any given time, enabling the user to run larger and more complex problems. To facilitate handling of the data file on which the collision parameters are written, J01 sorts the data by energy supergroups. This sorting is accomplished by reading the collision data from the H01 data file, writing all collisions that occur in the first (highest) energy supergroup on another data file, then rereading the H01 data file, and writing the collisions in the second energy supergroup on the J01 data file. This process is continued until all data have been sorted into the proper supergroup. The J01 data file is then used as input to the analysis routines (A01 and A02). When all data can be placed in core storage at the same time, only one supergroup is used and the J01 routine is not required. Obviously, the most economical procedure as far as machine running time is concerned is to use the smallest number of energy supergroups possible.

1.5 A01 ROUTINE

The analysis routine, A01, estimates the scattered, unscattered (virgin), and total fluence at specified point detectors. The fluence at each detector is recorded in user-specified energy, time, polar angle, and azimuth angle intervals. By inputting fluence-to-dose conversion factors in each energy interval, the dose in each energy, time, polar angle, and azimuth angle also can be computed. The problem geometry is similar to the H01 geometry, and the nuclear data and cross sections are subsets of the H01 input. The collision data required by A01 includes

- Spatial coordinate
- Direction cosines of incoming particle

- Energy of incoming particle
- Weight of after collision particle
- Age of after collision particle
- Type of collision
- Scattering nuclide
- Region of scattering.

The scattered fluence estimate is made by summing the value of f in the following expression over all collision points and then normalizing as

$$f = W P \left[\frac{\exp(-\lambda)}{r^2} \right]$$

where

W - weight of after collision particle

P - probability of the particle being scattering through the angle between the direction before collision and the direction from the collision point to the detector

λ - number of mean free paths from the collision point to the detector

r - distance between collision point and detector.

The unscattered fluence is calculated by the above estimator; however, only source points are summed and P is set equal to $1/4\pi$.

1.6 A02 ROUTINE

The second analysis routine of CAVEAT, A02, estimates the average particle track length within each geometric region. Thus by dividing by the volume of the region, the fluence can be determined. The geometric regions used in A02 routine do not necessarily have to correspond to those regions of H01. The fluences are recorded for each region by user-specified energy and time intervals. The A02 routine also gives the angular distribution of current leaking out of the problem geometry and records the data on a specified data file. These

data can be used as input source data to the H01 routine. Because each collision point generates a leakage particle, an energy cutoff and a weight-dependent Russian Roulette scheme have been added to A02 to reduce the number of leakage particles. The A02 routine will not compute time-dependent fluences or fluxes and has not been revised to handle the real atmosphere model as have the H01 and the A01 routines.

1.7 PASS OPTIONS

In order to expedite the running of CAVEAT on certain computers (such as the IBM 360 and UNIVAC 1108), a pass option has been programmed into each routine so that several routines can be run in succession (e.g., for the IBM 360, the user can run S01, H01, A01 as job steps for a single job). Thus, unlike COHORT, it is possible to go from source generation to final answers such as fluence or doses in one run. This progression is accomplished by writing on data files that input data, for subsequent routines, that are normally generated as output data by some preceding routine. Then the pass option instructs the routine to accept the input data from the data file rather than from the input data cards. The routines that generate pass data are S01, H01, S02, J01, and A02. Appropriate explanation is given in the input instructions for each routine so that pass data can be both generated and/or accepted.

1.8 INPUT DATA FORMS

The input data that are entered by computer cards for a given routine are divided into two types

- Problem deck data
- Library data.

The problem deck data generally consist of data that will change for each different problem, such as type of source particles, number of

histories, materials, elements, regions, etc. The library data decks include cross section data, anisotropic scattering data, inelastic scattering data, and problem geometry description. With the exception of the problem geometry, library data are applicable to a number of different problems; usually only the control (or first) card of each library data deck is changed with each new problem. The problem deck data must precede any library data, but the routines have been written so that any input order for the library decks is acceptable. Unlike previous versions of COHORT, CAVEAT does not require card sequencing in any of its data decks.

Within a given data deck, each card or set of cards is denoted by an alphabetic identifier. For each set of cards, a formula is given to compute the number of cards in that set. For example, if the number of elements (or nuclides), NEL, in a given problem is 15 and the card format is 6E10.4, then the number of input cards for inputting the atomic weights of these elements is given by

$$\text{No. Cards} = 1 + \text{INT}[(\text{NEL} - 1)/6]$$

where INT is the truncation function. Hence

$$\begin{aligned} \text{No. Cards} &= 1 + \text{INT}[(15 - 1)/6] \\ &= 1 + \text{INT}(2.333\dots) \\ &= 1 + 2 = 3 \end{aligned}$$

Of these three cards, the first two cards will contain six entries and the third card will contain three.

When inputting doubly dimensioned arrays, [e.g., $\text{DN}(I, J)$], a change in the slower changing index will require that the data begin on a new card. For example, if the element number subscript, J, runs

through the element range from 1 to NEL (= 15) everytime the material subscript, I, takes on any value from 1 to NMAT (= 5), then the number of cards required to input the array DN in a 6E10.4 format is

$$\begin{aligned}\text{No. cards} &= \text{NMAT} * \{1 + \text{INT} [(15 - 1)/6]\} \\ &= 5 * 3 \\ &= 15.\end{aligned}$$

Note that each third card will contain only three entries.

Card A of each library deck has an identification symbol input. This symbol is for the benefit of the user and does not affect the running of the problem. The symbol is placed to the far right of the input card so that the beginning of each library can be detected easily in the card image printout.

Many of the CAVEAT routines have an intermediate printout option, to be used for checkout and debugging. Because of the enormous amount of printout produced, this option should be used only on problems of 50 histories or less.

2. S01 PRIMARY SOURCE ROUTINE INPUT DATA

The ultimate purpose of S01 is to place on a specified data file the 10 parameters that define each primary source particle for the history routine, H01. Fourteen sets of these parameters form one data record. All records are of this form with the exception of the first and last record written on the data file. The first record is a bookkeeping record that includes the source tape number, the number of records on the tape, the number of data sets on the last record, and other pertinent information. However, only the source tape number is read by H01, which checks this number against input data to determine whether the correct source data have been input. The last record also contains the data sets, but not necessarily 14 of them as in the previous data records.

The S01 data file assignments are given below:

<u>Data File Symbol</u>	<u>Logic Number</u>	<u>Purpose</u>
NT5	5	System input
NT6	6	System output
NT8	8	S01 pass information
JJJ5	11	Source data

The logic number of each data file can be changed easily by changing the appropriate FORTRAN assignments, which are located at the beginning of the S01 main program of the FORTRAN source deck. Of course, the source data on JJJ5 should be saved for input into H01; and if the pass option is used, then NT8 should also be saved. For runs in which the pass option is not used, it would probably be advisable to set up NT8 as a scratch unit, even though this unit will not be used.

2.1 S01 PROBLEM DECK

The problem deck data cards constitute the first part of the S01 data deck. This deck will always include two cards, A and B, and will contain Card C only if the parameter IC (in Card A) is equal to 6. The input format for each input item is specified in Table 2-1.

TABLE 2-1. S01 PROBLEM INPUT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	N	Number of source particles to be generated. Must be less than the largest integer number for the machine used.
	6-10/I5	NG	Type of particle NG = 0, neutron NG = 1, gamma
	11-15/I5	IC	Source coordinate option IC = 0, point source (located at center of coordinate system) IC = 1, rectangular volume, area, or line source IC = 2, spherical volume source IC = 3, cylindrical volume source IC = 4, circular area source (z = 0 plane) IC = 5, spherical surface source (angular distribution outward radially) IC = 6, cylindrical surface source (angular distribution outward radially)
	16-20/I5	ID	Direction cosine option ID = 0, direction cosine defined as in IC options 5 or 6 ID = 1, monodirectional source ID = 2, isotropic source ID = 3, anisotropic source (input polar angle θ distribution, azimuthal angle evenly distributed between 0 and 2π) ID = 4, anisotropic source (input both polar and azimuthal angular distributions) ID = 5, isotropic in 2π space (positive x direction) ID = 6, isotropic in 2π space (negative x direction) ID = 7, isotropic in 2π space (positive y direction) ID = 8, isotropic in 2π space (negative y direction) ID = 9, isotropic in 2π space (positive z direction)

TABLE 2-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
A			ID = 10, isotropic in 2π space (negative z direction)
	21-25/I5	IE	IE = 1, monoenergetic source energy IE = 2, input energy spectrum (Library 9)
	26-30/I5	IT	IT = 1, all source particles born at time T (see Card B below) IT = 2, input time spectrum (Library 10)
	31-35/I5	ITAPE	Identification number for output source data file
	36-40/I5	IO	IO = 0, no listing of input data cards is given IO = 1, all input data cards are printed
	41-45/I5	LIST	LIST = 0, no intermediate printout is given LIST = 1, intermediate printout is given
	46-50/I5	IP	IP = 0, no pass information is written IP = 1, pass information for use in H01 is written on data file NT8
	51-60/I10	NRI	Input random number (should be odd positive integer, and less than the largest integer the computer can accept)
	61-65/IX,A4	PID	Problem identification symbol
	66-70/I5	NO	Problem number
B	1-10/E10.4	E	Energy of monoenergetic source if IE = 1 (leave blank if IE = 2)
	11-20/E10.4	R	Radius of disk, sphere, or cylinder source when IC = 2, 3, 4, 5, or 6 (leave blank if IC = 0 or 1)

TABLE 2-1 - Concluded

Card(s)	Field/Format	Input Symbol	Description
B	21-30/E10.4	Z3	Lower z plane for end of cylindrical source when IC = 3 or 6; otherwise leave blank
	31-40/E10.4	Z4	Upper z plane for end of cylindrical source when IC = 3 or 6; otherwise leave blank
	41-50/E10.4	T	For IT = 1, time of source particle birth (in seconds). If IF $\neq$ 1, leave blank
C			(Omit card if IC $\neq$ 6)
	1-10/E10.4	THETA1	Minimum angle (radians) to corner of cylindrical source when IC = 6
	11-20/E10.4	THETA2	Maximum angle (radians) to corner of cylindrical source when IC = 6

2.2 S01 LIBRARY ONE

Library One is needed only when $IC = 1$. The data in Library One give information for dividing a rectangular volume, area, or line source into subregions and the fraction of source particles to be generated in each subregion. The rectangular volume source degenerates into an area source whenever the upper and lower planes of a given direction (x , y , or z) for all subregions are set equal to the same value. By setting two sets of upper and lower planes equal, the volume source is degenerated to a line source. For example, if all upper and lower z planes are set equal to 0, then the source becomes a rectangular z -plane (i. e., perpendicular to the z -axis) at $z = 0$. If in addition, the upper and lower y planes are set equal to -10, then the source is a line source in the z -plane, parallel to the x -axis at $y = -10$. (The further degeneracy to a point is handled by $IC = 0$.) Table 2-2 contains the necessary information for inputting data to generate rectangular volume, area, or line sources.

TABLE 2-2. S01 LIBRARY ONE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 1)
	6-10/I5	I	Number of subregions into which the source region is divided
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(I - 1)/6]$
	1-60/6E10.4	P(M)	Fraction of source particles to be generated in subregion M (M = 1, I)
C			Number of cards = I
	1-10/E10.4	X1(M)	Lower x plane for subregion M
	11-20/E10.4	X2(M)	Upper x plane for subregion M
	21-30/E10.4	Y1(M)	Lower y plane for subregion M
	31-40/E10.4	Y2(M)	Upper y plane for subregion M
	41-50/E10.4	Z1(M)	Lower z plane for subregion M
	51-60/E10.4	Z2(M)	Upper z plane for subregion M
			Items X1(M), X2(M), Y1(M), Y2(M), Z1(M), and Z2(M) describe one subregion so there should be one card containing these items for each subregion (M = 1, I)

2.3 S01 LIBRARY TWO

Library Two should be omitted unless $IC = 2$ or 4 . The data in Library Two give the radial distribution for either a spherical volume source ($IC = 2$) or a circular disk source ($IC = 4$).

The distribution in any given subregion is assumed to be uniform with area for $IC = 4$ and with volume for $IC = 2$. This means that within any spherical volume shell, the density (in source particles/unit volume) is constant. Likewise, for $IC = 4$, the density (in source particles/unit area) is the same throughout a given circular disk ring (or subregion). The format to be used in making up a Library Two deck is shown in Table 2-3.

TABLE 2-3. S01 LIBRARY TWO DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 2)
	6-10/I5	I	Number of radial subregions into which the source will be divided (≤ 999)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(I - 1)/6]$
	1-60/6E10.4	P(M)	Fraction of source particles to be generated in subregion M ($M = 1, I$)
C			Number of cards = $1 + \text{INT} (I/6)$
	1-60/6E10.4	X1(M)	Radii bounding the subregions, beginning with the smallest ($M = 1, I + 1$)

2.4 S01 LIBRARY THREE

If $IC = 3$, then Library Three is required input. This library describes the distribution of source particles in a cylindrical volume. It is required that the radial and axial distributions be independent, so that they can be input as one-dimensional arrays. The input format for Library Three is given in Table 2-4. Note that the product, $I * J$, of the input variables in Card A is the total number of subregions into which the cylindrical source is divided.

TABLE 2-4. S01 LIBRARY THREE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 3)
	6-10/I5	I	Number of disk sections into which the cylindrical source is cut by z-planes (≤ 999)
	11-15/I5	J	Number of cylindrical sections into which the cylindrical source is cut (≤ 999)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(I - 1)/6]$
	1-60/6E10.4	P(M)	Fraction of source particles to be generated between two consecutive z-plane ($M = 1, I$)
C			Number of cards = $1 + \text{INT} (I/6)$
	1-60/6E10.4	Z1(M)	z-planes dividing the cylindrical source where $z - Z1(M) = 0$ ($M = 1, I + 1$)
D			Number of cards = $1 + \text{INT} [(J - 1)/6]$
	1-60/6E10.4	Q(M)	Fraction of source particles to be generated between two consecutive cylindrical boundaries ($M = 1, J$)
E			Number of cards = $1 + \text{INT} (J/6)$
	1-60/6E10.4	X1(M)	Radii bounding cylindrical sections ($M = 1, J + 1$)

2.5 S01 LIBRARY FOUR

Library Four, which is omitted unless $IC = 5$, describes a source distributed over the surface of a sphere. The angular distribution for this source will be dependent upon the distribution of the source points over the surface of the sphere, since the direction of a given particle will be assumed radially outward from the center of the sphere through the source coordinates. Hence this source is equivalent to a point source with a uniform distribution azimuthally (but not necessarily uniform in the polar angle), where the particles have been transported through a void to the surface of the sphere. The input format for this library is given in Table 2-5.

TABLE 2-5. S01 LIBRARY FOUR DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 4)
	6-10/I5	I	The number of subdivisions on the spherical surface formed by the intersection of the sphere with cones symmetrical about the z-axis (≤ 999)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(I - 1)/6]$
	1-60/6E10.4	P(M)	The fraction of source particles leaking through the surface of the sphere within the Mth subdivision ($M = 1, I$)
C			Number of cards = $1 + \text{INT}(I/6)$
	1-60/6E10.4	Z1(M)	The half angle of the cones (or polar angles) in radians whose intersections with the sphere describe the subdivisions ($M = 1, I + 1$)

2.6 S01 LIBRARY FIVE

Library Five, which is omitted unless $IC = 6$, describes a source distributed over the surface of a cylinder. The angular distribution for this source will be dependent upon the distribution of the source points over the surface of the cylinder, since the direction for a given particle will be assumed radially outward from the center of the cylinder through the point on the curved surface of the cylinder giving the source location. This source is equivalent to an anisotropic point source whose particles are transported in a void to the curved surface of the cylinder. No particles are allowed to escape through the top and bottom disk surfaces. The cylindrical surface source is subdivided by the intersections of the cylinder with cones symmetric about the z -plane having vertices at the origin. The input format for Library Five is given in Table 2-6.

TABLE 2-6. S01 LIBRARY FIVE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 5)
	6-10/I5	I	Number of subdivisions of the cylindrical surface source (≤ 999)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(I - 1)/6]$
	1-60/6E10.4	P(M)	Fraction of source particles leaking through the cylindrical surface within the Mth subdivision ($M = 1, I$)
C			Number of cards = $1 + \text{INT} (I/6)$
	1-60/6E10.4	X1(M)	Half angles (radians) of the cones whose intersection with the cylindrical surface from the subdivisions ($M = 1, I + 1$)

2.7 S01 LIBRARY SIX

For a monodirectional source, (ID = 1), Library Six is used to input the direction cosines. Only two input cards are required. The required input format is given in Table 2-7.

