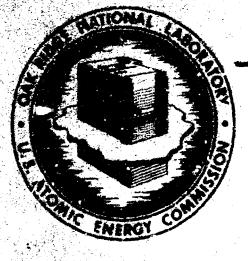
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ORNL-4744 UC-32 - Mathematics and Computers

## OPERATING INSTRUCTIONS FOR THE HIGH-ENERGY NUCLEON-MESON TRANSPORT CODE HETC

K. C. Clandler T. W. Armstrong



#### OAK RIDGE NATIONAL LABORATORY

operated by UNION CARBINE CORPORATION for the U.S. ATOMIC ENERGY COMMISSION

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Prints: in the United States of America: Available from Noticisal Technical Information Service U.S. Department of Commune 5285 Port Royal Read, Springfield, Virginia 22151 Price: Brinsed Copy \$3.55; Microfiche 50.95

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#### Neutron Physics Division

#### OPERATING INSTRUCTIONS FOR THE HIGH-ENERGY NUCLEON-MESON TRANSPORT CODE HETC

K. C. Chandler\* and T. W. Armstrong

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#### **JANUARY 1972**

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#### Abstract

The high-energy nucleon-meson transport code HETC computes the transport of nucleons, charged pions, and muons through matter for energies up to several hundred GeV by using Monte Carlo methods. This report is primarily concerned with the programming aspects of HETC. Instructions for operating the code are given, and the code input is described. HETC is written in FORTRAN IV for the IBM 360/75 and IBM 360/91 computers.

#### ACKNOWLEDGMENT

We wish to thank Dr. T. A. Gabriel for helpful discussions concerning the incorporation of the extrapolation model into HETC.

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#### 1. INTRODUCTION

The high-energy nucleon-meson transport code HETC is basically an extension of the nucleon-meson transport code NMTC<sup>1</sup> to allow particle transport at energies  $\geq 3$  GeV.<sup>\*</sup> Although the transport of particles  $\leq 3$  GeV in HETC is essentially the same as in NMTC, there are several minor differences. HETC also contains several programming options not available in NMTC. Throughout much of this report the operation of HETC is compared with that of NMTC. Therefore, the reader is assumed to have some familiarity with NMTC.

The version of 05R used with HET is the same as the version used with NMT except for one very minor programming modification relating to buffering (see Sec. 3). The input description for 05R is the same as described in the NMTC manual.<sup>1</sup> As with NMT, HET may be readily coupled with codes other than 05R (e.g., ANISN,<sup>2</sup> DOT,<sup>3</sup> MORSE<sup>4</sup>) to obtain the low-energy neutron transport.

The principal differences between HET and NMT with respect to both the transport physics and programming options are discussed in Sec. 2. The tape buffering option available in HETC is described in Sec. 3, and the input description for HET is given in Sec. 4.

<sup>\*</sup>A few words about code nomenclature: Physically, NMTC consists of two transport codes: (a) NMT, a transport code for neutrons ( $\geq$  15 MeV), protons, charged pions, and muons, and (b) a code for low-energy ( $\leq$  15 MeV) neutron transport. For the standard version of NMTC, a modified version of the 05R code is used for the low-energy neutron transport. A similar convention is used for HETC; i.e., HET is designated as the transport code for neutrons ( $\geq$  15 MeV), protons, charged pions, and muons, and HETC includes both HET and O5R.

#### 2. DIFFERENCES BETWEEN HET AND NMT

#### 2.1 Physics

#### 2.1.1 Maximum Energy

NMT is limited to nucleon transport  $\leq 3.5$  GeV and charged-pion transport  $\leq 2.5$  GeV because of certain restrictions imposed by the intranuclear-cascade routines. HET will accommodate nucleons and charged pions with energies up to several hundred GeV. There is no programming restriction on the maximum allowable muon energy by either NMT or HET.

