

LA-UR- 99- 1992

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Submitted to: Being made available on the WWW

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HTAPE3X for Use with MCNPX

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April 16, 1999

Abstract

HTAPE3X is a code for processing medium- and high-energy collision data written to a history file by MCNPX. In addition, it provides surface flux and current edits which supplement the standard MCNP tallies.

1. THE HTAPE3X CODE

HTAPE3X is a modification of the HTAPE code from the LAHET Code System[1] designed to provide analysis of the history file HISTP optionally written by MCNPX[2]. It is primarily intended to provide an analysis of the outcome of collisions in the medium- and high-energy range where the interaction physics is obtained from LAHET.

However, all appropriate features have been retained even when they duplicate existing MCNP flux and current tallies[3]. The latter features relate to editing a "surface source write (SSW)" file (default name WSSA). For experienced LAHET users, they do provide some options not available with standard MCNP F1 and F2 tallies.

Note that the information written to HISTP comes *only* from interactions processed by the medium- and high-energy modules in MCNPX; low-energy neutron and proton (and any photon/electron) collisions which utilize MCNP library data *do not* contribute to the collision information on the history file and will not contribute to edits by HTAPE3X of collision data. Surface crossing edits from data on the file WSSA will apply to all particle types and all energies.

2. Input for HTAPE3X

The input structure is largely unchanged from the description in reference [1]. In general, energy units are MeV, *time units are nanoseconds*, and length units are centimeters. Note the difference in the time scale from MCNP practice.

The input file (default name INT) for HTAPE3X has the following structure:

1. Two records of title information, 80 columns each.
2. An option control record.
3. Additional input as required by the chosen option.

Items 2 and 3 above are written as "list-directed input"[1]. Repeat counts are allowed, including repeat counts for commas to take default values (i.e., "4*" expands to ",,,"). Multiple cases may be processed; for each case the above structure applies. Slashes "/" are allowed *only* in the first pair of title cards *unless* each title card containing one or more slashes has a " \$" in column 1.

The option control record defines the options to be used and the additional input information that must be specified for the problem. The structure of this record is

**IOPT,NERG,NTIM,NTYPE,KOPT,NPARM,NFPRM,FNORM,KPLOT,
IXOUT,IRS,IMERGE,ITCONV,IRSP,ITMULT/**

Some of the parameters in this record may optionally be preceded by a minus sign whose meaning is defined below (see Table 2 for applicability). Thus if NTIM is specified by inserting "-3" in the option control record, it is interpreted as NTIM = 3 with a *minus-sign flag*

attached. In the discussion which follows, input control parameters are treated as positive or zero quantities, even though the flag may be present.

IOPT	NERG	NTIM	NTYPE	NPARM	NPPRM	KPLOT	IXOUT	IMBRGE	ITCONV	IRSP	ITMULT
1	O	O	R	R	O	N	N	O	O	O	O
101	O	O	R	R	O	N	N	O	O	O	O
2, 102	O	O	R	R	N	N	N	O	O	O	O
3	O	O	N	O	N	O	N	N	O	N	N
103	O	O	N	R	N	O	N	N	O	N	N
5	N	N	N	O	N	O	N	N	N	N	N
105	N	N	N	R	N	O	N	N	N	N	N
8	N	N	N	O	N	O	O	N	N	N	N
108	N	N	N	R	N	O	O	N	N	N	N
9, 109	O	O	R	R	O	N	N	O	O	O	O
10, 110	O	O	R	R	N	N	N	O	O	O	O
11, 111	O	N	R	R	O	N	N	O	N	N	N
12, 112	O	N	R	R	O	N	N	O	N	N	N
13	O	O	R	O	O	N	N	O	O	O	O
14	N	N	N	O	N	N	N	N	N	N	O
114	N	N	N	R	N	N	N	N	N	N	O
15	N	N	N	O	N	O	O	N	N	N	N
115	N	N	N	R	N	O	O	N	N	N	N
16	O	N	N	O	N	O	N	N	N	N	N
116	O	N	N	R	N	O	N	N	N	N	N

R ≡ required O ≡ optional N ≡ not used

IRS is optional with any value of IOPT

Table 1: Applicability of Input Control Parameters

IOPT defines the editing option to be applied as defined below. For all but **IOPT = 13**, **100** may be added to the basic option type to indicate that the tally over a list of cell, surface, or material numbers will be combined in a single tally. Prefixing **IOPT** by a minus sign, when allowed, indicates an option-dependent modification to the tally.