TABLE 2-7. S01 LIBRARY SIX DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 6)
	73-76/A4	FLIB	Library identification
B	1-10/E10.4	ALPHA	Cosine of angle between the source direction and the positive x axis
	11-20/E10.4	BETA	Cosine of angle between the source direction and the positive y axis
	21-30/E10.4	GAMMA	Cosine of angle between the source direction and the positive z axis

2.8 S01 LIBRARY SEVEN

When ID = 3, Library Seven data are input, giving the angular distribution of an anisotropic source that has a specified polar angle distribution and a uniform azimuthal distribution. Note that the cosine of the polar angle (measure from the positive z axis) is the required input in Card Set C and not just the angle. Table 2-8 gives the required input data format for Library Seven.

TABLE 2-8. S01 LIBRARY SEVEN DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 7)
	6-10/I5	I	Number of polar angle intervals used to describe the anisotropic source (≤ 49)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(I - 1)/6]$
	1-60/6E10.4	CP(M)	Fraction of source particles emitted through the Mth polar angle interval ($M = 1, I$)
C			Number of cards = $1 + \text{INT} (I/6)$
	1-60/6E10.4	GAM(M)	Cosines of the angles bounding the polar angle intervals ($M = 1, I + 1$)

2.9 S01 LIBRARY EIGHT

Library Eight, which is input when ID = 4, gives the polar and azimuthal distribution for an anisotropic source. It is assumed that the polar and azimuthal distributions are dependent, that the polar angles are measured from the positive z axis, and that the azimuthal angles are measured from the positive x axis.

Although the azimuthal intervals can be different for each polar interval, the number of azimuthal intervals must be the same in each polar interval. The data format for Library Eight is given in Table 2-9. Note that the cosines of the polar angles are input, whereas the azimuthal angles (in radians) are required.

TABLE 2-9. SOI LIBRARY EIGHT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 8)
	6-10/I5	K	Number polar angle intervals used to describe the anisotropic source distribution (≤ 49)
	11-15/I5	L	Number of azimuthal angle intervals in each polar interval (≤ 49)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(K - 1)/6]$
	1-60/6E10.4	CP(M)	Fraction of source particles being emitted through the Mth polar angle interval ($M = 1, K$)
C			Number of cards = $1 + \text{INT} (K/6)$
	1-60/6E10.4	GAM(M)	Cosines of angles bounding the polar angle intervals ($M = 1, K + 1$)
D			Number of cards = $L * \{1 + \text{INT} [(K - 1)/6]\}$
	1-60/6E10.4	DCP(M,N)	Fraction of the total particle emitted through the Mth polar angle interval that emerge through the Nth azimuthal angle interval. N is the more rapidly varying index ($N = 1, L; M = 1, K$)
E			Number of cards = $(L + 1) * \{1 + \text{INT} [(K - 1)/6]\}$
	1-60/6E10.4	PHI(M,N)	Azimuthal angles (radians) bounding the Nth azimuthal interval in the Mth polar angular interval. N is the more rapidly varying index ($N = 1, L + 1; M = 1, K$)

2.10 S01 LIBRARY NINE

For IE = 2, the energy spectrum is input by Library Nine. The energy units (eV, keV, MeV) are arbitrary but must be consistent throughout all of the CAVEAT routines. Table 2-10 presents the format to be used in making up a Library Nine deck.

TABLE 2-10. S01 LIBRARY NINE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 9)
	6-10/I5	K	Number of energy groups used to define the spectrum (≤ 49)
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT} [(K - 1)/6]$
	1-60/6E10.4	ECP(M)	Fraction of the source particles emitted in the Mth energy interval (M = 1, K)
C			Number of cards = $1 + \text{INT} (K/6)$
	1-60/6E10.4	EG(M)	Energies bounding the energy intervals (M = 1, K + 1)

2-11 S01 LIBRARY TEN

Library Ten, input when IT = 2, describes the time spectrum of the source particles. Since H01, A01, and A02 calculate time in seconds, the unit for the input spectrum should be seconds. Note that the cumulative probability is required and not the fraction of particles generated in each interval. The input data format is given in Table 2-11. Since the cumulative probability is required for TP(I), in Card Set C, then $TP(K) = 1.0$.

TABLE 2-11. S01 LIBRARY TEN DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 10)
	6-10/I5	K	Number of time intervals used to define the time spectrum
	73-76/A4	FLIB	Library identification
B			Number of cards = $1 + \text{INT}(K/6)$
	1-60/6E10.4	TG(I)	Times (seconds) which bound the time intervals ($I = 1, K + 1$)
C			Number of cards = $1 + \text{INT}[(K - 1)/6]$
	1-60/6E10.4	TP(I)	Probability that a particle is born in or before the Ith time interval ($I = 1, K$)

3. H01 HISTORY ROUTINE INPUT DATA

The H01 routine determines the history of the input source particles as they scatter through the problem geometry. The primary output from H01 is a data file which contains data on each collision of the particles. Included in the printed output is an energy deposition table. This table is normalized by the number of histories parameter, NHIST.

Input data consist of both the problem deck and library decks, plus the input source data and, if the pass option is used, the pass data, which resides on an input data file. Any given problem may require several libraries of the same type; e. g. , a Library Four is required for each energy supergroup for every element. The number of different libraries needed for each library type is given in the library description. Routine H01 calculates the total number of libraries needed and compares this number to the NLIB parameter given in the problem deck. If these two numbers do not agree, then an error print is given and the problem is terminated. Using other parameters given in the problem deck, the required core storage for each variably dimensioned array is computed. A table showing the storage requirements and entry points in the common array (Array name-S) is printed in the output.

The H01 data file assignments are given below:

<u>Data File Symbol</u>	<u>Logic Number</u>	<u>Purpose</u>
NT5	5	System input
NT6	6	System output
NT8	8	Scratch
NT10	10	Source input
NT11	11	Collision data storage (No. 1)
NT13	13	Collision data storage (No. 2)
NT15	15	Cross section data
NT16	8	Source pass data (input)
NT17	8	H01 pass data (output)

The logic number of each data file is assigned in a BLOCK DATA sub-program and thus can be changed easily for compatability with other computer facilities. Except for checkout runs, the collision data files (NT11 and NT13) and the cross section data file (NT15) should be saved for input into other CAVEAT routines. If the source pass data are to be used, then NT16 should be given a unique logic number; otherwise, NT16 is not used and can be assigned any number (e. g. , the same logic number as the scratch file). H01 pass data are always written on some data file. If this pass option is used, NT17 also should be given a unique logic number and saved. If the pass data are not desired, then NT17 should be assigned the same logic number as NT8.

The overlay structure for H01 is shown in Figure 3-1. MAIN, which calls the other overlays into core, XCLOCK, and BLOCK DATA, resides in core at all times during execution of a problem. The first overlay called is controlled by SETIN. When this overlay is in core, the variably dimensioned arrays are set up and the input data are read and stored. Next, MAIN calls HIGENE, which controls the history tracing calculations. Finally, the output subroutine DAWN is called into core. All three of these overlays are completely independent; i. e. , no subroutine in one overlay is called by a subroutine in another overlay. The H01 routine is written so that each overlay is called only once.

3.1. H01 PROBLEM DECK

The problem deck of H01 contains the information needed to set up core storage requirements for a particular problem, plus other problem dependent data. The input formats are specified in Table 3-1. Note that in Card A the maximum size of the common block must be input. This value should be at least as large as that needed to store all

variably dimensioned arrays but must not exceed core storage capability. In Card B, many of the parameters will not be known until the data tables for Libraries One, Two, Four, Six, and Seven are determined.

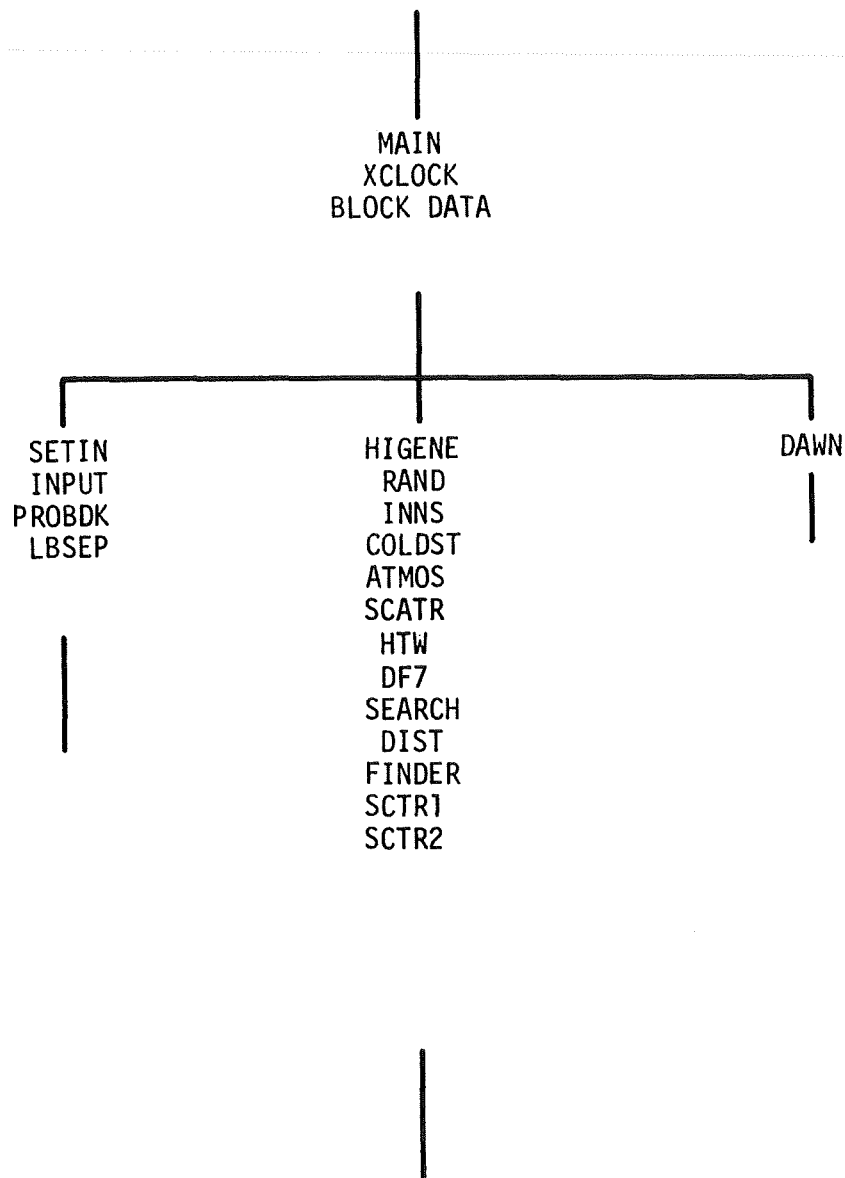


FIGURE 3-1. HOI OVERLAY STRUCTURE

TABLE 3-1. HOI PROBLEM INPUT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	MSIZE	Maximum size of common block for S-Array (machine dependent)
	11-20/I10	NRI	Initialization number for random number sequence (must not exceed largest integer number for machine)
	21-30/I10	IO	Option that controls the listing of input data cards and intermediate print IO = 0, no listing is given IO = 1, only the problem deck is listed IO = 2, both the problem deck and library deck are listed IO = 3, intermediate printout of each history is given as output
	31-35/1X,A4	PID	Problem identification symbol
	36-40/I2,3X	NN	Problem number
	41-80/10A4	ID	Problem description
B	1-5/I5	NRG	Type of particles: NRG = 0 - neutrons NRG = 1 - primary gammas NRG = 2 - secondary gammas
	6-10/I5	NSG	Number of energy supergroups
	11-15/I5	NREG	Number of geometric regions
	16-20/I5	NEL	Number of elements (and/or nuclides)
	21-25/I5	NMAT	Number of materials
	26-30/I5	NBD	Number of boundaries
	31-35/I5	MBD	Maximum number of boundaries needed to define any one region {i.e., Max [NB (K), K = 1, NREG]}
	36-40/I5	MEP	Maximum number of energy data points for any energy supergroup [i.e., Max (NENEGY)] in Library 4

TABLE 3-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
B	41-45/I5	NMESH	*Maximum number of incident energies for exciting various levels of the target nucleus for any element and for any supergroup (Library 6) {i.e., Max [NMESH(J), J = 1, NEL]}
	46-50/I5	MEXP	*Maximum number of excitation levels for any element in any energy group (Library 6) - {i.e., Max [NEXP(J), J = 1, NEL for all supergroups]}
	51-55/I5	NELM	*Number of elements for which Library 6 data (i.e., Cards B, C, and D) are input (i.e., those elements in energy supergroup 1 for which INEO(J) $\neq$ 0)
	56-60/I5	MCROS	*Maximum number of incident-energy groups for which scattering probabilities are input for any element in any energy supergroup (Library 7) {i.e., Max [NCROS(J), J = 1, NEL for all supergroups]}
	61-65/I5	MEPI	*Maximum number of equal scattering probability intervals for any element in any energy supergroup (Library 7) {i.e., Max [NEPI(J), J = 1, NEL for all supergroups]}
	66-70/I5	MNEL	*Number of elements for which Library 7 are input
C	1-5/I5	ISRCTP	Source data file option: ISRCTP = 0, input source parameters available on data file. (When a leakage data file is used, all leakage surfaces must be bounded by inside regions.) ISRCTP = 1, source data on card input. (Source data given in Library 3.)
	6-10/I5	MTPREC(1)	Number of records on source (or leakage) data file. [If MTPREC(1) is negative, the values of the number of records on the source data file will be input from the pass option parameters on NT16]

*Set equal to 0 for primary and secondary gamma problems

TABLE 3-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
C	11-15/I5	MTPREC(2)	Number of source (or leakage) particles on last record. Leave blank if MTPREC(1) < 0
	16-20/I5	NHIST	Number of histories
	21-25/I5	NRCD	Maximum number of records to be written on any collision data file. (A function of the amount of space available on the NT11 data file. Each record has 440 words)
	26-30/I5	IHTAPE	Identification number of the first collision data file to be generated
	31-35/I5	NTAP	Cross section option: NTAP = 0, cross sections input on cards NTAP = 1, cross sections input on data file
	36-40/I5	IQID	Cross section data file identification number (if NTAP = 0, this number is written on the generated cross section data file for later identification. If NTAP = 1, this number is checked against the identification number on the input data file)
	41-45/I5	MAXCOL	Maximum number of collisions per particle within a given energy supergroup
	46-50/I5	NLIB	Number of libraries input on cards for this problem (This number is checked against the number actually input.) Consider each library type 4, 6, and 7 as separate libraries even though there may be several of the same type.
	51-55/I5	NCBW	Number of collision records to be written before a time interval print is given
	56-60/I5	NER	Specifies the energy units of the input data, which must be consistent for a given problem NER = 1: MeV energy units NER = 2: KeV energy units NER = 3: eV energy units

TABLE 3-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
C	61-65/I5	IAIR	If IAIR is nonzero, the real air density table is needed for air model. If IAIR is zero, no air model is used.
	66-70/I5	MATAIR	IAIR $\neq$ 0: Material number is DN array (see Card I below) in which the atmospheric concentrations are given. IAIR = 0: Leave blank.
D	1-10/E10.0	X0	Source coordinate translation distance in the x-direction
	11-20/E10.0	Y0	Source coordinate translation distance in the y-direction
	21-30/E10.0	Z0	Source coordinate translation distance in the z-direction
	31-40/E10.0	DMAX	Maximum distance restriction. (Tracking of particles is terminated when their distance from the origin exceeds DMAX)
	41-50/E10.0	EMIN	Minimum energy termination value
	51-60/E10.0	WMIN	Minimum weight termination value
	61-70/E10.0	TMAX	Maximum time restriction. (Tracking of the particle is terminated when their time in seconds exceeds TMAX)
E	1-10/E10.0	ELD	Energy below which energy deposition is neglected
	11-20/E10.0	ELOW	*Upper limit of energy range at which the target nucleus velocity will be considered in the scattering process (ELOW $\geq$ ETM)
	21-30/E10.0	ETM	*Energy at which neutron scattering is assumed isotropic in laboratory system with no energy loss
	31-40/E10.0	TEMP	*Temperature in $^{\circ}$ K for the target nucleus when ELOW $\neq$ 0