For nucleons  $\leq$  3.5 GeV and charged pions  $\leq$  2.5 GeV, HET treats nonelastic nuclear interactions by using the intranuclear-cascade-evaporation model in the same manner as does NMT. For nucleon-nucleus and pion-nucleus conelastic collisions at higher energies, HET first calls the intranuclear-cascade routines to determine the collision products at 3.5 GeV (if the incident particle is a neutron or proton) or at 2.5 GeV (if the incident particle is a charged pion). The information (particle types, energies, direction cosines, etc.) obtained from the intranuclear cascade is then input to scaling routines that use an extrapolation model<sup>5</sup> to obtain the description of the collision products corresponding to the actual energy of the particle. Scaling is not used for nucleon and charged-pion interactions with hydrogen at energies > 3.5 GeV. These interactions are treated using the formulae of Ranft<sup>6</sup> in the manner described by Gabriel and Santoro.<sup>7</sup>

Unlike NMT, HET does not have an internal check on the energy of the particle returned by subroutine SØRS. Thus, in principle, there is no restriction on the maximum energy of the source particles in HETC. In practice, the maximum energy is restricted both by the physics used for the high-energy nonelastic nuclear interactions (as the energy increases, the extrapolation

model becomes more approximate) and by programming considerations (dimensions for arrays pertaining to particle storage during a cascade may be exceeded at very high energies). Thus, the maximum allowable energy in HET is not well defined. HET has been run successfully for source particles with energies up to 1 TeV.

#### 2.1.2 Intranuclear-Cascade Routines

The intranuclear-cascade routines used by NMT correspond to version 2 of Bertini's medium-energy cascade code (MECC2)<sup>8\*</sup> whereas the latest version of the cascade routines (MECC7)<sup>9</sup> has been incorporated into HET. The main differences between MECC2 and MECC7 concern the particle-particle cross sections, the angular distributions for isobar states, and the neutron and proton cutoff energies.

The nucleon-nucleon cross sections above 1 GeV and the pion-nucleon cross sections at all energies used in MECC2 have been updated for use in MECC7.

In MECC2 the angular distribution of isobars is an input option which can be selected (for all energies) as either isotropic, forward-backward, or 50% isotropic and 50% forward-backward. (In the NMT input this option corresponds to the variable ANDIT.) In MECC7 the angular distribution is specified internally (in subroutine ANGID) as an energy-dependent mixture of isotropic and forward-backward distributions. (The distributions used are given elsewhere.<sup>10</sup>) Therefore, ANDIT does not appear in the HET input.

The intranuclear-cascade cutoff energies for neutrons and protons are specified by a variable called CTØFE in both the NMT and HET inputs. However, the cutoff energies used when CTØFE is input as 0. is not the same

<sup>\*</sup>Reference 8 gives a description of the MECC3 version of the intranuclearcascade routines. The only difference between MECC2 as referred to here and MECC3 described by Bertini in ref. 8 is in the options available for cutoff energies used in the intranuclear-cascade calculations.

in MECC7 as in MECC2. In the NMT input,  $CT \not PFE = 0$ . means that the MECC2 cutoff energy for both neutrons and protons will be set equal to one-half the Coulomb barrier. In the HET input,  $CT \not PFE = 0$ . means that the MECC7 cutoff energy for protons will be set equal to the Coulomb barrier and the cutoff energy for neutrons will be set to 0. The action taken when  $CT \not PFE \neq 0$ is the same in both MECC2 and MECC7; i.e., the input value for  $CT \not PFE$  is used for both the neutron and proton cutoff energies. In both MECC2 and MECC7 the  $\pi^+$  cutoff energy is set equal to the proton cutoff energy and the  $\pi^0$ and  $\pi^-$  cutoff energies are set equal to the neutron cutoff energy.

#### 2.1.3 Multiple Coulomb Scattering

An option to include multiple Coulomb scattering by <u>primary</u> charged particles (protons,  $\pi^+$ ,  $\pi^-$ ,  $\mu^+$ ,  $\mu^-$ ) has been incorporated into HET. The routines for Coulomb scattering were taken from Kinney's NTC code<sup>11</sup> and modified to include scattering by charged pions and muons. The multiple Coulomb scattering theory used<sup>12</sup> is based on Fermi's joint distribution function for angular and lateral spread and Rutherford's single-scattering cross-section formula.