NERG, when applicable, defines the number of energy bins for the tally; the maximum is 2000. The default is 0, implying that only a total over energy will be produced. If **NERG** is > 1 and is preceded by a minus sign, the tally in each energy bin will

IOPT	-IOPT	-NERG	-NTIM	-NTYPE	-NPARM	-NFPRM
1, 101	O	O	O	N	O	O
2, 102	O	O	O	N	O	N
3, 103	O	O	O	N	O	N
5, 105	O	N	N	N	O	N
8, 108	O	N	N	N	O	N
9, 109	O	O	O	N	O	O
10, 110	O	O	O	N	O	N
11, 111	N	O	N	N	O	O
12, 112	N	O	N	N	O	O
13	O	O	O	N	N	N
14, 114	N	N	N	N	O	N
15, 115	O	N	N	N	O	N
16, 116	O	O	N	N	O	N

O ≡ optional N ≡ not used

Table 2: Applicability of Minus-sign Flags on Input Control Parameters

be divided by the bin width to normalize per MeV. The total over energy will be unnormalized.

NTIM defines the number of time bins for the tally when applicable; the maximum is 100. The default is 0, implying that only a total over time will be produced. If NTIM is > 1 and is preceded by a minus sign, the tally in each time bin will be divided by the bin width to normalize per nanosecond; the total over time will be unnormalized.

NTYPE defines the number of particle types for which the edit is to be performed for those options where it is applicable; the particle type is that of the particle causing the event which is recorded on the history tape. The default is 0; however, some options require that a value be supplied.

KOPT defines a sub-option for tally option IOPT. *The default is 0.*

NPARM usually defines the number of cells, materials, or surfaces over which the tally is to be performed when applicable; the maximum is 400. If NPARM is preceded by a minus sign, NPARM+1 normalization divisors will be read in as described below. *The default is 0;* however, some options require that a value be supplied.

NFPRM, at present, is used only to define the number of cosine bin boundaries to read in for particle current tallies; the maximum is 400. If NFPRM is preceded by a minus

Type	LAHET Usage	MCNPX Usage
0	proton	proton, \bar{p}
1	neutron	neutron, \bar{n}
2	π^+	π^+, π^-
3	π^0	π^0
4	π^-	
5	μ^+	
6	μ^-	μ^-, μ^+
7	deuteron	deuteron
8	triton	triton
9	${}^3\text{He}$	${}^3\text{He}$
10	alpha	alpha
11	photon	photon
12	K^+	K^+, K^-
13	K^0 long	K^0 long
14	K^0 short	K^0 short
15	K^-	
16	\bar{p}	
17	\bar{n}	
18	electron	electron, positron
19	positron	
20	neutrino	neutrino, antineutrino
21	antineutrino	

Table 3: Particle Type Identification in HTAPE3X

sign, cosine bin tallies will be normalized per steradian: the total over cosine bins will remain unnormalized (i.e., angle integrated). *The default is 0.*

FNORM may be used to apply an overall multiplicative normalization to all bins, except for IOPT = 11, 111, 12, or 112. For these cases, FNORM multiplies the time variable (e.g., use FNORM = 0.001 to convert from nanoseconds to microseconds). *The default is 1.0.*

KPLOT is a plot control flag; plotting is available for some options (provided it has been installed with the code using the LANL CGS and CGSHIGH Common Graphics System libraries). Using a 0 indicates that no PLOT file will be produced and is the default.

IXOUT is a flag to indicate that the tally will be written to a formatted auxiliary output

file for post-processing. The details (and the file name) are option dependent; however, a 0 indicates that no such file will be written, and is the default.

IRS is the RESOURCE option flag. A non-zero value indicates that the option will be turned on; 0 is the default (see section 19 below).

IMERGE is not used in HTAPE3X; see section 20 below.

ITCONV is the TIME CONVOLUTION option flag. A non-zero value indicates that the option will be turned on; 0 is the default (see section 21 below).

IRSP is the RESPONSE FUNCTION option flag. IRSP > 0 indicates that the tally will be *multiplied* by a user-supplied response function; IRSP < 0 indicates that the tally will be *divided* by a user-supplied response function. The default is 0. For a discussion, see section 22 below.

ITMULT is the TIME MULTIPLIER flag. ITMULT > 0 indicates that the weights tallied will be *multiplied* by the event time. This option applies only when the basic option type is 1, 2, 4, 9, 10, or 13.

The standard definitions for these input variables may not apply for some options. The applicability of the option control parameters is summarized in Table 1.

According to the parameters specified on the option record, the following records are required in the order specified:

- For NERG > 0, a record defining NERG upper energy bin boundaries, from low to high, defined as the array ERGB(I), I=1,NERG. The first lower bin boundary is implicitly always 0.0. The definition may be done in four different ways. First, the energy boundary array may be fully entered as ERGB(I), I=1,NERG. Second, if two or more, but less than NERG, elements are given (with the record terminated by a slash), the array is completed using the spacing between energy boundaries obtained from the last two entries. Third, if only one entry is given, it is used as the first upper energy boundary and as a constant spacing between all the boundaries. Fourth, if only two entries are given with the first negative and the second positive, the second entry is used as the uppermost energy boundary, ERGB(NERG), and the first entry is interpreted as the lethargy spacing between bin boundaries. Thus the record "-0.1,800./" will specify ten equal-lethargy bins per decade from 800 MeV down.
- For NTIM > 0, a record specifying NTIM upper time bin boundaries, from low to high, defined as the array TIMB(I), I=1,NTIM. The first lower time boundary is always 0.0. The same four methods that are allowed for defining the energy boundaries may also be used to define the time bin boundaries.