*Leave blank for gamma problems

TABLE 3-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
E	41-50/E10.0	RR	Russian Roulette parameter for terminating a particle with weight less than or equal to WMIN
	51-60/E10.0	EPSL	Distance to be added vectorially to a particle's coordinates to move the particle off of a boundary. (When EPSL is added to the maximum distance to any boundary, the distance should change at least in the eighth significant figure.)
F			Number of Cards = $1 + \text{INT}[(\text{NSG}-1)/3]$
	1-60/6E10.0	EGRP(K)	Lower energy bound for energy super-group K
		EMAX(K)	Upper energy bound for energy super-group K
			Input EGRP(1), EMAX(1), EGRP(2), EMAX(2), . . . from K = 1 to NSG
G			Number of Cards = $1 + \text{INT}[(\text{NEL}-1)/6]$ for neutron problems = 0 for gamma problems
	1-60/6E10.0	ESI(K)	Energy at which elastic scattering becomes isotropic in the center-of-mass system for element K (K = 1, NEL)
H			Number of Cards = $1 + \text{INT}[(\text{NEL}-1)/6]$
	1-60/6E10.0	ATWT(K)	Atomic weight of element K (K = 1, NEL)
I			Number of Cards = $\text{NMAT} * \{1 + \text{INT}[(\text{NEL} - 1)/6]\}$
	1-60/6E10.0	DN(J,K)	Density of element K in material J or concentration for material MATAIR when using the air model (IAIR $\neq$ 0). K varies most rapidly (K = 1, NEL; J = 1, NMAT)

TABLE 3-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
J			Number of Cards = $1 + \text{INT}[(\text{NREG}-1)/14]$
	1-70/14I5	NB(K)	Number of boundaries defining region K (K = 1, NREG) as defined in Library 2
K			Number of Cards = $1 + \text{INT}[(\text{NREG}-1)/14]$
	1-70/14I5	MATREG(K)	Material number (as defined by DN array) in region K (K = 1, NREG). Set void regions equal to 0.
L	1-10/2X, 2A4	T(K)	Label of source data file (usually SOURCE) K = 1, 2
	11-15/I5	ISTAP	Input source data file number
M			Number of Cards = $1 + \text{INT}[(\text{NEL}-1)/6]$ for neutron problem (ELOW > 0) = 0 for neutron problem (ELOW = 0) = 0 for gamma problem
	1-60/6E10.0	ASTAR(K)	Effective Atomic Weight for element K (K = 1, NEL) when using the low energy scattering routine
N			Number of Cards = $1 + \text{INT}[(\text{NEL}-1)/14]$ for neutron problem = 0 for gamma problem
	1-70/14I5	LB6(K)	LB6(K) = 0: No Library 6 data are input for the Kth element for any energy supergroup [INEO(K) = 0] LB6(K) = N: Library 6 data are input for the Kth element in at least one of the energy supergroups [INEO(K) ≠ 0] N is an integer sequencing of those elements for which LB6(K) ≠ 0 K = 1, NEL (e.g., if Library 6 data are needed for the second and fourth elements of a 4-element problem, then: LB6(1) = 0, LB6(2) = 1, LB6(3) = 0, LB6(4) = 2)

TABLE 3-1 - Concluded

Card(s)	Field/Format	Input Symbol	Description
0			Number of Cards = $1 + \text{INT}[(\text{NEL}-1)/14]$ for neutron problem = 0 for gamma problem
	1-70/14I5	LB7(K)	LB7(K) = 0: No Library 7 is input for the Kth element for any energy supergroup LB7(K) = N: A Library 7 is input for the Kth element in at least one of the energy supergroups. N is an integer sequencing of those elements for which LB7(K) $\neq$ 0. K = 1, NEL.
P			Number of Cards = 233 if IAIR > 0 and NTAP = 0 = 0 otherwise
	1-54/3D18.10	YM(K) XLRHO(K) F(K)	Real atmospheric density table for 0 to 466 km at 2-km increments

3.2 H01 LIBRARY ONE

Library One describes the boundaries that are used to specify the different geometric regions in a CAVEAT problem. Normally, this problem geometry will be identical in H01, A01, and A02; therefore, this library will also be used in A01 and A02 runs. However, the problem geometries are not required to be identical. The format to be used for Library One is given in Table 3-2.

TABLE 3-2. H01 LIBRARY ONE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 1)
	6-10/I5	NBD	Number of boundaries described in Library One (same as NBD in Card B of problem deck)
	41-80/10A4	LID	Library identification
B			Number of cards = NBD
	1-5/I5	K	Boundary number (boundaries can be input in any order, but $K \leq NBD$)
	6-10/I5	IBT(K)	Type of boundary for boundary K
			IBT(K) = 1: Sphere, Ellipsoid or Hyperboloid $(X-XF)^2 + (Y-YF)^2 - AF(Z-ZF)^2 - CF = 0$
			IBT(K) = 2: Paraboloid $(X-XF)^2 + (Y-YF)^2 - AF(Z-ZF) = 0$
			IBT(K) = 3: Cone $[(X-XF)^2 + (Y-YF)^2]^{1/2} - AF(Z-ZF) = 0$
			IBT(K) = 4: Cylinder $[(X-XF)^2 + (Y-YF)^2]^{1/2} - AF = 0$
			IBT(K) = 5: Plane containing Z axis $\theta - AF = 0$ (AF in radians)
			IBT(K) = 6: Plane perpendicular to Z axis $Z - AF = 0$
			IBT(K) = 7: Plane perpendicular to X axis $X - AF = 0$
			IBT(K) = 8: Plane perpendicular to Y axis $Y - AF = 0$
			IBT(K) = 9: Plane arbitrarily oriented $AF \cdot X + ZF \cdot Y + CF \cdot Z - XF = 0$
	11-20/E10.4	AF(K)	Curve fit coefficients for boundary K
	21-30/E10.4	ZF(K)	
	31-40/E10.4	CF(K)	
	41-50/E10.4	XF(K)	
	51-60/E10.4	YF(K)	

3.3 H01 LIBRARY TWO

In Library Two, the different geometric regions of the problem geometry are defined by giving the boundary number of those boundaries surrounding a particular region. The material within a given region will be taken to be a homogenous mixture. If the problem geometry is identical for the A01 and/or A02 run, then this library can be used in those routines. Since H01 computes energy deposition and A02 computes track lengths within regions, consideration should be given in choosing the size that gives the best statistical results. Each source particle is checked to determine the region in which it falls. Since S01 sets the source region number to 1, then, if possible, Region 1 should be the source region. However, if more than one source region is needed, then the lowest numbered regions should be used, except for Region 2. Region 2 is used for the outside region; i. e., the volume outside of the problem geometry. All other regions are inside regions, since they are completely bounded. The CAVEAT program assumes that any particle leaking into Region 2 will not reenter the problem geometry and hence will terminate the tracking of that particle. Region 2 is also special in the fact that it is not defined in Library Two, since the boundaries of Library One cannot completely define this region. The code senses that a particle is in Region 2 by checking the $MPR(K, N)$ parameter, which gives the most probable region into which a particle will enter, upon leaving the Nth region across boundary K. If $MPR(K, N)$ is 2, then the particle is assumed to be entering Region 2. The material in Region 2 is void, designated by a "0" in the MATREG array. Inside regions should be designated in such a manner that if a particle exits the region through a given boundary into Region 2, then any other particle exiting the region through that boundary cannot enter any region than Region 2. Inside regions can be listed in any order. However, since the code searches cyclically (beginning at MPR) to determine the next region a particle enters, judicious selection of the MPR's and the region numbers can reduce computation time.

Boundaries used in describing a region should not extend into the region. For example, consider the cross-sectional area of the cylindrical region shown in Figure 3-2. Boundaries 2, 3, and 5 are Z-planes (planes perpendicular to the Z-axis) and Boundaries 1 and 4 are cylinders about the Z-axis. A particle traveling in the direction shown in Figure 3-2 will intersect Boundary 4 before Boundary 3, and the code will incorrectly determine that the particle has exited from the region. This error can be prevented by extending either Boundary 3 or 4, as shown by the dashed line, thus dividing the cylindrical region into two correctly defined regions. The same type of geometry error can occur (and often does) when defining regions such as that depicted in Figure 3-3. If the cylindrical region with a hemispherical top is described by using only Boundaries 1, 2, and 3, then the particle shown will "falsely" exit the region when it intersects with the bottom half of Boundary 1, which is a sphere. To correct the geometry error, the region should be separated into two regions by Boundary 4, which is a Z-plane.

Another common geometry error is shown by the "blowup" in Figure 3-3. This error is caused by the inability of the computer to have curved surfaces intersect exactly. Thus small undefined regions, such as cross-hatched area in the blowup, are formed. This problem can be overcome by extending vectorially the path of the particle by a distance of EPSL, which is specified in the problem deck.

The final geometry error that should be avoided in setting up the problem geometry is shown in Figure 3-4. This error is caused by a reflected region appearing in the geometry. Figure 3-4 depicts an annular region bounded on the bottom by Boundary 1, a Z-plane, on the top by Boundary 4, an ellipsoid, and on either side by the two concentric cylinders, 2 and 3. This region is completely defined for any particle inside of the region. However, any particle inside the shaded region meets the geometry requirements to be inside of the above defined

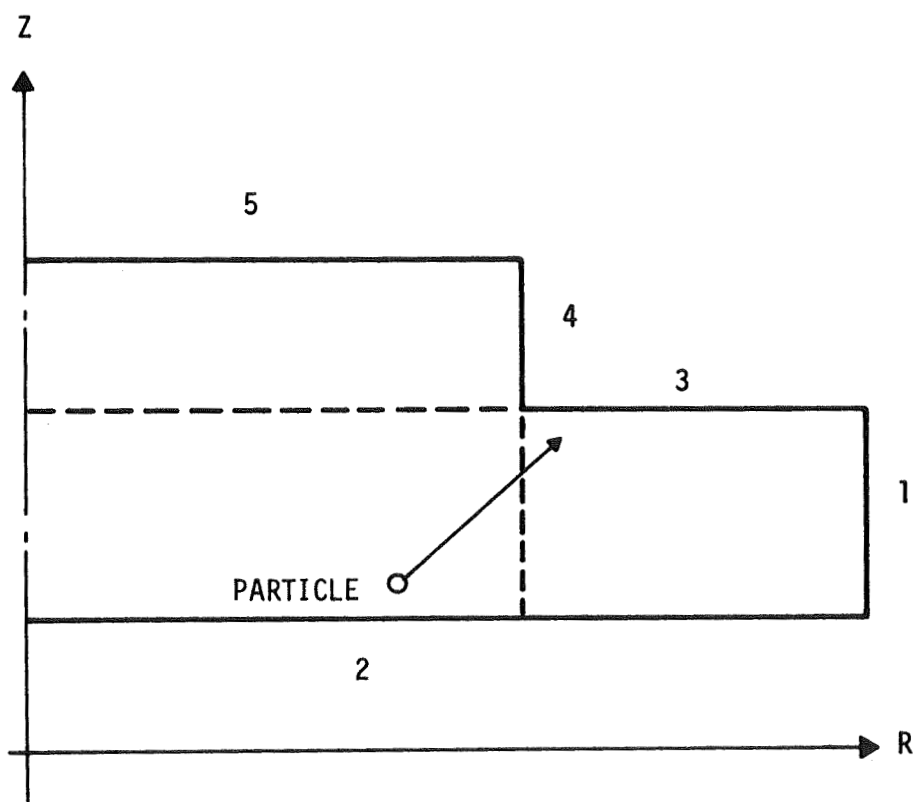


FIGURE 3-2. GEOMETRY ERROR EXAMPLE 1

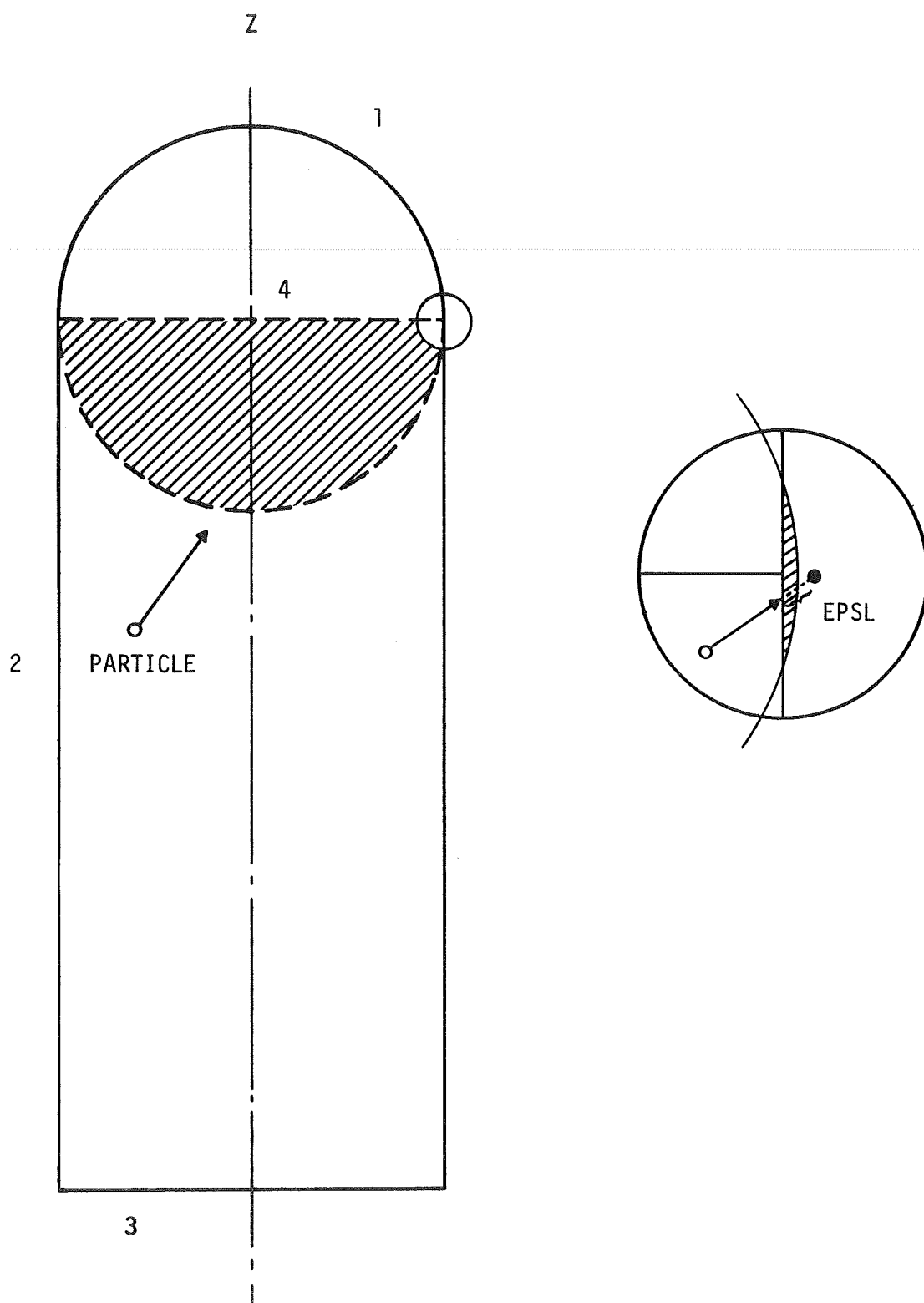


FIGURE 3-3. GEOMETRY ERROR EXAMPLE 2

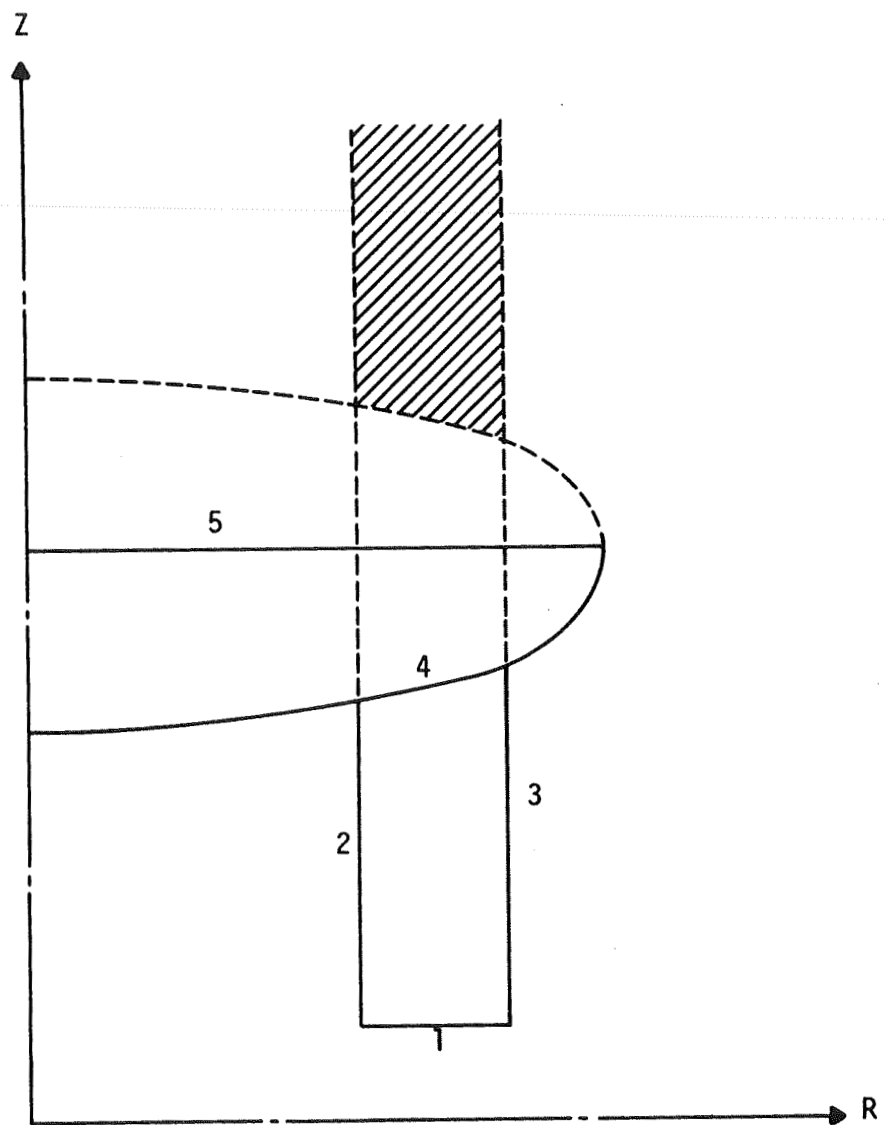


FIGURE 3-4. GEOMETRY ERROR EXAMPLE 3

annular region. A particle in either the shaded region or the annular region must be "outside" of Boundaries 1, 2, and 4, and "inside" Boundary 3. To prevent this error for particles in the shaded area, use the fictitious boundary, 5, as part of the boundary description of the annular region. Then particles must be "inside" of Boundary 5 to be in the annular region, while particles in the shaded region are "outside" of Boundary 5.