#### 2.2 Programming

#### 2.2.1 Tape Buffering

In NMTC the writing and reading of history tapes is performed using the standard FORTRAN  $I/\emptyset$  routines. When a tape error is encountered using FORTRAN  $I/\emptyset$ , control is given to the operating system rather than the user's program. Thus, a tape error results in the termination of the job at the point at which the error occurs.

In HETC an option has been added so that the ORNL tape buffering package can be used. With buffering, in most instances information can be written and read after a tape error occurs. The use of tape buffering with HETC is described in Section 3.

#### 2.2.2 Joint Muon and Nucleon-Pion Transport

In NMT two options exist for muon transport: (a) muon transport only, in which the muon source is defined in subroutine SØRS, and (b) muon transport following a nucleon-pion transport, in which the muon source is obtained by reading a previously generated nucleon-pion history tape. Option (b) requires two separate NMT runs for the nucleon-pion and muon transport.

In HET a third option has been added to allow the nucleon-pion and muon transport calculations to be carried out jointly during the same HET run. In this option, the muons produced are stored in arrays for subsequent transport during the cascade in the same manner as nucleons and pions. Thus, the nucleon-pion-muon history tape will have records containing the muon transport information intermittent with records containing nucleon and pion information. The muon information can be identified by analysis programs from the particle-type variable (TIP) which is included in the records (TIP = 5. for  $\mu^+$ , TIP = 6 for  $\mu^-$ ).

#### 2.2.3 Storage Requirements

The minimum memory requirement for NMT is approximately 575,000 bytes. HET requires approximately 1,000,000 bytes.

#### 3. TAPE BUFFERING WITH HETC

#### 3.1 General Comments

#### 3.1.1 Tape Buffering

The ORNL tape buffering package can be used to both output and input data on magnetic tape and, in some instances, can be used to input data from a tape which was created with FOPTRAN write statements. Both output and input buffering are used for the HET nucleon-pion-muon history tape, but only input buffering is used with the HET low-energy neutron tape and the \$5R collision tape.

Depending upon the choice of RECFM, LRECL, and BLKSJZE, one or more logical records, in part or in entirety, may be contained within a given physical record on a tape created with FORTRAN write statements. Since there are no blocking factors built into the buffering package per se, a physical record will be created each time an output buffering command is issued. Similarly, the contents of an entire physical record must be input with a single buffering request if all of the data in that physical record are to be retrieved.

If a tape error occurs during a buffering operation, control is returned to the calling program along with a flag indicating that an error has occurred. In most instances, the outcome of subsequent buffering operations will not be affected. As a general rule, if an error occurs during execution of an input buffering request, the contents of the entire physical record should be ignored.

The buffering package does not automatically request a new tape to be mounted when the end of tape is reached during input or output buffering. However, the calling program may indicate that a new tape is to be used

by simply using a different logical unit number in the next buffering request.

There must be a separate data definition card supplied for each reel of tape on which buffering operations are to be performed, and each tape must be defined by a unique logical unit number. In order to use one tape drive for more than one reel of tape, the unit-affinity (UNIT = AFF) option may be invoked. If the affinity option is used, the DD cards for the tapes affected should precede those for all other tapes.

3.1.2 Data Definition Control Cards

The most general form of the data definition control card for a tape on which buffering operations are to be performed is as follows:

//G\$\u00c6.BUjjFOO1 DD UNIT=TAPE1,LABEL=(,NL),

// VØLUME=SER=kk,DISP=ØLD,

//\_DCB=(DEN=\_\_\_\_,TRICH=\_\_\_\_\_

where jj = logical unit number for the tape, (58<jj<99),

kk = jj, (normally), and

i = 7 or 9.

Note that the DCB field is only applicable for 7-track tapes and may be omitted for 9-track tapes.