(-)IOPT, . . .	option control record (always required)
ERGB(I),I=1,NERG	upper energy bin limits
TIMB(I),I=1,NTIM	upper time bin limits
ITIP(I),I=1,NTYPE	particle type identifiers
LPARM(I),I=1,NPARM	surface, cell, or material identifiers
FPARM(I),I=1,NFPRM	upper cosine bin boundaries
DNPARM(I),I=1,NPARM+1	normalization divisors
	original source definition record for RESOURCE option
	new source definition record for RESOURCE option
ITOPT,TWIT,TPEAK,TWIT	parameters for TIME CONVOLUTION
ERESP(I),I=1,NRESP	energy grid for RESPONSE FUNCTION
FRESP(I),I=1,NRESP	function values for RESPONSE FUNCTION
IRESP(I),I=1,NRESP-1	interpolation scheme for RESPONSE FUNCTION
	segment definition record or window definition record
CN(I),I=1,3	arbitrary direction vector for defining cosine binning

Table 4: Order of HTAPE3X Input Records

- For NTYPE > 0, a record containing NTYPE particle types in any order, defined as the array ITIP(I),I=1,NTYPE. In the present MCNPX version 2.1.5, the contents of a surface source file WSSA are insufficient to distinguish between a particle and its antiparticle; it is to be expected that this condition will be remedied in future releases of MCNPX. The allowed particle types are listed in Table 3, which also indicates the overlapping particle/antiparticle tally definition which follows the column "MCNPX Usage".
- For NPARM > 0, a record containing NPARM *user-defined* cell, material, or surface numbers (integers), in any order, for which one wishes a tally to be made; these are defined as the array LPARM(I),I=1,NPARM. If a null record ("/") is supplied with NPARM > 0, it is treated as "1,2,3, ... ,NPARM/". (Note: a different meaning for NPARM is used for IOPT = 13.)
- For NFPRM > 0, a record containing NFPRM upper cosine bin boundaries, defined as the array FPARM(I),I=1,NFPRM. The first lower cosine boundary is always -1.0. If a null record is supplied, equal cosine bin boundaries from -1.0 to 1.0 will be defined by default.

- If NPARM is preceded by a minus sign, a record containing NPARM or NPARM+1 normalization divisors; these are defined in HTAPE3X as the DNPARM array. The NPARM values are in a one-to-one correspondence with the LPARM array. The last (NPARM+1) entry applies to a total over the NPARM entities where applicable; if omitted, it defaults to 1.0. Through this feature it is possible to input a list of volumes, areas, or masses, as appropriate, obtained from a MCNP calculation. When IOPT > 100, the NPARM cell, surface, or material identifiers are treated as a single entity in constructing a tally edit. In this case, the NPARM normalization divisors are summed to a single divisor. Consequently, one may supply the full list of divisors, if appropriate, or just supply one value for the common tally.
- For IRS > 0, the original source definition record (in LAHET format as described in Section 2.4 of reference [1]) followed by the new source definition record (also in LAHET format).
- For ITCONV \neq 0, a LAHET source time distribution record as described in Section 2.4 of reference [1].
- For IRSP \neq 0, three records defining the user-supplied response function:

ERESP(I),I=1,...,NRESP a monotonically increasing energy grid on which the value of the response function is tabulated;

FRESP(I),I=1,...,NRESP the values of the response function at the above energies;

IRESP(I),I=1,...,NRESP-1 interpolation scheme indicators, where IRESP(I) indicates the interpolation scheme to be used for the response function in the I-th energy interval.

The length NRESP \leq 200 is obtained from the array ERESP input (terminated by a "/"). The user must maintain the proper correspondence among the arrays (see section 22 below).

- Any additional input required for the particular option. For basic option types 1, 2, or 11, this may be the specification of surface segmenting. For basic option types 9, 10, or 12, it is the collimating window definition. Also, for basic option types 1, 9, 11, or 12, an arbitrary vector for angular binning may be input.

The order of the input records as they appear in the INT file is illustrated in Table 4.