Table 3-3 describes the input data format to be used for Library Two. Note that the IBN parameter requires a sign. As discussed in Volume I, the sign results from substituting the coordinates of a point inside the region into the boundary equation. Since the point is not the boundary, the result will be nonzero.

TABLE 3-3. HOI LIBRARY TWO DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 2)
	41-80/10A4	LIB	Library identification
B			Number of Cards*
	1-60/12I5	IBN(K,N)	**The Nth boundary surrounding region K (with proper sign), except for K = 2
		MPR(K,N)	**The most probable region of entry across the Nth boundary of region K (K ≠ 2)

*If NB(K) is the number of boundaries of the region K and N_m is the number of inside regions that have from $[6(m-1) + 1]$ to $6m$ boundaries, then

$$\text{the number of cards} = \sum_{m=1}^{\infty} m N_m$$

**K = 1, NREG, but Region 2 is excluded. Begin a new card for each region.

3.4 H01 LIBRARY THREE

This library is used to input the 10 source parameters when $ISRCTP = 1$; that is, when source data are input on cards instead of a data file. Two options are allowed for card input of source data, these options being controlled by the variable JOPT. When $JOPT = 0$, a maximum of 140 source particles can be described on the card input as shown in Table 3-4. Normally, the number of source particles will equal the NHIST value in the problem deck. However, if the source is a monoenergetic, monodirectional point source with all particles being born at the same time, the source parameters can be input once and the code will duplicate these parameters NHIST times during execution. The input for this option, $JOPT = 1$, is also explained in Table 3-4.

TABLE 3-4. HOI LIBRARY THREE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 3)
	6-10/I5	I	Number of sets of source particle parameters to be input (≤ 140)
	11-15/I5	JOPT	Option determining use of source particle parameters: JOPT = 0: "I" sets of source particle data required JOPT = 1: Only one set of source particle parameters is required. This set will be duplicated internally NHIST times
	41-80/10A4	LID	Library identification
B ₁ *			Number of cards = 2*I
	1-10/E10.4	XS(N)	Spatial coordinates of the source particle position
	11-20/E10.4	YS(N)	
	21-30/E10.4	ZS(N)	
	31-40/E10.4	AS(N)	Direction cosines of the source particles direction
	41-50/E10.4	BS(N)	
	51-60/E10.4	CS(N)	
B ₂ *	1-10/E10.4	ES(N)	Source particle energy
	11-20/E10.4	WS(N)	Source particle weight
	21-30/E10.4	TS(N)	Time of birth of source particle
	31-40/I10	NR(N)	Region containing source particle

*Reading order: [(XS(N), YS(N), ZS(N), AS(N), BS(N), CS(N), ES(N), WS(N), TS(N), NR(N), N = 1, I]

3.5 H01 LIBRARY FOUR

Library Four is used to input the total, total scattering, and elastic scattering cross sections for neutrons or the total, Compton plus pair production, and Compton cross sections for gammas. Since a Library Four is required for each energy supergroup for every element, the number of Library Fours required for a given problem is $NSG * NEL$. The cross sections are listed at arbitrarily spaced energy points within a given supergroup; however, within that supergroup, the energy points must be the same for all elements. The energy data points should be input in descending order. Different Library Fours can be input in any order after the problem deck. The code first records these data on a scratch data file and then rearranges these data by supergroups after all library data are read in. A cross section data file that contains the data from Libraries Four, Six, and Seven is then generated. This data file should be saved for subsequent H01, A01, and A02 runs on this problem. If this cross section file is not retained, then the Library Fours data decks generated for the H01 problem can be used without modification for the analysis runs, even though only the total cross sections are needed in A01 and A02.

Units for the cross sections are arbitrary but must be consistent with the density table (DN) units input in the problem deck. For example, if the density units are measured in atoms/barn-cm, then the cross sections should be measured in barns/atom; or if the density units are g/cm^3 , then the cross sections should be in cm^2/g . The required input data format for Library Four is given in Table 3-5.

TABLE 3-5. HO1 LIBRARY FOUR DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 4)
	6-10/I5	K	Number of energy points at which cross sections are read in (same for all elements in any given supergroup)
	11-15/I5	J	Element number (elements are numbered in the order that their atomic weights are listed in the ATWT array)
	16-20/I5	L	Energy supergroup number (energy supergroups must be numbered beginning with the supergroup of highest energies as 1 and increasing with decreasing supergroup energies)
	41-80/10A4	LID	Library identification
B*			Number of cards = K
	1-10/E10.4	ENERGY(M)	Energy within a supergroup at which the cross section is defined in descending order (these energies should be the same for all Library Fours for a given supergroup)
	11-20/E10.4	TM(J,M)	Total cross section for element J NRG = 0: neutron total cross section NRG > 0: gamma total cross section
	21-30/E10.4	SM(J,M)	Total scattering cross section for element J NRG = 0: neutron total scattering cross section NRG > 0: gamma Compton plus pair production cross section
	31-40/E10.4	ESM(J,M)	Elastic scattering cross section for element J NRG = 0: neutron elastic scattering cross section NRG > 0: gamma Compton scattering cross section

*M = 1, K

3.6 H01 LIBRARY FIVE

Library Five input determines the manner in which the exponential transformation will be applied to each region in the problem geometry. The pseudo-cross section is obtained by multiplying the actual cross section, $\sum_T(E)$, by the nonnegative term, $[1 - XK * EXT(M)]$. The XK parameter is usually a directionally dependent parameter, which is determined by the particle direction cosines, (α, β, γ) , and the collision point-to-bias point direction cosines, $(\alpha_B, \beta_B, \gamma_B)$, but XK can also be made independent of direction by setting XK equal to 0 or 1. The EXT(M) term is a weighting factor where $0 \leq EXT(M) < 1$. The CAVEAT H01 routine will allow the exponential transformation to be used to bias toward a selected point in space. If this option is selected for any region, then the coordinates of the bias point must be input. The necessary input data formats are explained in Table 3-6.

TABLE 3-6. HOI LIBRARY FIVE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 5)
	6-10/I5	I	Number of regions (this number should be the same as NREG in the problem deck)
	11-15/I5	J	Bias point option J = 0: NEXT(M) $\neq$ 9 for any region M, M = 1, NREG (Card C not required) J = 1: NEXT(M) = 9 for at least one region (Card C is required input)
	41-80/10A4	LID	Library identification
B			Number of cards = NREG (or I)
	1-5/I5	M	Region number
	6-10/I5	NEXT(M)	Exponential transformation option for region M NEXT(M) = 1: XK = 0 NEXT(M) = 2: XK = 1 NEXT(M) = 3: XK = α NEXT(M) = 4: XK = $-\alpha$ NEXT(M) = 5: XK = β NEXT(M) = 6: XK = $-\beta$ NEXT(M) = 7: XK = γ NEXT(M) = 8: XK = $-\gamma$ NEXT(M) = 9: XK = $\alpha \cdot \alpha_B + \beta \cdot \beta_B + \gamma \cdot \gamma_B$
	11-20/E10.4	EXT(M)	Weighting factor used to obtain a pseudo-cross section for a bias sampling of path lengths in region M
C	1-10/E.0.4	XB	Spatial coordinates of the bias point
	11-20/E10.4	YB	
	21-30/E10.4	ZB	

3.7. H01 LIBRARY SIX

Library Six contains inelastic scattering data that will allow the code to represent the neutron energy spectrum after an inelastic scattering event. Obviously, this library is not needed for gamma problems; however, a Library Six is required for each energy supergroup for every element except hydrogen. Nevertheless, many of these libraries will consist of only one card (Card A). The required input and format for Library Six is given in Table 3-7. Note that the energy supergroups that are specified in the problem data decks are broken down into incident neutron energy groups. The number of energy groups, specified by NMESH(J), can vary for different elements and for different energy supergroups.

TABLE 3-7. HO1 LIBRARY SIX DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 6)
	6-10/I5	NMESH(J)	The number of incident neutron energy groups for element J and supergroup L for which probabilities of exciting the various levels of the target nucleus are listed
	11-15/I5	J	Element number (the elements are numbered in the order they appear in the ATWT array in the problem data deck)
	16-20/I5	L	Energy supergroup number
	21-25/I5	NEXT(J)	Number of excitation levels for which probabilities are given for element J and supergroup L
	26-30/I5	INEO(J)	Option to determine if inelastic scattering with element J is possible for neutron energies within supergroup L INEO(J) = 0: inelastic scattering is not possible (omit Cards B, C, and D) INEO(J) = 1: inelastic scattering is possible
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT}\{[\text{NEXP}(J) - 1]/6\}$
	1-60/6E.0.4	EEK(J,N)	Energy excitation levels listed in ascending order for element J [N = 1, NEXP(J)]
C			Number of cards = $1 + \text{INT}\{[\text{NMESH}(J) - 1]/6\}$
	1-60/6E10.4	EMESH(J,M)	Upper bounds of the incident energy groups listed in descending order for element J [M = 1, NMESH(J)]

TABLE 3-7 - Concluded

Card(s)	Field/Format	Input Symbol	Description
D			Number of cards = $NMESH(J) * (1 + INT \{ [NEXP(J) - 1] / 6 \})$
	1-60/6E10.4	SEP(J,M,N)	Inelastic scattering probability for element J, incident energy M, and excitation level N (Probabilities are entered for each excitation level for the first neutron incident energy group, then for each excitation level for the second incident energy group, and so on. Probabilities are cumulative probabilities so the input probability of exciting the second level should actually be the sum of the probabilities for exciting the first two levels.)

Anisotropic scattering data of elastic scattered neutrons are input to the code by Library Seven. Library Seven is required for each energy supergroup and for every element except hydrogen in which the value of $ESI(J)$ (see problem data deck) is less than or equal to the maximum value of the energy supergroup $[EMAX(L)]$. Gamma problems and the element hydrogen in neutron problems do not require Library Sevens.

Library Seven information includes the cosines of the center-of-mass scattering angles that divide the total area under a differential elastic scattering curve for a given neutron energy range into $NEPI(J)$ equal areas. This information is equivalent to specify those cosines of the center-of-mass scattering angles at those angles where the cumulative probability equals $K/NEPI(J)$, $K = 1, NEPI(J)$. For example, if $NEPI(J) = 20$, then the cosines are given where the cumulative probability equals 0.05, 0.10, 0.15, . . . , 0.90, 0.95, 1.0. These cosines are given for a specified neutron incident energy group contained in an energy supergroup. All input data can vary with different elements and different supergroups. The format to be used in preparing a Library Seven deck is given in Table 3-8.

TABLE 3-8. H01 LIBRARY SEVEN DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 7)
	6-10/I5	NEPI(J)	Number of probabilities for which the cosines of the scattering angles are listed for element J and supergroup L
	11-15/I5	J	Element number (the elements are numbered in the order they appear in the ATWT array in the problem data deck)
	16-20/I5	L	Energy supergroup number
	21-25/I5	NCROS(J)	Number of incident energy groups for which scattering probabilities are input for element J and supergroup L
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT}[(\text{NCROS}-1)/6]$
	1-60/6E10.4	ESCAT(J,N)	Upper bound of the incident energy groups listed in descending order for element J and supergroup L [N = 1, NCROS(J)]
C			Number of cards = $\text{NCROS}(J) * (1 + \text{INT}\{[\text{NEPI}(J)-1]/6\})$
	1-60/6E10.4	DES(J,N,M)	Cosines of the center-of-mass scattering angles for element J and supergroup L tabulated for equal probability intervals of $1.0/\text{NEPI}(J)$ from $1.0/\text{NEPI}(J)$ to 1.0 and for each incident energy group N (M = 1, NEPI(J) varies most rapidly; N = 1, NCROS(J))

4. S02 SECONDARY SOURCE ROUTINE INPUT DATA

The S02 routine generates a secondary gamma source data file, using as input the H01 collision data file. The source data file produced by S02 is identical in format to that produced by S01 and includes the same 10 source parameters. Routine S02 allows the generation of either an inelastic or capture gamma data file, or both. Proper manipulation of the input data will allow the user to include other secondary gamma producing events.

The S02 data file assignments are given below:

<u>Data File Symbol</u>	<u>Logic Number</u>	<u>Purpose</u>
NT5	5	System input
NT6	6	System output
JJJ3	10	Input collision data (No. 1)
JJJ10	12	Input collision data (No. 2)
JJ8	11	Inelastic gamma source
JJ5	13	Capture gamma source
JJJ4	8	Scratch
JJJ2	9	Scratch
NT16	8	Inelastic gamma pass data
NT17	8	H01 pass data (input)
NT18	8	Capture gamma pass data

The logic number for each data file is assigned in a BLOCK DATA sub-program, and the user can reassign the logic numbers as required to assure compatibility with the computer system being used. Note that the pass data files have been assigned a logic number of 8. The purpose of this assignment is to reduce the number of data files when the pass option is not used. If the pass option is used, then NT16, NT17, and/or NT18 should be assigned a unique logic number as required. Other data files that will not be used for a particular run can also be assigned a scratch data file logic number (e. g., set JJ5 = 8 for an inelastic gamma only run).

When preparing library data for S02, Library Nine should be prepared either before or concurrently with Libraries One, Two, and Three. Likewise, Library Ten should be prepared either before or concurrently with Libraries Five, Six, and Seven, because Libraries Nine and Ten specify the energy data points for the other libraries.

The overlay structure for S02 is shown in Figure 4-1. MAIN, BLOCK DATA, and FINDER reside in the core at all times during the execution of the program. MAIN calls in each overlay once, beginning with S02, which sets up the variably dimensioned arrays and reads in the input data. Next, TAPS is called and finally, the 10 source parameters are generated when SOURCE is placed in the core. The three overlays are independent of each other.

4.1. S02 PROBLEM DECK

The problem deck of S02 contains the necessary information to set up core storage requirements for the problem being run, specifies the options being used, and defines other problem-dependent data. The S-array is the array in common that is used to set aside core storage for the variably dimensioned arrays. The input data formats are given in Table 4-1.

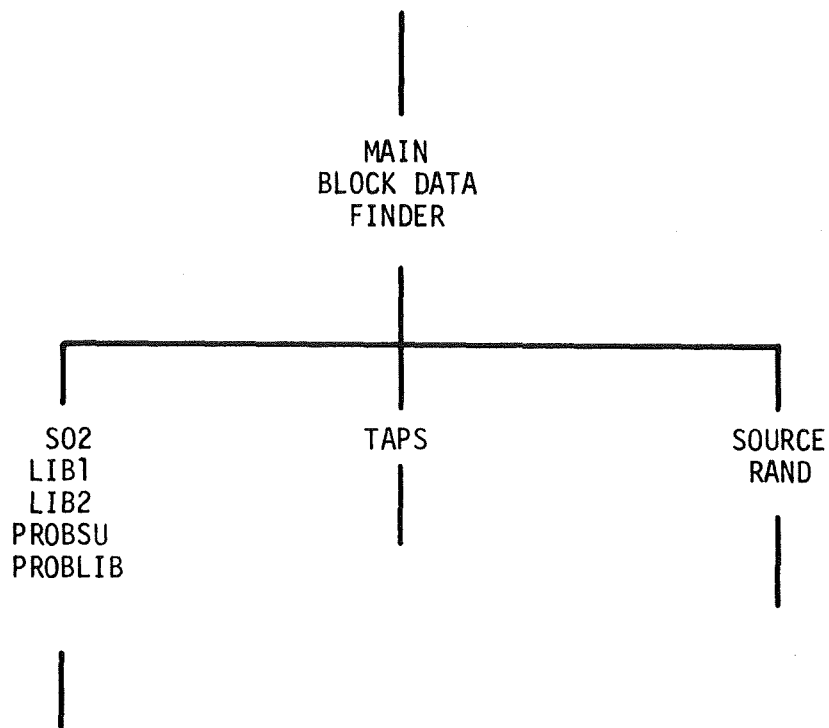


FIGURE 4-1. S02 OVERLAY STRUCTURE

TABLE 4-1. SO2 PROBLEM INPUT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	MSIZE	Maximum size in S array for program
	6-10/I5	IO	Input data listing option. If IO > 0, all input data are printed out
	11-15/I5	MNCS13	Maximum number of energy data points per element for inelastic scattering in Library 9
	16-20/I5	MNCS57	Maximum number of energy data points per element for the capture events in Library 10
	21-25/I5	MNRSTI	Maximum number of records to be put on the inelastic data file
	26-30/I5	MNRSTC	Maximum number of records to be put on the capture data file
	31-35/I5	INTAPE(1)	First input collision data file number
B	1-5/I5	NMAT	Number of materials
	6-10/I5	NEL	Number of elements
	11-15/I5	NREG	Number of regions
	16-20/I5	NGI	Number of gamma rays of different energy given off by all elements over the inelastic energy range
	21-25/I5	NGC	Number of gamma rays of different energy given off by all elements over the capture energy range
	26-30/I5	INEL	Problem Type -1 Inelastic only 0 Capture only +1 Inelastic and Capture
	31-35/I5	NRCO	Maximum number of records written on a collision data file

TABLE 4-1 - Continued

Cards(s)	Field/Format	Input Symbol	Description
B	36-40/I5	ITAPE	Inelastic data file number
	41-45/I5	ITAPE1	Capture data file number
	46-50/I5	NIT	Number of input collision data files (≤ 2). For pass cases, set $NIT < 0$. The pass case is used when a problem combines the use of H01, S02, and the analysis routines, and these programs are linked together as job steps within a given job.
	51-55/I5	NIO	Number of elements for $\sigma_{n,n'} = 0$ (IF INEL = 0, NIO = 0). NIO is used to determine NZ1
	56-60/I5	NCO	Number of elements for which $\sigma_{n,\gamma} = 0$ (IF INEL = -1, NCO = 0). NCO is used to determine NZ2
	61-66/2X,A4	PID	Problem identification symbol
	67-68/I2	NN	Problem number
C	1-10/E10.4	EMAX	Maximum neutron energy for cross section input
	11-20/E10.4	EIN	Threshold energy (minimum) for inelastic scattering
	21-30/E10.4	ESEC	Threshold energy (maximum) for capture events
	31-40/E10.4	EMIN	Minimum neutron energy for cross section input
D	1-10/I10	NRI	Initial number of random number generator
	21-25/I5	NI	Number of neutron energy boundaries minus one in inelastic range (between these boundaries the probabilities of getting a different inelastic gamma are considered constant)

TABLE 4-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
D	26-30/I5	NC	Number of neutron energy boundaries minus one in the capture range (between these boundaries the probabilities of getting different capture gammas are considered constant)
	31-40/I10	ITP	Option for intermediate printout =0; no intermediate printout =1; intermediate printout
E			Omit if INEL = 0 (Card B)
	1-10/E10.4	FINEL1	All values of the inelastic gamma weight greater or equal to FINEL1 are retained for use in the transport of gamma particles.
	11-20/E10.4	FINEL2	All values of the inelastic gamma weight greater than FINEL2 but less than FINEL1 are allowed to play Russian Roulette by the value of WFIN1. If these particles succeed the RR game, the weight of the inelastic gamma is divided by WFIN1 and retained for gamma transport. If the particles lose the game of RR, the particles are terminated. Similarly, values of the inelastic gamma weight less than FINEL2 are allowed to play Russian Roulette according to the value of WFIN2.
	21-30/E10.4	WFIN1	Russian Roulette parameter for inelastic gamma particles of weight between FINEL1 and FINEL2.

TABLE 4-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
F	31-40/E10.4	WFIN2	Russian Roulette parameters for inelastic gamma particles of weight less than FINEL2. (For example, if WFIN2 = 0.001, all particles with weight less than FINEL1 are given a chance 1:1000 of surviving with the resultant weight being WEIGHT = WEIGHT/WFIN2)
			Omit if INEL = -1 (Card B)
	1-10/E10.4	CAPL1	Same as for FINEL1 except for capture gammas
	11-20/E10.4	CAPL2	Same as for FINEL2 except for capture gammas
	21-30/E10.4	WFCAL	Same as for WFIN1 except for capture gammas
G	31-40/E10.4	WFCAL2	Same as for WFIN2 except for capture gammas
			Number of cards = $1 + \text{INT} [(2 * \text{NMAT} - 1)/12]$
	1-60/12I5	IOP(I)	Option to determine number of gammas produced per event by event type and material IOP(I) = 0: random selection of gamma producing events IOP(I) = 1: each event produces a gamma reduced in weight {I = 1 to 2 * NMAT; where for an odd integer, say I = N, IOP(N) is for inelastic events in the [1 + INT (N/2)]th material, and for an even integer, say I = M, IOP(M) is for capture events in the (M/2)th material}

TABLE 4-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
H			Number of cards = $1 + \text{INT}[(\text{NEL} - 1)/6]$
	1-60/6E10.4	A(J)	Atomic weight of element J (J = 1, NEL)
I			Number of cards = $\text{NMAT} * \{1 + \text{INT}[(\text{NEL} - 1)/6]\}$
	1-60/6E10.4	DN(I,J)	Density (or concentration) of element J in material I. J varies most rapidly (J = 1, NEL; I = 1, NMAT)
J			Number of cards = $\begin{cases} 0 & \text{if INEL} = 0 \\ 1 + \text{INT}(\text{NI}/6) & \text{if INEL} \neq 0 \end{cases}$
	1-60/6E10.4	ENI(I)	Neutron incident energy boundaries in the inelastic energy range [once an inelastic event with element J has been selected, the inelastic gammas are given off for all incident energies between ENI(K), and ENI (K + 1) are determined from the same probability density table Q1(J, K, M) from S02 Library 4] (I = 1, NI + 1)
K			Number of cards = $\begin{cases} 0 & \text{if INEL} = 0 \\ 1 + \text{INT}[(\text{NEL} - 1)/12] & \text{if INEL} \neq 0 \end{cases}$
	1-60/12I5	LIBIN(I)	LIBIN(I) = 0: Libraries 2, 3, and 4 are not needed for element I since inelastic scattering does not occur over the specified energy range. LIBIN(I) = N: Libraries 2, 3, and 4 are input for element I. N is an integer sequencing of those elements for which LIBIN(I) $\neq$ 0. (I = 1, NEL)

TABLE 4-1 Concluded

Card(s)	Field/Format	Input Symbol	Description
L			Number of cards = $\begin{cases} 0 & \text{if INEL} = -1 \\ 1 + \text{INT}(\text{NC}/6) & \text{if INEL} \neq -1 \end{cases}$
	1-60/6E10.4	ENC(I)	Neutron incident energy boundaries in capture energy range {once a capture event with element J has been selected, the capture gammas are given off for all incident neutron energies [between ENC(K) and ENC (K + 1)] and determined from the same probability density table Q2 (J, K, M) from S02 Library 8} (I = 1, NC + 1)
M			Number of cards = $\begin{cases} 0 & \text{if INEL} = -1 \\ 1 + \text{INT}(\text{NC}/12) & \text{if INEL} \neq -1 \end{cases}$
	1-60/12I5	LIBCP(I)	LIBCP(I) = 0: Libraries 6, 7, and 8 are not needed for element I since capture events do not occur over the specified energy range. LIBCP(I) = N: Libraries 6, 7, and 8 are input for element I. N is an integer sequencing of those elements for which LIBCP(I) $\neq$ 0. (I = 1, NEL)
N			Number of cards = $1 + \text{INT}[(\text{NREG} - 1)/12]$
	1-60/12I5	MATREG(K)	Material reference number of region K. Material number should correspond to material I of DN (I, K) MAT REG(2) = 0, region 2 is always outside region (K = 1, NREG)
0*	1-10/I10	MTPREC(1)	Number of records on the last input collision data file
	11-20/I10	MTPREC(2)	Number of sets of collision data on the last record of the above data file

*When NIT < 0, Card 0 is omitted and the pass data is used.

4.2. S02 LIBRARY ONE

Library One contains total neutron microscopic cross sections, $TCS1(J, K)$, in the energy range in which inelastic scattering is possible. The index J is the element index and is ascertained by the input of the atomic weight of the element on the first card of this library; therefore, Library Ones may be input in any order. The index K is the energy index and the energy it refers to is equal to the K th energy of Library Nine. The cross sections should be input at the energy points listed in Library Nine since the code performs a linear interpolation to obtain the cross sections at energies between those tabulated in Library Nine. One Library One has to be input for each element used in the problem whenever $INEL \neq 0$. If $INEL = 0$, Library Ones are not needed. The format to be used in making up Library One decks is presented in Table 4-2.

TABLE 4-2. S02 LIBRARY ONE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 1
	11-20/I10	NM	Number of cross sections to be input for element J (same as NM in S02 Library 9)
	21-30/E10.4	AW	Atomic weight of element J
	41-80/10A4	LID(I)	Library identification ($I = 1, 10$)
B			Number of cards = $1 + \text{INT}[(NM - 1)/6]$
	1-60/6E10.4	$TCS1(J, K)$	Total microscopic cross section for element J at the K th energy of Library 9 ($K = 1, NM$)

4.3. S02 LIBRARY TWO

Library Two contains the microscopic inelastic scattering cross sections, $SCSI(J, K)$, where J denotes the element number and K denotes the K th energy in Library Nine. A Library Two must be input for each element which has inelastic scattering in the energy range defined in Library Nine. These elements are the same as those for which $LIBIN(I) \neq 0$ in Card(s) K of the S02 problem deck. Library Two data are input as shown in Table 4-3.

TABLE 4-3. S02 LIBRARY TWO DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 2
	11-20/I10	NM	Number of cross sections to be input for element J (same as NM in Library 9)
	21-30/I10	AW	Atomic weight of element J
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT} [(NM - 1)/6]$
	1-60/E10.4	SCSI(J,K)	Microscopic inelastic scattering cross section for element J at the K th energy of Library 9 ($K = 1, NM$)

4.4. S02 LIBRARY THREE

Library Three contains NM values of $TTSC1(J,K)$, covering the inelastic scattering energy range. These values are the average number of gammas produced per inelastic event by element J at an incident neutron energy of the Kth value in Library Nine. A Library Three must be input for each element I such that $LIBIN(I) \neq 0$ in Card(s) K of the S02 problem deck. The input data format for Library Three is given in Table 4-4.

TABLE 4-4. S02 LIBRARY THREE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 3
	11-20/I10	NM	Number of cross sections to be input for element J (same as NM in Library 9)
	21-30/E10.4	AW	Atomic weight of element J
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT} [(NM - 1)/6]$
	1-60/6E10.4	$TTSC1(J,K)$	Average number of gammas per inelastic scattering for element J at the Kth energy in Library 9 ($K = 1, NM$)

4.5. S02 LIBRARY FOUR

Library Four contains a complete list of the gamma energies, EGAM(M), that are possible from inelastic collisions with all elements. Each Library Four contains this list, and all these lists have to be identical (M = 1 to NGI). Each Library Four also contains a probability density table, Q1(J, N, M).

The index J is the element index and is obtained by the program from the value of the atomic weight, AW, input in this library. The index N is the incident-neutron energy group index, with group N being from ENI(N) to ENI(N+1), N = 1 to NI[ENI(N) > ENI(N+1)]. The index M is the resultant gamma energy index; i. e., if the gamma-ray index K is picked by a random process in the program, the resulting gamma energy is EGAM(K). One Library Four is required for each element I used in the problem for which LIBIN(I) $\neq$ 0. The Q1 array of each Library Four consists of a matrix of NI rows and NGI columns. The sum of the Q1 in any row must lie within the interval 1.000 ± 0.0001 . Each Q1(J, N, M) in row N should be calculated to be the average probability of getting a gamma ray of energy EGAM(M) from an inelastic event with element J for incident neutrons with energies from ENI(N) down to ENI(N+1). Input data for Library Four are to be input according to the format shown in Table 4-5.

TABLE 4-5. S02 LIBRARY FOUR DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 4
	11-20/I10	NI	Number of neutron incident energy groups for the inelastic scattering range (same as NI in Card D of problem deck)
	21-30/I10	AW	Atomic weight of element J
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT}[(\text{NGI} - 1)/6]$
	1-60/6E10.4	EGAM(M)	Inelastically produced secondary gamma energies for which Q1(J, M, N) values are input (M = 1, NGI)
C			Number of cards = $\text{NI} * \{1 + \text{INT}[(\text{NGI}-1)/6]\}$
	1-60/6E10.4	Q1(J,N,M)	Probability that a gamma of energy EGAM(M) will be produced from an inelastic event by a neutron with energy in energy group N colliding with element J (M = 1, NGI varies most rapidly; N = 1, NI)

4.6. S02 LIBRARY FIVE

Library Five contains the total neutron microscopic cross sections, $TCS2(J,K)$, in the energy range for which neutron capture can occur. The index J is the element index and is ascertained by the input of the atomic weight of the element on the first card of each library. The index K is the energy index and the energy it refers to is equal to the K th energy in Library Ten. One Library Five has to be input for each element used in the problem whenever $INEL \neq -1$. The input data format shown in Table 4-6 should be used in preparing a Library Five input deck.

TABLE 4-6. S02 LIBRARY FIVE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 5
	11-20/I10	NM	Number of cross sections to be input for element J (same as NM in S02 Library 10)
	21-30/E10.4	AW	Atomic weight of element J
	41-80/10A4	LID(I)	Library identification ($I = 1, 10$)
B			Number of cards = $1 + \text{INT}[(NM - 1)/6]$
	1-60/6E10.4	TCS2(J,K)	Total microscopic cross section for element J at the K th energy of Library 10 ($K = 1, NM$)

4.7. S02 LIBRARY SIX

Library Six contains the microscopic radiative capture cross sections, $SCS2(J, K)$, where J denotes the element number and K denotes the K th energy in Library Ten. A Library Six must be input for each element that has capture events in the energy range defined in Library Ten. These elements are the same as those for which $LIBCP(I) \neq 0$ in Card(s) M of the S02 problem deck. Library Six data are input as shown in Table 4-7.

TABLE 4-7. S02 LIBRARY SIX DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 6
	11-20/I10	NM	Number of cross sections to be input for element J (same as NM in Library 10)
	21-30/I10	AW	Atomic weight of element J
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT}[(NM - 1)/6]$
	1-60/E10.4	SCS2(J,K)	Microscopic radiative capture cross section for element J at the Kth energy of Library 10 ($K = 1, NM$)

4.8. S02 LIBRARY SEVEN

Library Seven contains NM values of TTSC2(J,K), covering the radiative capture energy range. These values are the average number of gammas produced per capture event by element J at an incident neutron energy of the Kth value in Library Ten. A Library Seven must be input for each element I such that LIBCP(I) $\neq$ 0 in Card(s) M of the S02 problem deck. The input data format for Library Seven is given in Table 4-8.