3. Edit Option IOPT = 1 or 101 : Surface Current

Option 1 tallies the particle current across the NPARM designated surfaces; it is analogous to the MCNP F1 tally. If IOPT is preceded by a minus sign, the weight binned is multiplied

by the particle energy. The number of energy bins is given by NERG. The number of particle types for which surface crossing data is to be tallied is given by NTYPE and must be > 0 . Current will be tallied on NPARM surfaces; a total over surfaces is not performed. Any of the above particle types may be specified. Binning into NFPRM cosine bins is defined by the value of KOPT. For KOPT = 0 or 5, the cosine is taken with respect to the normal to the surface at the crossing point. For KOPT = 1 or 6, the cosine is taken with respect to the x-axis. For KOPT = 2 or 7, the cosine is taken with respect to the y-axis. For KOPT = 3 or 8, the cosine is taken with respect to the z-axis. For KOPT = 4 or 9, the cosine is taken with respect to an arbitrary vector to be read in.

If KOPT = 5, 6, 7, 8, or 9, the current tallies are binned according to a slicing of each surface into NSEG+1 segments by NSEG planes. In this case, an additional record of the following form is required: "IFSEG,NSEG,FSEG(1), . . . ,FSEG(NSEG)/". For IFSEG = 1 the segmenting planes are perpendicular to the x-axis, for IFSEG = 2 the y-axis, and for IFSEG = 3 the z-axis. The FSEG(I) are the coordinates of the NSEG planes in increasing order.

Segmenting may also be accomplished by using segmenting cylinders. The input has the same format as segmenting by planes; however, IFSEG negative designates cylindrical segmenting. IFSEG = -1 indicates that the segmenting cylinders are concentric with the x-axis; IFSEG = -2 indicates that the segmenting cylinders are concentric with the y-axis; IFSEG = -3 indicates that the segmenting cylinders are concentric with the z-axis. The values of the FSEG array are the radii of nested concentric cylinders and must be in increasing order. Segmenting cylinders are *concentric* with an axis, not just parallel.

For KOPT = 4 or 9, an additional record must be supplied with the direction cosines of the arbitrary vector with which cosine binning is to be made. The form of this record is "CN(1),CN(2),CN(3)/", where the parameters input are the direction cosines of the arbitrary vector with respect to the x-, y-, and z-axes. The vector need not be normalized.

The surface current tally represents the time-integrated current integrated over a surface area and an element of solid angle. Unless otherwise normalized, it is the weight of particles crossing a surface within a given bin per source particle. As such, it is a dimensionless quantity.

4. Edit Option IOPT = 2 or 102 : Surface Flux

The surface flux tally is analogous to an MCNP F2 tally. All particle types listed above may be specified. The number of energy bins is given by NERG. The number of particle types for which surface flux data is to be tallied is given by NTYPE and must be > 0 . NFPRM is unused. If KOPT = 1, surface segmenting is performed as in option 1 above; the same input record to designate the segmenting planes or cylinders must be included as in option 1. If IOPT is preceded by a minus sign, the particle weight is multiplied by its energy before tallying.

The surface flux tally represents the time-integrated flux integrated over surface areas. Unless otherwise modified, it is a dimensionless quantity.

5. Edit Option IOPT = 3 or 103 : Particle Production Spectra

Option 3 may be used to tally the spectra of particles produced in nuclear interactions. It accesses all collision records on HISTP for all particles causing collisions. If IOPT is preceded by a minus sign, the edit is performed only for events initiated by the primary (source) particles. For KOPT = 0 or 1, separate edits are performed for cascade and evaporation phase production. In addition, total nucleon production from either phase is edited. For KOPT = 2 or 3, only the cascade production is edited. For KOPT = 4 or 5, only the evaporation phase production is edited. For KOPT = 6 or 7, only the total particle production is edited. For KOPT = 8 or 9, only the pre-fission evaporation production is edited. For KOPT = 10 or 11, only the post-fission evaporation production is edited. If KOPT is even, the edit is over cell numbers; if KOPT is odd, the edit is over material numbers. If NPARM is zero, the edit is over the entire system. The parameters NTYPE and NFPRM are not used. If KPLOT = 1, a plot is made of each edit table. With KOPT = 0 or 1, the cascade production for neutrons and protons is simultaneously plotted (as a dotted line) with the total production.

Unless otherwise modified, tally option 3 (or 103) represents the weight of particles emitted in a given bin per source particle. As such, it is a dimensionless quantity.

6. Edit Option IOPT = 4 or 104 : Track Length Estimate for Neutron Flux

Option 4 is not available in this version; use a standard F4 flux tally.

7. Edit Option IOPT = 5 or 105 : Residual Masses and Average Excitation

Option 5 provides an edit by mass number A of the calculated residual masses and the average excitation energy for each mass. Only *nonelastic* interactions are included. The option accesses the records on HISTP for all interacting particle types. The edit is performed for both the final residual masses and the residuals after the cascade phase. If IOPT is preceded by a minus sign, the edit is performed for events initiated by primary (source) particles only. For KOPT = 0, the edit is by cell numbers; if KOPT = 1, the edit is by material numbers. If NPARM = 0, the edit is over the entire system. The parameters NTIM, NTYPE, and NFPRM are immaterial. KPLOT = 1 will produce plots of each edit table.