TABLE 4-8. S02 LIBRARY SEVEN DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 7
	11-20/I10	NM	Number of cross sections to be input for element J (same as NM in Library 10)
	21-30/E10.4	AW	Atomic weight of element J
	41-80/10A4	LID	Library identification
B			Number of cards = 1 + INT [(NM - 1)/6]
	1-60/6E10.4	TTSC2(J,K)	Average number of gammas per capture event for element J at the Kth energy in Library 10 (K = 1, NM)

4.9. S02 LIBRARY EIGHT

Library Eight contains a complete list of the gamma energies, EGAMC(M) that are possible from radiative capture events with all elements. Each Library Eight contains this list, and all these lists have to be identical (M = 1 to NGC). Each Library Eight also contains a probability density table, Q2(J, N, M).

The index J is the element index and is obtained by the program from the value of the atomic weight, AW, input in this library. The index N is the incident-neutron energy group index, with group N being from ENC(N) to ENC(N+1), N = 1 to NC [ENC(N) > ENC(N+1)]. The index M is the resultant gamma energy index; i. e., if the gamma-ray index K is picked by a random process in the program, the resulting gamma energy is EGAMC(K). One Library Eight is required for each element I used in the problem for which LIBCP(I) $\neq$ 0. The Q2 array of each Library Eight consists of a matrix of NC rows and NGC columns. The sum of the Q2 in any row must lie within the interval 1.000 ± 0.0001 . Each Q2(J, N, M) in row N should be calculated to be the average probability of getting a gamma ray of energy EGAMC(M) from a capture event with element J for incident neutrons with energies from ENC(N) down to ENC(N+1). Input data for Library Eight are to be input according to the format shown in Table 4-9.

TABLE 4-9. SO2 LIBRARY EIGHT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 8
	11-20/I10	NC	Number of neutron incident energy groups for the capture energy range (same as NC in Card D of problem deck)
	21-30/I10	AW	Atomic weight of element J
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT}[(\text{NGC} - 1)/6]$
	1-60/6E10.4	EGAMC(M)	Radiative capture-produced secondary gamma energies for which Q2(J,M,N) values are input (M = 1, NGC)
C			Number of cards = $\text{NC} * \{1 + \text{INT}[(\text{NGC} - 1)/6]\}$
	1-60/6E10.4	Q2(J,N,M)	Probability that a gamma of energy EGAMC(M) will be produced from a capture event by a neutron with energy in energy group N colliding with element J (M = 1, NGC varies most rapidly; N = 1, NC)

4.10. S02 LIBRARY NINE

The set of energies at which neutron data in the inelastic scattering energy range are defined is given in Library Nine. This set of energies is used by Library One for defining total microscopic cross sections, by Library Two for inelastic scattering cross sections, and by Library Three for the average number of gammas given off per inelastic event. Library Nine is the same for all elements. Table 4-10 gives the format to be used in preparing Library Nine.

TABLE 4-10. S02 LIBRARY NINE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 9
	11-20/I10	NM	Number of energies for which cross sections in the inelastic scattering energy range are listed
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT} [(NM - 1)/6]$
	1-60/6E10.4	ENERG1(K)	Energy values for which cross sections are given. List in descending order (K = 1, NM)

4.11. S02 LIBRARY TEN

Library Ten specifies the energy data points at which the nuclear data of Libraries Five, Six, and Seven are given. Then energies should cover the energy range over which the neutron radiative capture event is important for any element in the problem being considered, and this set of energies is the same for all elements. Table 4-11 presents the formats to be used in preparing a Library Ten data deck.

TABLE 4-11. S02 LIBRARY TEN DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	LIBNO	Library number = 10
	11-20/I10	NM	Number of energies for which cross sections in the radiative capture energy range are listed
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT} [(NM - 1)/6]$
	1-60/6E10.4	ENERG2(K)	Energy values for which cross sections are given. List in descending order (K = 1, NM)

5. J01 DATA FILE SORT ROUTINE INPUT DATA

For problems in which more than one energy supergroup has been used to input cross section data, the J01 routine must be executed before the collision data from H01 can be input to the analysis codes, A01 and A02. Routine J01 sorts the collision data by energy supergroups, placing all collisions that occurred with energies in the first supergroup at the beginning of another data file. Following these data, the collision data for the subsequent supergroup are written in the proper order. The sorted collision data are written in the same format as the original data.

The J01 data file assignments are given below:

<u>Data File Symbol</u>	<u>Logic Number</u>	<u>Purpose</u>
NT5	5	System input
NT6	6	System output
NT10	10	Input collision data (No. 1)
NT11	11	Sorted collision data (No. 1)
NT12	12	Input collision data (No. 2)
NT13	13	Sorted collision data (No. 2)
NT16	8	H01 pass data (input)
NT17	8	J01 pass data (output)

The logic numbers of the data files are assigned in a DATA statement in the J01 source deck and can be changed to be compatible with the requirements of other computer facilities. If there is only one input collision data file, this file should be designated as NT10 and the sorted data file, as NT11. The sorted collision data file should be retained for input into the analysis routines. At least one data file should be assigned to handle the pass information, even if the pass data will not be used. If desired, these data files can be the same, but then the H01 pass information is destroyed.

Unlike the other CAVEAT routines, J01 does not require library data decks. The input format for J01 is given in Table 5-1.

TABLE 5-1. J01 PROBLEM INPUT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	NHT	Number of input collision data files [set NHT < 0 if the pass data giving NHT, MKREC(1), and MKREC(2) are to be used]
	6-10/I5	NSG	Number of energy supergroups
	11-15/I5	JHTAPE	Number to be assigned to first out- put (sorted) collision data file (second data file will be numbered JHTAPE +1, if needed)
	16-25/2X,2A4	H(1) H(2)	Label of sorted collision data file (usually SORTED)
	26-35/2X,2A4	HU(1) HU(2)	Label of input collision data file (usually HISTORY)
	36-40/I5	MKREC(1)	Number of records on last input collision data file (leave blank if NHT < 0)
	41-45/I5	MKREC(2)	Number of sets of collision data on final record of last input collision data file (leave blank if NHT < 0)
	46-50/I5	NRCD	Maximum number of collision records written on either the input or the sorted collision data file
	51-55/I5	IMHT1	Number assigned in H01 problem deck to the first collision data file to be generated (i.e., IHTAPE)
B			Number of cards = $1 + \text{INT}[(\text{NSG}-1)/3]$
	1-60/6E10.4*	EMAX(K)	Upper bound of energy supergroup K (K = 1, NSG)
		EMIN(K)	Lower bound of energy supergroup K (K = 1, NSG)

*Reading order: [EMAX(K), EMIN(K), K = 1, NSG]

6. A01 ANALYSIS ROUTINE INPUT DATA

The A01 routine estimates the time-dependent fluence (or flux) at specified point detectors. Energy and angular distributions of the radiation environment can also be determined, and the dose (or dose rate) can be computed. All output is normalized by dividing by the number of histories parameter, NHIST.

Input for A01 may consist of the H01 (or J01) collision data file, pass option data file, cross section data file, problem deck, and several library decks. Most of the data required in the problem deck and library decks will have been determined during the setup of the H01 routine. Like H01, many different libraries of the same type may be required for a single problem, and the routine checks to see whether the proper number and types of libraries are input. Routine A01 is also variably dimensioned, with the common array named V. A table showing the storage requirements and entry points of each variably dimensioned array is printed in the output.

The A01 data file assignments are given below:

<u>Data File Symbol</u>	<u>Logic Number</u>	<u>Purpose</u>
NT5	5	System input
NT6	6	System output
NT8	8	Cross section data
NT10	10	Input collision parameters (No. 1)
NT11	11	Latent collision parameters
NT12	12	Input collision parameters (No. 2)
NT13	13	Latent collision parameters
NT17	11	Collision pass data

The logic number of each data file is assigned in a BLOCK DATA subprogram and easily can be changed for compatibility with the requirements of other computer facilities. Data file NT8 can be either input from a previous H01 or A01 run of the same problem or generated from the card input. If NT8 is generated, then it should be saved for future

runs. The collision data, either from H01 (one energy supergroup) or J01 (more than one supergroup), are put on NT10 and NT12. If only one collision data file was generated, this file is placed on NT10; and NT12 is not needed. The latent collision parameters are written on NT11 and NT13, so that these two data files must be assigned logic numbers. These files act as scratch units and need not be saved. In cases where the pass option is used (i. e. , pass data from either H01 or J01), NT17 should be assigned a unique logic number. If the pass option is not used, then NT17 can be given a scratch unit logic number, as done above.

The overlay structure for A01 is given in Figure 6-1. The MAIN subroutine, which calls in the different overlays, and the BLOCK DATA subprogram remain in core at all times. The three overlays shown are completely independent and are called into core only one time each.

6.1. A01 PROBLEM DECK

The input formats for the A01 problem decks are given in Table 6-1.

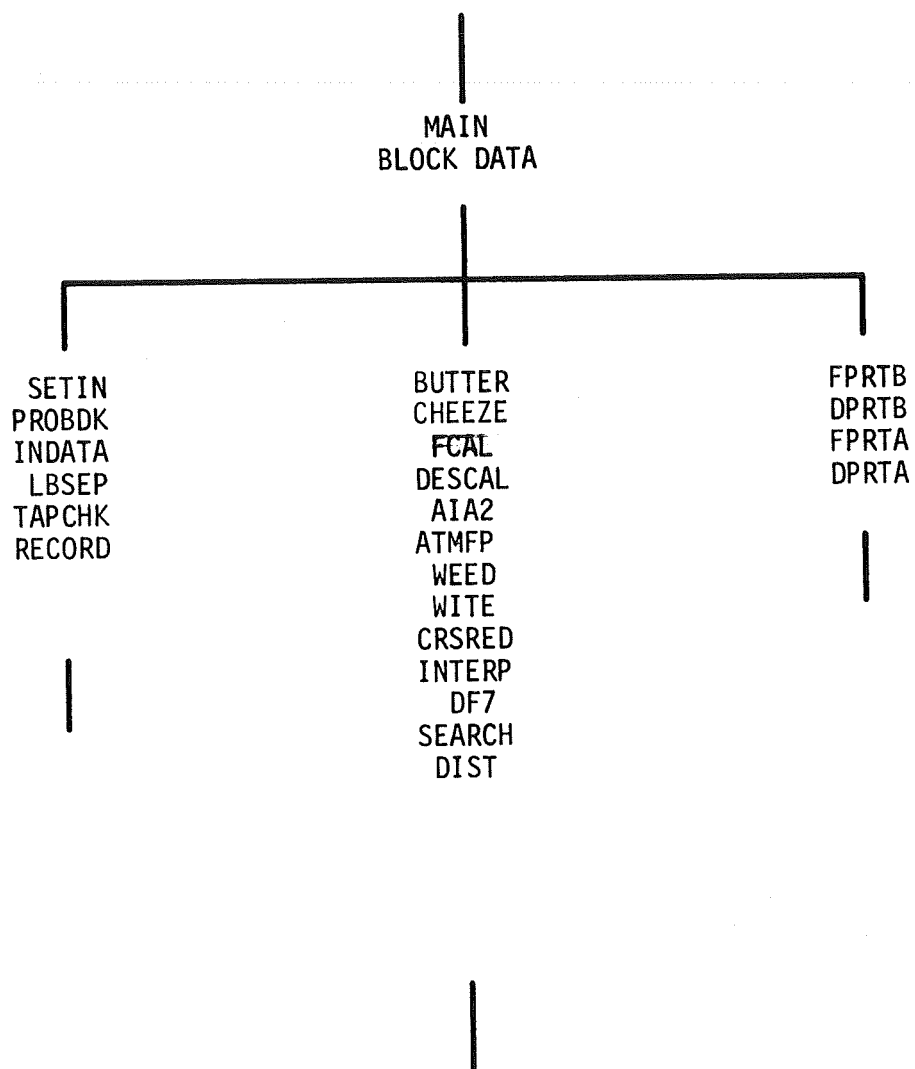


FIGURE 6-1. A01 OVERLAY STRUCTURE

TABLE 6-1. A01 PROBLEM INPUT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	MSIZE	Maximum size of common block for V-array
	11-15/I5	JSENSE	Intermediate data printout option JSENSE = 0: No intermediate data printout JSENSE = 1: Printout of intermediate data
	16-20/I5	I0	Option that controls the listing of input data cards I0 = 0: No listing given I0 = 1: Only the problem deck is listed I0 = 2: Both the problem deck and library decks are listed
	21-22/I2	IFPRT(1)	Controls printout of fluence (or flux) which gives angular distribution for each energy and time interval for each detector IFPRT(1) = 0: Printout omitted IFPRT(1) > 0: Printout given
	23-25/I3	IFPRT(2)	Controls printout of fluence (or flux) which gives only energy interval as function of time interval values for each detector (no angular dependence) IFPRT(2) = 0: Printout omitted IFPRT(2) > 0: Printout given
	26-27/I2	IFPRT(3)	Controls printout of dose (or dose rate) which gives angular distribution for each energy and time interval for each detector IFPRT(3) = 0: Printout omitted IFPRT(3) > 0: Printout given
	28-30/I3	IFPRT(4)	Controls printout of dose (or dose rate) which gives only energy interval as function of time

TABLE 6-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
A			interval values for each detector IFPRT(4) = 0: Printout omitted IFPRT(4) > 0: Printout given
	31-35/1X,A4	PID	Problem identification symbol
	35-40/3X,I2	NN	Problem number
	41-80/10A4	ID(I)	Problem description (I = 1, 10)
B	1-5/I5	NG	Type of particle: NG = 0: Neutrons NG = 1: Primary gammas NG = 2: Secondary gammas
	6-10/I5	NSG	Number of energy supergroups
	11-15/I5	NEL	Number of elements
	16-20/I5	NMAT	Number of materials
	21-25/I5	NREG	Number of geometric regions
	26-30/I5	NBD	Number of boundaries
	31-35/I5	MBD	Maximum number of boundaries needed to define any region {i.e., Max [NB(K), K = 1, NREG]}
	36-40/I5	MEP	Maximum number of energy data points for any energy supergroup [i.e., Max (NENEGY)] in Library 4
	41-45/I5	MCROS	*Maximum number of incident-energy groups for which scattering probabilities are input for any element in any energy supergroup (Library 7) {i.e., Max [NCROS(J), J = 1, NEL for all supergroups]}
	46-50/I5	MEPI	*Maximum number of equal scattering probability intervals for any element in any energy supergroup (Library 7) {i.e., Max [NEPI(J), J = 1, NEL for all supergroups]}

*Set equal to 0 for primary and secondary gamma problems

TABLE 6-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
B	51-55/I5	MNEL	*Number of elements for which Library 7 is input
	55-60/I5	NLIB	Number of libraries input on cards for this problem (this number is checked against the number actually input). Consider each Library 4 and 7 as separate libraries even though there may be several of the same type.
	61-65/I5	IAIR	IAIR $\leq$ 0, No atmosphere model used IAIR > 0, Real atmosphere model used
	66-70/I5	MATAIR	IAIR > 0: Material number is DN array (see Card I below) in which the atmospheric concentrations are given IAIR $\leq$ 0: Leave blank
C	1-5/I5	IPPMAX	Number of angles bounding printout azimuthal angle groups
	6-10/I5	IGPMAX	Number of angles bounding printout polar angle groups
	10-15/I5	IEPMAX	Number of energies bounding printout energy groups
	16-20/I5	ITPMAX	Number of times bounding printout time intervals
	21-25/I5	ND	Number of detector points
	26-30/I5	NHIST	Number of histories
	31-35/I5	ISRCTP	Collision data input option: ISRCTP = 0 - HISTORY or SORTED collision data file is available ISRCTP = 1 - Collision data will be supplied by Library 3

*Set equal to 0 for primary and secondary gamma problems

TABLE 6-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
C	36-40/I5	NHT	Number of input collision data files (maximum of 2) [If NHT is negative, the value of MKREC(1), MKREC(2), and BEG are provided by the pass file option parameters on unit NT17 for job steps to be linked and executed as one job.]
	41-45/I5	MHTAPE(1)}	Input collision data file numbers. If only one data file is input, MHTAPE(2) is left blank and the input file symbol is NT10. For two files, the partially filled file [MHTAPE(2)] symbol is NT12.
	46-50/I5	MHTAPE(2)}	
	51-55/I5	MKREC(1)	Number of records on the last (or partially filled) collision data file
	56-60/I5	MKREC(2)	Number of sets of collision data on the last record of the above data file
	61-65/I5	NTAP	Cross section input option (for Libraries 4 and 7): NTAP = 0: cross sections input on cards NTAP = 1: cross sections input on data file
	66-70/I5	IQID	Cross sections data file number
D	1-10/E10.0	EPSL	Distance to be added vectorially to a particle's coordinates to move the particle off of a boundary (when EPSL is added to the maximum distance to any boundary, the distance should change at least in the eighth significant figure)
	11-20/E10.0	DPMIN	Minimum separation distance between collision point and detector point for that collision to contribute to the flux estimate at specified detector

TABLE 6-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
D	21-30/2X,2A4	H(I)	Label for the input collision data file(s). (I = 1, 2)
	31-35/I5	NER	Specifies the energy units of the input data, which must be consistent for a given problem. NER = 1: MeV energy units NER = 2: keV energy units NER = 3: eV energy units
	36-40/I5	IEF	Option to determine whether particle or energy fluence (flux) is calculated: IEF = 0: Particle fluence (flux) IEF = 1: Energy fluence (flux)
	41-45/I5	NRCD	Maximum number of records to be written on any collision data file (as specified in H01)
E			Number of cards = $NHT * 1 + INT \left[\frac{(NSG-1)}{6} \right]$ if $NHT > 0$ = 0 if $NHT \leq 0$
	1-60/E10.0	BEG(I,J)	Number of collisions (with 0.5 added to each value) for supergroup J on collision data file I. The J index varies most rapidly (J = 1, NSG). Begin a new card for each data file (I = 1, NHT)
F			Number of cards = $1 + INT[(IPPMAX-1)/6]$
	1-60/E10.0	PPRINT(K)	Angles bounding printout azimuthal angle groups (in degrees, ascending order). The first value should be 0.0 and the remaining values are the upper bounds of the first through the last group. The last value should be 360.0 (K = 1, IPPMAX)

TABLE 6-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
G			Number of cards = $1 + \text{INT}[(\text{IGPMAX}-1)/6]$
	1-60/6E10.0	GPRINT(K)	Angles bounding printout polar angle groups (in degrees, ascending order). The first value should be 0, and the remaining values are the upper bounds of the first through the last group. That last value should be 180 (K = 1, IGPMAX)
H			Number of cards = $1 + \text{INT}[(\text{IEPMAX}-1)/6]$
	1-60/6E10.0	EPRINT(K)	Energies bounding printout energy groups (in ascending order). The first values should be less than or equal to EMIN (from H01) and the remaining values are the upper bounds of the first through last energy groups. The last value should be greater than the maximum value possible on the input collision data file or cards (K = 1, IEPMAX)
I			Number of cards = $1 + \text{INT}[(\text{ITPMAX}-1)/6]$
	1-60/6E10.0	TPRINT(K)	Times bounding printout time intervals in ascending values. First value should be zero, last value should be TMAX in H01 code (K = 1, ITPMAX)
J			Number of cards = $1 + \text{INT}[(\text{IEPMAX}-1)/6]$ if IFPRT(3) or IFPRT(4) $\neq$ 0 = 0 if IFPRT(3) and IFPRT(4) = 0
	1-60/6E10.0	FTOD(K)	Fluence-to-dose conversion constants by energy group specified in card(s) H above

TABLE 6-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
K			Number of cards = $1 + \text{INT}[(\text{NSG}-1)/3]$
	1-60/6E10.0	EGRP(K)	Lower energy bound for energy super-group K
		EMAX(K)	Upper energy bound for energy super-group K
		Input EGRP(1), EMAX(1), EGRP(2), EMAX(2), . . . from K = 1 to NSG	
L			Number of cards = $1 + \text{INT}[(\text{NEL}-1)/6]$ for neutron problems = 0 for gamma problems
	1-60/6E10.0	ESI(K)	Energy at which elastic scattering becomes isotropic in the center-of-mass system for element K (K = 1, NEL)
M			Number of cards = $1 + \text{INT}[(\text{NEL}-1)/6]$
	1-60/6E10.0	ATWT(K)	Atomic weight of element K (K = 1, NEL)
N			Number of cards = $\text{NMAT} * \{1 + \text{INT}[(\text{NEL}-1)/6]\}$
	1-60/6E10.0	DN(J,K)	Density of element K in material J or concentration for material MATAIR when using the air model (IAIR $\neq$ 0). K varies most rapidly (K = 1, NEL; J = 1, NMAT).
O			Number of cards = $1 + \text{INT}[(\text{NREG}-1)/14]$
	1-70/14I5	NB(K)	Number of boundaries defining region K (K = 1, NREG) as defined in Library 2
P			Number of cards = $1 + \text{INT}[(\text{NREG}-1)/14]$
	1-70/14I5	MATREG(K)	Material number (as defined by DN array) in region K (K = 1, NREG) (Voids are designated by the number 0)

TABLE 6-1 - Concluded

Card(s)	Field/Format	Input Symbol	Description
Q			Number of cards = $1 + \text{INT}[(\text{NEL}-1)/14]$ for neutron problem = 0 for gamma problem
	1-70/14I5	LB7(K)	LB7(K) = 0: No Library 7 is input for the Kth element for any energy supergroup. LB7(K) = N: A Library 7 is input for the Kth element in at least one of the energy supergroups. N is an integer sequencing of those elements for which LB7(K) $\neq$ 0. K = 1, NEL.
R			Number of cards = ND (one per detector point)
	1-10/I10	NRD(K)	Region in which the Kth detector is located
	11-40/3E10.0	XD1(K) YD1(K) ZD1(K)	Spatial coordinate of detector K (K = 1, ND)
S			Number of cards = 233 if IAIR > 0 and NTAP = 0 = 0 otherwise
	1-54/3D19.10	YM(K) XLRHO(K) F(K)	Real atmospheric density table for 0 to 466 km at 2-km increments

6.2. A01 LIBRARY ONE

The input format for A01 Library One is identical to that of H01 Library One in Section 3.2. In most problems, the boundaries used to describe the A01 problem geometry will be the same as for the H01 geometry. However, under some situations, some boundaries may be changed or deleted; an example is found in reducing the description of a reactor core to one geometric region in the A01 run when the core was subdivided into several regions in the H01 run to obtain a more detailed core heating description. Since in the A01 run the additional regions only increase the computer running time, those boundaries not needed to describe the core as one region can be omitted. However, boundaries can be described in Library One and not used in Library Two. Sometimes retaining unnecessary boundaries in Library One, but omitting regions in the problem geometry, is better than omitting unnecessary boundaries, so that the boundary numbers of needed regions remain the same as in the H01 run. The input format for Library One is given in Table 6-2.

TABLE 6-2. A01 LIBRARY ONE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 1)
	6-10/I5	NBD	Number of boundaries described in Library One (same as NBD in Card B of problem deck)
	41-80/10A4	LID	Library identification
B			Number of cards = NBD
	1-5/I5	K	Boundary number (boundaries can be input in any order, but $K \leq NBD$)
	6-10/I5	IBT(K)	Type of boundary for boundary K IBT(K) = 1: Sphere, Ellipsoid or Hyperboloid $(X-XF)^2 + (Y-YF)^2 - AF(Z-ZF)^2 - CF = 0$ IBT(K) = 2: Paraboloid $(X-XF)^2 + (Y-YF)^2 - AF(Z-ZF) = 0$ IBT(K) = 3: Cone $[(X-XF)^2 + (Y-YF)^2]^{\frac{1}{2}} - AF(Z-ZF) = 0$ IBT(K) = 4: Cylinder $[(X-XF)^2 + (Y-YF)^2]^{\frac{1}{2}} - AF = 0$ IBT(K) = 5: Plane containing Z axis $\theta - AF = 0$ (AF in radians) IBT(K) = 6: Plane perpendicular to Z axis $Z - AF = 0$ IBT(K) = 7: Plane perpendicular to X axis $X - AF = 0$ IBT(K) = 8: Plane perpendicular to Y axis $Y - AF = 0$ IBT(K) = 9: Plane arbitrarily oriented $AF \cdot X + ZF \cdot Y + CF \cdot Z - XF = 0$
	11-20/E10.4	AF(K)	Curve fit coefficients for boundary K
	21-30/E10.4	ZF(K)	
	31-40/E10.4	CF(K)	
	41-50/E10.4	XF(K)	
	51-60/E10.4	YF(K)	

6.3. A01 LIBRARY TWO

Library Two for the A01 routine has the same input format as Library Two of H01 in Section 3.3. As discussed in the previous section, having the same input format does not mean that the geometry description for the A01 run must be the same as for the H01 run. However, in most cases the geometry for A01 will be exactly like the geometry for H01, so that the H01 Library Two deck can be used as the A01 Library Two deck. Because the input format for A01 in Library Two is identical with that of the H01 Library Two, the suggestions given in Section 3.3 to aid in setting up this library will not be repeated; however, these suggestions should be considered whenever changes in the A01 Library Two geometry description are made. For completeness, the input format for A01 Library Two is given in Table 6-3.

TABLE 6-3. A01 LIBRARY TWO DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 2)
	41-80/10A4	LIB	Library identification
B			Number of cards*
	1-60/12I5	IBN(K,N)	**The Nth boundary surrounding region K (with proper sign), except for K = 2
		MPR(K,N)	**The most probable region of entry across the Nth boundary of region K (K ≠ 2)

*If NB(K) is the number of boundaries of the region K and N_m is the number of inside regions that have from $[6(m-1) + 1]$ to $6m$ boundaries, then the Number of cards = $\sum_{m=1}^{\infty} m N_m$

**K = 1, NREG, but Region 2 is excluded. Begin a new card for each region.

6.4. A01 LIBRARY THREE

Library Three is used to input collision data by cards (i. e. , $ISRCTP = 1$ in Card C of the problem deck), instead of by collision data files for a normal run. The main purpose of Library Three is to provide control over input variables for checkout purposes. The number of collision points must be less than or equal to 20. The collision points must be sorted according to energy so that all collisions with incident energy E in the first energy supergroup [$EGRP(1) < E \leq EMAX(1)$] are input first, those in the second supergroup, next, and so on. The format to be used when preparing Library Three is shown in Table 6-4.

TABLE 6-4. A01 LIBRARY THREE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 3)
	6-10/I5	ISRCRC	Number of collisions for which collision parameters are to be input (<u>≤</u> 20)
	41-80/10A4	LID	Library identification
B			Number of cards = 2 * ISRCRC
	1-10/E10.0	X1(L)	X-coordinate of the Lth collision point
	11-20/E10.0	Y1(L)	Y-coordinate of the Lth collision point
	21-30/E10.0	Z1(L)	Z-coordinate of the Lth collision point
	31-40/E10.0	A0(L)	Direction cosine of particle's direction with X-axis before the Lth collision
	41-50/E10.0	B0(L)	Direction cosine of particle's direction with Y-axis before the Lth collision
	51-60/E10.0	C0(L)	Direction cosine of particle's direction with Z-axis before the Lth collision
B ₂ *	1-10/E10.0	E0(L)	Particle's energy before Lth collision
	11-20/E10.0	AW(L)	Atomic weight of element with which the Lth collision occurred
	21-30/E10.0	W1(L)	Particle's weight after the Lth collision
	31-40/I10	NR1(L)	Region in which the Lth collision occurred
	41-50/E10.0	EX1(L)	Excitation level of target nucleus of the Lth collision
	51-60/E10.0	T1(L)	Particle's age (time) at the Lth collision

*Reading order: [X1(L), Y1(L), Z1(L), A0(L), B0(L), C0(L), E0(L),
AW(L), W1(L), NR1(L), EX1(L), T1(L), L = 1, ISRCRC]

6.5. A01 LIBRARY FOUR

A01 Library Four is used to input the total microscopic cross section for neutrons or gammas at a specified energy point. The input format for A01 Library Four is identical to that of H01 Library Four except that the SM(J, M) and ESM(J, M) values in Cards B are not required. However, a Library Four deck prepared for H01 can be used in A01, since the additional data are just ignored by the code. The number of Library Fours required for a given problem are the product of NSG and NEL, since a Library Four is required for each energy supergroup for every element. The suggestions given in Section 3.5 for preparing H01 Library Fours are valid for A01 Library Fours and will not be repeated here. However, the input format for an A01 Library Four deck is given in Table 6-5.

TABLE 6-5. A01 LIBRARY FOUR DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 4)
	6-10/I5	K	Number of energy points at which cross sections are read in (same for all elements in any given supergroup)
	11-15/I5	J	Element number (elements are numbered in the order that their atomic weights are listed in the ATWT array)
	16-20/I5	L	Energy supergroup number (energy supergroups must be numbered beginning with the supergroup of highest energies as 1 and increasing with decreasing supergroup energies)
	41-80/10A4	LID	Library identification
B*			Number of cards = K
	1-10/E10.4	ENERGY(M)	Energy within a supergroup at which the cross section is defined in descending order (these energies should be the same for all Library Fours for a given supergroup)
	11-20/E10.4	TM(J,M)	Total cross section for element J NRG = 0: neutron total cross section NRG > 0: gamma total cross section

*Reading Order: [ENERGY(M), TM(J,M), M = 1, K]

6.6 A01 LIBRARY SEVEN

The A01 Library Seven is identical to that of H01 in Section 3.8. Normally the library decks or the cross section data file used in the H01 run will be used in the A01 run. However, more detailed anisotropic scattering data can be input to A01 than H01, if desired. If Library Sevens are input by cards, then all Library Fours must also be input by cards. The input data formats for A01 Library Seven are given in Table 6-6.

TABLE 6-6. A01 LIBRARY SEVEN DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library Number (= 7)
	6-10/I5	NEPI(J)	Number of probabilities for which the cosines of the scattering angles are listed for element J and supergroup L
	11-15/I5	J	Element numbers (the elements are numbered in the order they appear in the ATWT array in the problem data deck)
	16-20/I5	L	Energy supergroup number
	21-25/I5	NCROS(J)	Number of incident energy groups for which scattering probabilities are input for element J and supergroup L
	41-80/10A4	LID	Library identification
B			Number of cards = $1 + \text{INT}[(\text{NCROS}-1)/6]$
C	1-60/6E10.4	ESCAT(J,N)	Upper bound of the incident energy groups listed in descending order for element J and supergroup L [N = 1, NCROS(J)]
	1-60/6E10.4	DES(J,N,M)	Cosines of the center-of-mass scattering angles for element J and supergroup L tabulated for equal probability intervals of $1.0/\text{NEPI}(J)$ from $1.0/\text{NEPI}(J)$ to 1.0 and for each incident energy group N. [M = 1, NEPI(J) varies most rapidly; N = 1, NCROS(J)]

7. A02 ANALYSIS ROUTINE INPUT DATA

The analysis routine, A02, estimates the average track length in each region of the problem geometry. Like H01 and A01, A02 is variably dimensioned, but will not compute time-dependent values or handle the real atmosphere model. However, A02 will calculate the angular distribution of the current leaving the system (which could be used as a point source for certain extensions of the problem) and will generate a leakage source data file that can be used as input into H01.

The code requires as input collision data either on cards (Library 3) or data files (H01 or J01), a problem deck, and library decks. In addition, input may include a pass option data file and a cross section data file.

The A02 data file assignments are given below:

<u>Data File Symbol</u>	<u>Logic Number</u>	<u>Purpose</u>
NT5	5	System input
NT6	6	System output
NT8	8	Cross sections
NT10	10	Collision data (No. 1)
NT11	11	Leakage source (No. 1)
NT12	12	Collision data (No. 2)
NT13	13	Leakage source (No. 2)
NT14	14	Collision pass data

The logic number of each data file is assigned in a BLOCK DATA sub-program and easily can be changed in order to be compatible with the requirements of other computer facilities. The cross section data can be input either by cards, in which case NT8 may be saved, or by previously generated data files on an H01, A01, or A02 run of the same problem. Collision data files are placed on NT10 and NT12, with the first file generated placed on NT10. For collision data from more than one energy supergroup, the sorted collision data files are required.

If desired, the parameters of particles leaking from the problem geometry can be placed on data files to produce a source data file for H01. These parameters are written on NT11 and NT13 (if needed). The input pass data are put on NT14 if the pass option is used.

The overlay structure for A02 is given in Figure 7-1. The A02VD subroutine calls in the other overlays as needed, with A02VD and BLOCK DATA remaining in core at all times. All three overlays are completely independent.

7.1. A02 PROBLEM DECK

The input formats for the A02 problem deck are given in Table 7-1.