Tally option 5 (or 105) represents the particle weight producing a given nuclide per source particle; as such it is a dimensionless quantity. The mean excitation is in units of MeV.

8. Edit Option IOPT = 6 or 106 : Energy Deposition

Option 6 is not available in this version.

9. Edit Option IOPT = 7 : Mass and Energy Balance

Option 7 is not available in this version.

10. Edit Option IOPT = 8 or 108 : Detailed Residual Mass Edit

Option 8 provides a detailed edit of residual masses by Z and N, by Z only, by N only, and by mass number A. The option accesses the records on HISTP for all interacting particle types. If IOPT is preceded by a minus sign, the edit is performed only for events initiated by primary (source) particles. If KOPT = 0 or 1, the edit is of the final residual masses, including *elastic* collisions. If KOPT = 2 or 3, the edit is of the residuals after the cascade phase and before evaporation. If KOPT = 4 or 5, the edit is of masses immediately preceding fission. If KOPT is even, the edit is by cell number; if KOPT is odd, the edit is by material number. If KPLOT = 1, plots will be produced for each edit table. Parameters NERG, NTIM, NTYPE, and NFPRM are unused. If IXOUT = 1, an auxiliary output file appropriate for input to the CINDER program will be written; the default file name is OPT8A. Unless otherwise modified, tally units are dimensionless (weight of a residual nuclide per source particle).

An additional tabulation is produced which shows the estimated metastable state production as a fraction of the total isotopic production. As illustrated in the example here, a state is identified by its excitation energy and half-life; the estimated fraction of total isotope production associated with the particular metastable state is shown with the estimated relative standard deviation.

z	a	e lev	t-half	fraction
*				
*				
47	110	0.11770	2.17730D+07	4.00000D-01 0.3465
47	111	0.05990	6.50000D+01	8.00000D-01 0.2001
47	116	0.08100	1.05000D+01	5.00000D-01 0.5001
48	113	0.26370	4.41500D+08	2.85714D-01 0.3195
48	115	0.17340	3.87070D+06	5.00000D-01 0.3536
48	117	0.13000	1.22400D+04	2.50000D-01 0.4331
48	119	0.14640	1.62000D+02	6.00000D-01 0.2829
*				
*				

11. Edit Option IOPT = 9 or 109 : Surface Current with Collimating Window

Option 9 is identical to option 1 except that a rectangular or circular "window" is imposed on each surface and the tally made within and without the window. The window is defined by the intersection of a rectangular or circular tube parallel to the x-,y-, or z-axis with the tally surface. A window definition record appears in place of the segmenting record of option 1. For KOPT = 0, 1, 2, 3, or 4, the window is formed by the rectangular tube; the window record has the following allowed forms:

parallel to x-axis: 1,y(min),y(max),z(min),z(max)/
parallel to y-axis: 2,z(min),z(max),x(min),x(max)/
parallel to z-axis: 3,x(min),x(max),y(min),y(max)/

For KOPT = 5, 6, 7, 8, or 9, the window is formed by a circular tube (cylinder); the window record has the following allowed forms:

parallel to x-axis: 1,y(center),z(center),radius/
parallel to y-axis: 2,z(center),x(center),radius/
parallel to z-axis: 3,x(center),y(center),radius/

12. Edit Option IOPT = 10 or 110 : Surface Flux with Collimating Window

Option 10 is identical to option 2 except that the edit is performed inside and outside a "window" defined as in option 9. Instead of the segmenting record of option 1 a window definition record appears, whose form is described in option 9. For KOPT = 0, the rectangular form is used, and for KOPT = 1, the circular form is used. Parameter NFPRM is unused.

13. Edit Option IOPT = 11 or 111 : Pulse Shape of Surface Current

For each defined bin, option 11 provides an edit of the current crossing a surface in an energy and angle bin, the mean time \bar{t} of crossing in the bin, the standard deviation σ of \bar{t} given by $(\bar{t}^2 - \bar{t}^2)^{\frac{1}{2}}$, the figure of merit FOM1 given by $(\text{current})/\sigma^2$, and the figure of merit FOM2 given by $(\text{current})/\sigma^3$.

Unless otherwise modified, the current tally is dimensionless. The units of \bar{t} and σ are nanoseconds, while FOM1 is in ns^{-2} and FOM2 is in ns^{-3} . The parameter FNORM is used to adjust the units of the time variable, which are nanoseconds in LAHET3, and does *not* modify the surface current edit. Thus to convert from nanoseconds to microseconds, use FNORM = 0.001. The bin definition is identical to option 1, *including surface segmenting*, except that NTIM is unused.