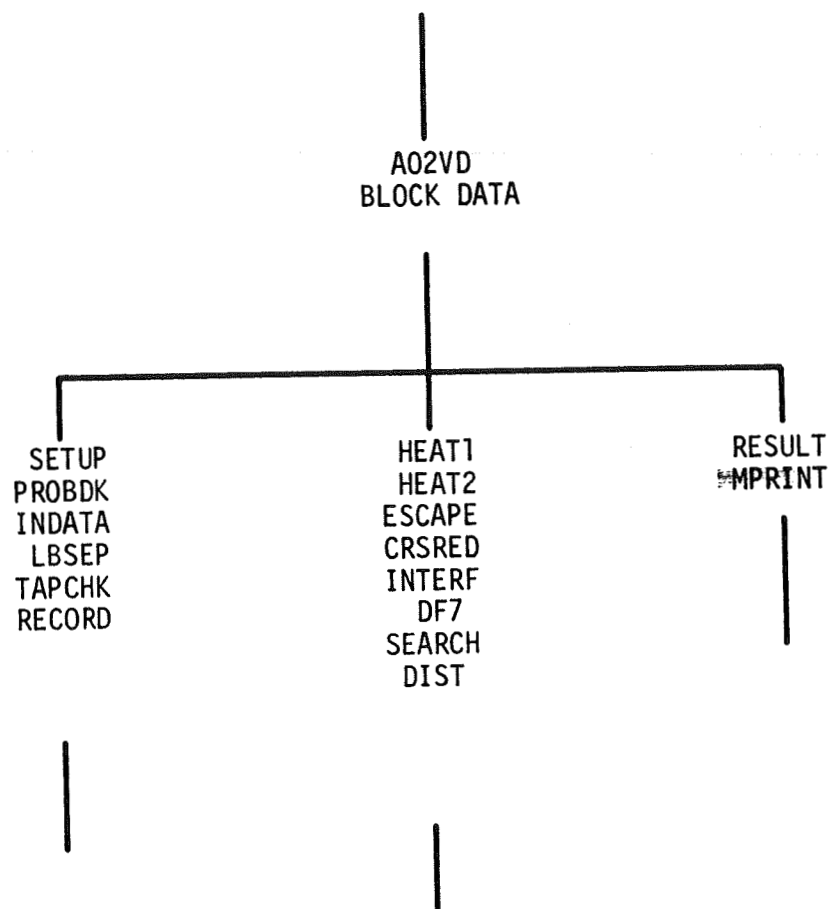


FIGURE 7-1. A02 OVERLAY STRUCTURE

TABLE 7-1. A02 PROBLEM INPUT DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-10/I10	MSIZE	Maximum size of common block for V-array
	11-20/I10	NRI	Initialization number for random number sequence (must not exceed largest integer number for machine)
	21-25/I5	JSENSE	Intermediate data printout option JSENSE = 0: No intermediate data printout JSENSE = 1: Printout of intermediate data
	26-30/I5	IO	Option that controls the listing of input data cards IO = 0: No listing given IO = 1: Only the problem deck is listed IO = 2: Both the problem deck and library decks are listed
	31-35/IX,A4	PID	Problem identification symbol
	36-40/3X,I2	NN	Problem number
	41-80/10A4	ID(I)	Problem description (I = 1, 10)
B	1-5/I5	NG	Type of particles NG = 0: Neutrons NG = 1: Primary gammas NG = 2: Secondary gammas
	6-10/I5	NSG	Number of energy supergroups
	11-15/I5	NEL	Number of elements
	16-20/I5	NMAT	Number of materials
	21-25/I5	NREG	Number of geometric regions
	26-30/I5	NBD	Number of boundaries
	31-35/I5	MBD	Maximum number of boundaries needed to define any region {i.e., Max [NB(K), K = 1, NREG]}

TABLE 7-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
B	36-40/I5	MEP	Maximum number of energy data points for any energy supergroup [i.e., Max (NENERGY) in Library 4]
	41-45/I5	IEPMAX	Number of energies bounding the printout energy group
	46-50/I5	IGPMAX	Number of angles bounding the printout polar angle groups
	51-55/I5	NRCD	Maximum number of records which could be written on any collision data file (as specified in H01)
	56-60/I5	MPRECS	Maximum number of records to be written on any leakage source data file
	61-65/I5	NHIST	Number of histories
	66-70/I5	NLIB	Number of libraries input on cards for this problem. Consider each Library 4 as separate libraries even though there may be several of the the same type
C	1-5/I5	LSO	Output option LSO = 0, Only track lengths as a function of region and particle energy will be printed LSO = 1, The number current leaking from a system as a function of angle and energy will be printed as well as the track lengths as a function of region and energy LSO = 2, The same printout is given as when LSO = 1 and, in addition, leakage source data files are written giving: the number current, the region before escaping into a vacuum, the final particle energy, the coordinates of the particle at the exit point, and the direction cosines, with age (time) set to zero

TABLE 7-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
C	6-10/I5	J2N0	Number to be assigned to the first leakage source data file
	11-15/I5	ISRCRC	Collision data input option ISRCRC = 0: HISTORY or SORTED collision data file is available ISRCRC > 0: Collision data will be supplied by Library 3
	16-20/I5	NHT	Number of input collision data files. If the pass option is to be used, set NHT < 0 and put the pass data file on NT14. NHT, MKREC(1), MKREC(2) and BEG values are provided by pass data
	21-25/I5	MHTAPE(1)	} Input collision data file numbers. If only one data file is input, MHTAPE(2) is left blank and the input file symbol is NT11. For two files, the partially filled file [MHTAPE(2)] symbol is NT13
	26-30/I5	MHTAPE(2)	
	31-35/I5	MKREC(1)	Number of records on the last (or partially filled) collision data file
	36-40/I5	MKREC(2)	Number of sets of collision data on the last record of the above data file
	41-45/I5	NTAP	Cross section input option (for Library 4) NTAP = 0: Cross sections input on cards NTAP = 1: Cross sections input on data file
	46-50/I5	IQID	Cross sections data file number
	1-10/2X,2A4	H(1)	} Label for the input H01 or J01 collision data files (usually HISTORY or SORTED)
D		H(2)	

TABLE 7-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
D	11-20/2X,2A4	HE(1) } HE(2) }	Label for the output leakage source data files (usually LEAKAGE)
	21-30/E10.0	ELOCUT	Leakage particles with energy less than ELOCUT will not be written on the leakage source data file
	31-40/E10.0	WLOCUT	Leakage particles with energy less than WLOCUT will not be written on the leakage source data file unless successful at Russian Roulette based on RR below
	41-50/E10.0	RR	Russian Roulette parameter for terminating a leakage particle with weight less than WLOCUT
	51-60/E10.0	EPSL	Distance to be added vectorially to a particle's coordinates to move the particle off of a boundary (when EPSL is added to the maximum distance to any boundary, the distance should change at least in the eighth significant figure)
E			Number of cards = $\begin{cases} \text{NHT} * \{1 + \text{INT}[(\text{NSG} - 1)/6]\} & \text{if NHT} > 0 \\ 0 & \text{if NHT} \leq 0 \end{cases}$
	1-60/E10.0	BEG(I,J)	Number of collisions (with 0.5 added to each value) for supergroup J on collision data file I. The J index varies most rapidly (J = 1, NSG). Begin a new card for each data file (I = 1, NHT)
F			Number of cards = $1 + \text{INT}[(\text{IGPMAX} - 1)/6]$
	1-60/6E10.0	GPRINT(K)	Angles bounding printout polar angle groups (in degrees, ascending order). The first value should be 0, and the remaining values are the upper bounds of the first through the last group. That last value should be 180 (K = 1, IGPMAX)

TABLE 7-1 - Continued

Card(s)	Field/Format	Input Symbol	Description
G			Number of cards = $1 + \text{INT}[(\text{IEPMAX} - 1)/6]$
	1-60/6E10.0	EPRINT(K)	Energies bounding printout energy groups (in ascending order). The first values should be less than or equal to EMIN (from H01), and the remaining values are the upper bounds of the first through last energy groups. The last value should be greater than the maximum value possible on the input collision data file or cards ($K = 1, \text{IEPMAX}$)
H			Number of cards = $1 + \text{INT}[(\text{NSG} - 1)/3]$
	1-60/6E10.0	EGRP(K) } EMAX(K) }	Lower energy bound for energy super group K Upper energy bound for energy super group K
			Input EGRP(1), EMAX(1), EGRP(2), EMAX(2) . . . from $K = 1$ to NSG
I			Number of cards = $\begin{cases} 1 + \text{INT}[(\text{NEL} - 1)/6] & \text{for neutron problems} \\ 0 & \text{for gamma problems} \end{cases}$
	1-60/6E10.0	ESI(K)	Energy at which elastic scattering becomes isotropic in the center-of-mass system for element K ($K = 1, \text{NEL}$)
J			Number of cards = $1 + \text{INT}[(\text{NEL} - 1)/6]$
	1-60/6E10.0	ATWT(K)	Atomic weight of element K ($K = 1, \text{NEL}$)

TABLE 7-1 - Concluded

Card(s)	Field/Format	Input Symbol	Description
K			Number of cards = $\text{NMAT} * \{1 + \text{INT}[(\text{NEL} - 1)/6]\}$
	1-60/6E10.0	DN(J,K)	Density of element K in material J. K varies most rapidly (K = 1, NEL; J = 1, NMAT)
L			Number of cards = $1 + \text{INT}[(\text{NREG} - 1)/14]$
	1-70/14I5	NB(K)	Number of boundaries defining region K (K = 1, NREG) as defined in Library 2
M			Number of cards = $1 + \text{INT}[(\text{NREG} - 1)/14]$
	1-70/14I5	MATREG(K)	Material number (as defined by DN array) in region K (K = 1, NREG) Voids are designated by the number 0.

7.2. A02 LIBRARY ONE

The input format for A02 Library One is identical to that of H01 and A01 Library Ones. Suggestions on the proper setup of this library can be found in Section 3.2. This fact does not mean that the geometry model used in H01 must be used in A02. Because A02 calculates track lengths within regions, a different geometry model may be needed to get the best statistical results. However, the regions should retain the same number as in the H01 run whenever possible, since the first region searched by the code to determine in what region the collision point took place in the collision region of H01. If this region is not the collision region of the A02 geometry, then the other regions are searched cyclically. The input format for Library One is given in Table 7-2.

TABLE 7-2. A02 LIBRARY ONE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 1)
	6-10/I5	NBD	Number of boundaries described in Library 1 (same as NBD in Card B of problem deck)
	41-80/10A4	LID	Library identification
B			Number of cards = NBD
	1-5/I5	K	Boundary number (boundaries can be input in any order, but $K \leq NBD$)
	6-10/I5	IBT(K)	Type of boundary for boundary K IBT(K) = 1: Sphere, Ellipsoid or Hyperboloid $(X-XF)^2 + (Y-YF)^2 - AF(Z-ZF)^2 - CF = 0$ IBT(K) = 2: Paraboloid $(X-XF)^2 + (Y-YF)^2 - AF(Z-ZF) = 0$ IBT(K) = 3: Cone $[(X-XF)^2 + (Y-YF)^2]^{\frac{1}{2}} - AF(Z-ZF) = 0$ IBT(K) = 4: Cylinder $[(X-XF)^2 + (Y-YF)^2]^{\frac{1}{2}} - AF = 0$ IBT(K) = 5: Plane containing Z axis $\theta - AF = 0$ (AF in radians) IBT(K) = 6: Plane perpendicular to Z axis $Z - AF = 0$ IBT(K) = 7: Plane perpendicular to X axis $X - AF = 0$ IBT(K) = 8: Plane perpendicular to Y axis $Y - AF = 0$ IBT(K) = 9: Plane arbitrarily oriented $AF \cdot X + ZF \cdot Y + CF \cdot Z - XF = 0$
	11-20/E10.4	AF(K)	Curve fit coefficients for boundary K
	21-30/E10.4	ZF(K)	
	31-40/E10.4	CF(K)	
	41-50/E10.4	XF(K)	
	51-60/E10.4	YF(K)	

7.3. A02 LIBRARY TWO

Library Two for the A02 routine has the same input format as Library Two of both H01 and A01. Suggestions as to the proper use of this library are contained in Section 3.3. When desired, the A02 geometry model can be different from either the H01 or the A01 model, and the input format for this new model is given in Table 7-3.

TABLE 7-3. A02 LIBRARY TWO DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number (= 2)
	41-80/10A4	LIB	Library identification
B			Number of cards*
	1-60/12I5	IBN(K,N)	**The Nth boundary surrounding region K (with proper sign), except for K = 2
		MPR(K,N)	**The most probable region of entry across the Nth boundary of region K (K ≠ 2)

* If NB(K) is the number of boundaries of the region K and N_m is the number of inside regions that has from $[6(m-1) + 1]$ to $6m$ boundaries,

$$\text{then the number of cards} = \sum_{m=1}^{\infty} m N_m$$

** K = 1, NREG, but Region 2 is excluded. Begin a new card with each region.

7.4. A02 LIBRARY THREE

Library Three is used to input collision data by cards (i. e. , $ISRCTC = 1$ in Card C of the problem deck), instead of by collision data files for a normal run. The main purpose of Library Three is to provide control over input variables for checkout purposes. The number of collision points must be less than or equal to 20. The collision points must be sorted according to energy so that all collisions with incident energy E in the first energy supergroup $[EGRP(1) < E \leq EMAX(1)]$ are input first, those in the second supergroup, next, and so on. The format to be used when preparing Library Three is shown in Table 7-4.

TABLE 7-4. A02 LIBRARY THREE DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number = 3
	6-10/I5	ISRCRC	Number collisions for which collision parameters are to be input (≤ 20)
	41-80/10A4	LID	Library identification
B ₁ *			Number of cards = 2 * ISRCRC
	1-10/E10.0	X0(L)	x - coordinate of the Lth collision point
	11-20/E10.0	Y0(L)	y - coordinate of the Lth collision point
	21-30/E10.0	Z0(L)	z - coordinate of the Lth collision point
	31-40/E10.0	A0(L)	Direction cosine of the particle's direction with x-axis after the Lth collision
	41-50/E10.0	B0(L)	Direction cosine of the particle's direction with y-axis after the Lth collision
	51-60/E10.0	C0(L)	Direction cosine of the particle's direction with z axis after the Lth collision
B ₂ *	1-10/E10.0	E0(L)	Particle's energy after Lth collision
	11-20/E10.0	AWL	Atomic weight of element with which the Lth collision occurred (not used by A02)
	21-30/E10.0	W0(L)	Particle's weight after the Lth collision
	31-40/I10	NRO(L)	Region in which the Lth collision occurred

TABLE 7-4 - Concluded

Card(s)	Field/Format	Input Symbol	Description
B ₂ *	41-50/E10.0	EXI	Excitation level of target nucleus of the Lth collision (not used by A02)

*Reading order: [X0(L), Y0(L), Z0(L), A0(L), B0(L), C0(L), E0(L), AWL,
W0(L), NRO(L), EXI, L = 1, ISRCRC]

7.5. A02 LIBRARY FOUR

A02 Library Four is used to input the total microscopic cross section for neutrons or gammas at a specified energy point. The input format for A02 Library Four is identical to that of H01 Library Four except that the SM(J, M) and ESM(J, M) values in Cards B are not required. However, a Library Four deck prepared for H01 can be used in A02, since the additional data are just ignored by the code. The input format for A02 Library Four and A01 Library Four is identical. The number of Library Fours required for a given problem are the product of NSG and NEL, since a Library Four is required for each energy supergroup for every element. The suggestions given in Section 3.5 for preparing H01 Library Fours are valid for A02 Library Fours and will not be repeated here. However, the input format for a A02 Library Four deck is given in Table 7-5.

TABLE 7-5. A02 LIBRARY FOUR DATA FORMAT

Card(s)	Field/Format	Input Symbol	Description
A	1-5/I5	LIBT	Library number = 4
	6-10/I5	K	Number of energy points at which cross sections are read in (same for all element in any given supergroup)
	11-15/I5	J	Element number (elements are numbered in the order that their atomic weights are listed in the ATWT array)
	16-20/I5	L	Energy supergroup number (energy supergroups must be numbered beginning with the supergroup of highest energies as 1 and increasing with decreasing supergroup energies)
	41-80/10A4	LID	Library identification
B*			Number of cards = K
	1-10/E10.4	ENERGY(M)	Energy within a supergroup at which the cross section is defined in descending order (these energies should be the same for all Library 4's for a given supergroup)
	11-20/E10.4	TM(J,M)	Total cross section for element J NRG = 0: neutron total cross section NRG > 0: gamma total cross section

* Reading Order: [ENERGY(M), TM(J,M), M = 1, K]