14. Edit Option IOPT = 12 or 112 : Pulse Shape of Surface Current with Window

Option 12 provides the same edits as option 11 with the same bin definition as option 9 using a collimating “window”. The input is identical to option 9, with the exception that NTIM is unused.

15. Edit Option IOPT = 13 : Global Emission Spectrum

The original definition[1] of option 13 was given by

Option 13 tallies the number of particles per unit solid angle entering the external void region with direction cosine falling within a segment of solid angle; as such, it represents the angular distribution of the emitted particles at a very large distance from the interaction region. The option uses any NCOL = 4 leakage records on HISTP and *all* records on HISTX indiscriminately.

Surface crossing records appearing on a SSW-written file are not distinguished as to whether they correspond to an internal surface crossing or to escape into the external void. Therefore for use with MCNPX, the original intent of this option may most easily be achieved by defining the external importance 0 (leakage) region as the exterior of a sphere containing the complete geometry; then *only* specifying the defining spherical surface on the SSW card that controls the contents of the surface crossing file.

Energy binning is specified by the usual methods. The number of energy bins is given by NERG. The number of particle types for which surface crossing data is to be tallied is given by NTYPE and must be > 0 . The polar angle bins (representing lines of latitude) are defined by entering the NFPRM cosine values in the FPARM array. Binning in the azimuthal angle ϕ , corresponding to lines of longitude, is determined by the value of NPARM, which defines NPARM equal azimuthal angle bins from a lower bound of 0° on the first bin to an upper bound of 360° on the last bin. The value of KOPT determines the orientation used to define the angles as shown in Figure 1. The allowed options are as follows:

KOPT = 1: the +z-axis defines the polar angle and ϕ is measured counter-clockwise from the +x-direction;

KOPT = 2: the +z-axis defines the polar angle and ϕ is measured counter-clockwise from the +y-direction;

KOPT = 3: the +x-axis defines the polar angle and ϕ is measured counter-clockwise from the +y-direction;

KOPT = 4: the +x-axis defines the polar angle and ϕ is measured counter-clockwise from the +z-direction;

KOPT = 5: the +y-axis defines the polar angle and ϕ is measured counter-clockwise from the +z-direction;

KOPT = 6: the +y-axis defines the polar angle and ϕ is measured counter-clockwise from the +x-direction.

A value of KOPT = 0 defaults to KOPT = 1. For NPARM \geq 1, a null record "/" must be supplied in place of the LPARM array; NPARM = 0 defaults to NPARM = 1, but the null record need not be supplied. If a null record is supplied for the FPARM array, NFPRM equal cosine bins from -1.0 to 1.0 are supplied.

The following is an example of the input for using option 13:

```
Title 1: Option 13 Example
Title 2: 100 Equal Solid Angle Bins
13,-10,,1,1,10,10/, ,
-0.5,800./
1/
/
/
/
```

In this case, the energy is binned in 10 equal lethargy intervals of half-decade width below 800 MeV and normalized per MeV. No time binning is done. Only neutrons are edited. The z-axis determines the polar angle and the azimuthal angle is measured from the x-axis. Ten azimuthal angle bins are used and 10 equal polar angle cosine bins are defined by taking the default. Note that the last four records could be written on one line as "-0.5,800./1///".

Tally option 13 may be considered as the time-integrated particle current integrated over a sphere in a void at a very large distance for the interaction region. Since it is normalized per unit solid angle, the units are dimensionless, being sr^{-1} per source particle.

16. Edit Option IOPT = 14 or 114 : Gas Production

Option 14 provides an edit of hydrogen and helium gas production, by isotope, by element, and total. Unless modified by FNORM, the units of gas production are atoms per source particle. If KOPT = 0, the edit is by cell number; if KOPT = 1, the edit is by material. NERG, NTIM, and NTYPE are unused. The estimate is made by tallying all H and He ions stopped in a cell or material, including source particles.

17. Edit Option IOPT = 15 or 115 : Isotopic Collision Rate

Option 15 has been added to provide a collision rate edit by target isotope. The input has the same meaning as for IOPT = 8, with the following exceptions: KOPT = 0 or 1 tabulates

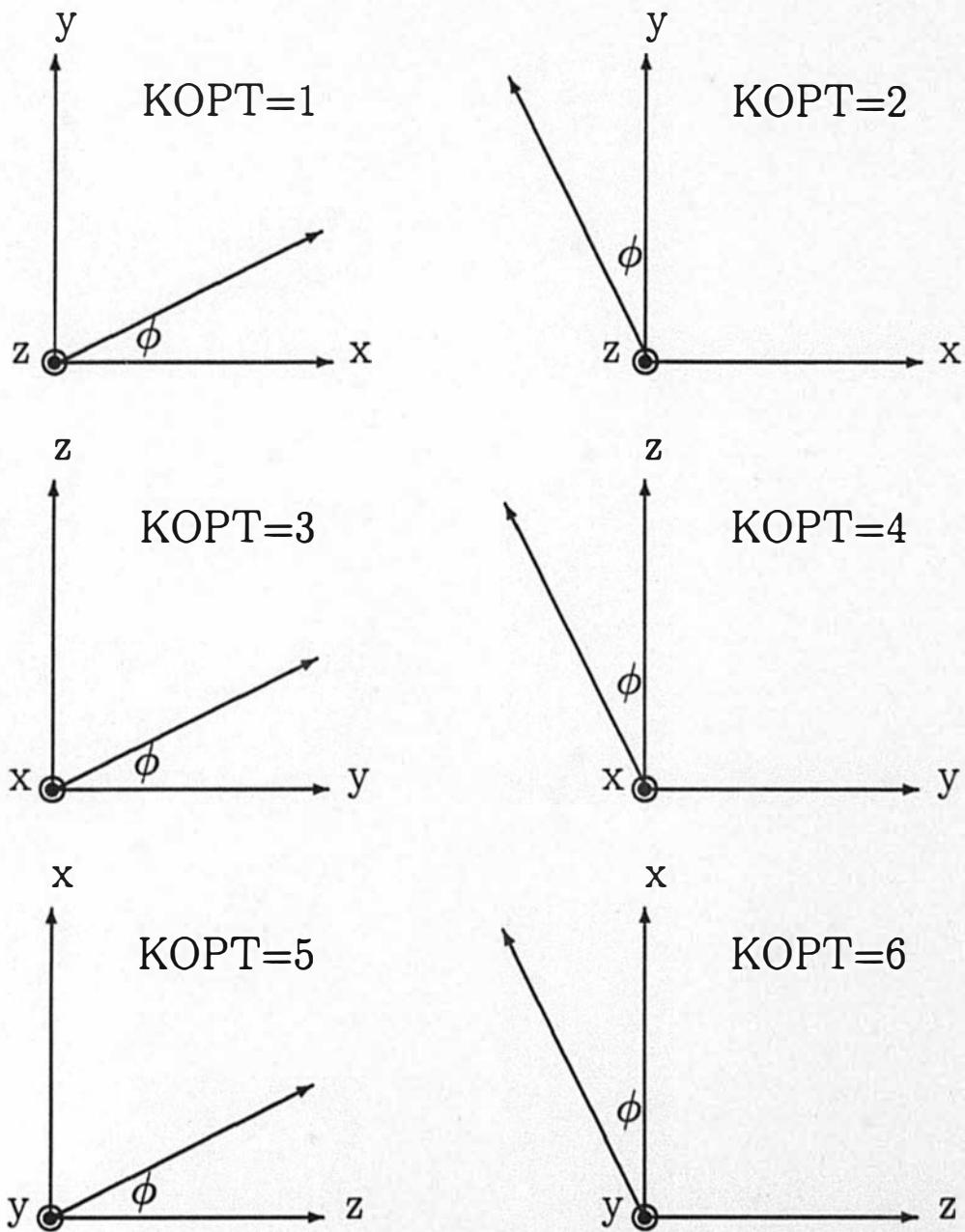


Figure 1: Use of the KOPT Parameter for HTAPE3X Option 13

all collisions; KOPT = 2 or 3 tabulates elastic scattering only; KOPT = 4 or 5 tabulates nonelastic events only. If KOPT is even, the edit is by cell number; if KOPT is odd, the edit is by material number. A CINDER removal rate input file will be produced for IXOUT > 0. The default CINDER file name is OPT15A.

18. Edit Option IOPT = 16 or 116 : Recoil Energy and Damage Energy Spectra

Option 16 provides an edit of the spectra of total recoil energy, elastic recoil energy, total damage energy, and elastic damage energy. Also estimated are the mean weight of recoiling fragments per history, mean weight of recoil (or damage) energy per history, and the mean energy per fragment (the ratio of the previous two estimates). NERG specifies the number of energy bins for the spectra; a minus sign on NERG will have the tabulation normed per MeV (recommended to produce a true spectrum). Input variables NTIM, NTYP, NFPRM, IXOUT, IRS, IMERGE, ITCONV, and IRSP are unused. KOPT = 0 indicates tally by cell; KOPT = 1 indicates tally by material. NPARM is the number of cells (or materials) to be read in for the tally. If a minus sign flag is used with IOPT (IOPT = -16), the weights tallied for the spectra will be multiplied by corresponding recoil (or damage) energy.

At any collision, the damage energy E_d is obtained from the recoil energy E_r of nucleus A_r, Z_r by the relation of Linhard[4]

$$E_d = E_r L(E_r)$$

using the formulation of Robinson[5]:

$$\begin{aligned} k_i &= \frac{0.133745 Z_r^{2/3} Z_i^{1/2}}{A_r^{3/2} A_i} \left(\frac{A_r + A_i}{2} \right)^2 \left(\frac{2}{Z_r^{2/3} + Z_i^{2/3}} \right)^{3/4} \\ \epsilon_i &= \frac{0.03252 A_i E_r}{(A_r + A_i) Z_r Z_i (Z_r^{2/3} + Z_i^{2/3})^{1/2}} \\ g(\epsilon_i) &= \epsilon_i + 0.40244 \epsilon_i^{3/4} + 3.4008 \epsilon_i^{1/6} \\ L(E_r) &= \sum_{i=1}^n \frac{f_i}{1 + k_i g(\epsilon_i)} \end{aligned}$$

where the summation is over the components of the material with atom fractions f_i .

19. The Resource Option

The RESOURCE option allows the user to edit the data available on a history file while altering the assumed spatial distribution of the source from that used in the original calculation. For its application, see reference [1]

20. The Merge Option

Not used in HTAPE3X. For any tally *either* the HISTP file *or* the HISTX file is edited, but not both.

21. The Time Convolution Option

Assume that an initial calculation has been made with the default source time distribution (i.e., all histories start at $t=0$). A time-dependent tally for *any* of the allowed LAHET source time distributions may then be made with HTAPE3X without rerunning the transport calculation. For details, see reference [1].

22. The Response Function Option

Any non-zero value of the IRSP parameter allows the user to apply an energy-dependent response function $F(E)$, where E is the particle energy, to the current and flux tallies given by edit option types 1, 2, 4, 9, 10, and 13. The user supplies a tabulation of the function $F(E)$ by the pairs of values FRESP(I), ERESP(I) which are input as the arrays ERESP(I), I=1,...,NRESP and FRESP(I), I=1,...,NRESP described in section 2 above. The element IRESP(I) of the third input array then specifies an interpolation scheme for computing the response function value within the interval $ERESP(I) < E \leq ERESP(I+1)$. For IRSP > 0 , the interpolated response function value *multiplies* the tally increment; for IRSP < 0 , it *divides* the tally increment.

There are five interpolation schemes that may be specified individually for each energy interval in the response function tabulation, using the following values for IRESP(I).

1. Constant: the response function value is the value at the lower energy of the interval.
2. Linear-linear: the response function is interpolated linearly in energy.
3. Linear-log: the response function is interpolated linearly in the logarithm of the energy.
4. Log-linear: the logarithm of the response function is interpolated linearly in energy.
5. Log-log: the logarithm of the response function is interpolated linearly in the logarithm of the energy.

Any value of IRESP(I) outside the range [1,5] is treated as 1 (i.e., constant over the interval).

The energy range for the specified response function need not span all possible particle energies in the problem. If a particle energy falls below ERESP(1), then FRESP(1) is used as the value of the response function. Similarly, if a particle energy exceeds ERESP(NRESP), then FRESP(NRESP) is used as the value of the response function.

23. Executing HTAPE3X

The default file name for the input is INT, the default file name for the output is OUTT, the default file name for the history file is HISTP, and the default file name for the surface crossing file is HISTX for input into HTAPE3X. (The latter is written by MCNPX with the default file name WSSA.) If option 8 is requested, the data file PHTLIB must be in the user's file space; if option 16 is requested, the data file BERTIN must be in the user's file space. All these file names may be defined by file replacement on the execute line:

```
HTAPE3X INT=my_input OUTT=my_output HISTP=file1 HISTX=file2
```

References

- [1] Richard E. Prael and Henry Lichtenstein, "User Guide to LCS: The LAHET Code System", LA-UR-89-3014, Los Alamos National Laboratory (September 1989).
<http://www-xdiv.lanl.gov/XCI/PROJECTS/LCS/lahet-doc.html>
- [2] H. G. Hughes, R. E. Prael, and R. C. Little, "MCNPX – The LAHET/MCNP Code Merger", X-Division Research Note XTM-RN(U)97-012, LA-UR-97-4891, Los Alamos National Laboratory (April 1997).
<http://www-xdiv.lanl.gov/XTM/hughes/LA.UR.97.4891/cover.html>
- [3] Judith F. Briesmeister, editor, "MCNPTM - A General Monte Carlo N-Particle Transport Code", Los Alamos National Laboratory report LA-12625-M (March 1997).
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- [4] J. Linhard, V. Nielsen, and M. Scharff, *Kgl. Dan. Vidensk. Selsk., Mat.-Fys. Medd.* **36**, No. 10 (1968)
- [5] M. Robinson, "The Dependence of Radiation Effects on Primary Recoil Energy", *Radiation Induced Voids in Metals*, AEC Symp. Ser. 26, p. 397, U. S. Atomic Energy Commission (1971).