3.2 Buffering in HET and HET Analysis

3.2.1 The HET Nucleon-Pion-Muon History Tape

In order to request output buffering on the HET nucleon-pionmuon history tape (NHSTP), the logical unit number for NHSTP must be input between 58 and 99 inclusive. Another input parameter, MXHIST, allows the user to specify the maximum number of buffered history tapes that may be filled. If MXHIST is left blank or zero, the program will set MXHIST

internally to five. When an "End of Tape" marker is encountered during an output buffering operation on NHSTP, a comparison is made between MXHIST and the current number of filled tapes. If the number of filled tapes is less than MXHIST, the program will increment the logical unit number of NHSTP by one and return to the normal sequence of instructions. If MXHIST tapes have been filled, the program will write out a message to that effect, set MAXBCH equal to the number of completed batches and proceed to the "End of Run" coding.

HET does an internal banking of particle event records in an effort to minimize the amount of blank tape used for record gaps. The bank, a dimensioned variable called BUFFER in subroutine BFØUT, can store a maximum of 4800 bytes of information. A variable named MXCØL, preset to 20 in subroutine BFØUT, determines the maximum number of particle-event records that may be stored. When either of these maxima is reached, the contents of the bank are buffered out, forming one physical record on the tape. This choice of blocking factors should make the effective amount of tape used comparable to the amount which might be used with the FORTRAN I/Ø package.

In the event that a tape error occurs during an output buffering request, a message to that effect will be written on the standard output unit. As many as fifteen attempts will be made to output each physical record. Unless a message indicates that the fifteenth attempt was unsuccessful, no information was lost in writing and these messages should be ignored.

In the HET card deck, there must be a separate DD card for each tape to be used for NHSTP. The logical unit number on the first DD card must be the same as the value of NHSTP in the HET input. For each subsequent card, the logical unit number should be incremented by one.

Given below is a sample set of DD cards for an HET run in which NHSTP is input as 59 and MXHIST is input as 3.

//GØ.BU59FOO1 DD UNIT=TAPE9,LABEL=(,NL),

//\_VØLUME=SER=59,DISP=ØLD\_\_\_

//G\$.BU60F001\_DD\_UNIT=AFF=BU59F001,

//\_LABEL=(,NL),VØLUME=SER=60,DISP=ØLD

//G\$.BU61F001 DD UNIT=AFF=BU59F001,

// LABEL=(,NL),VØLUME=SER=61,DISP=ØLD

The use of the UNIT = AFF option will cause BU60 and BU61 to use the same tape drive as BU59, and this should be noted under the "special handling" column on the job submission form.

#### 3.2.2 Subroutines BUFNMT and BFIN

Two new subroutines, BUFNMT and BFIN, have been written to retrieve data from an HET history tape created with the buffering package. In the normal course of events, subroutine BFIN will buffer in the contents of a physical record from the history tape and "de-bank" this information into single-particle-event records to be processed by subroutine BUFNMT. However, if a tape error occurs during the input buffering operation, no attempt will be made to analyze any of the particle-event records contained within the physical record. Instead, a message will be written on the standard output unit, and normal processing will continue with the contents of the next physical record. The amount of information lost when a tape error occurs will depend largely upon the banking factors used in HET.

If buffering efforts continue to be unsuccessful on subsequent records, NCØL will be set to -4, signalling "End of Run." In the event that a run is terminated prematurely, an internal batch counter, rather than the

number of batches requested to be analyzed, should be used for normalization purposes.

In order to incorporate the buffering option into existing analysis codes which read the HET history tape using FORTRAN I/Ø, the following statements, or their equivalent, should be inserted immediately before the first executable statement in subroutine REDNMT.

IF (NHST.LT.58) GØ TØ 1001

CALL BUFNMT

RETURN

1001 CONTINUE

To use these two routines, the logical unit number for NHSTP must be input between 58 and 99 inclusive. Subroutine BUFNMT will increment the logical unit number of the history tape by one for each continuation tape needed and each tape to be used must be defined by a separate control card.

#### 3.3 Buffering in \$5R and \$5R Analysis

3.3.1 **SR** Source Tape

An option has been added to the HETC version of  $\emptyset$ 5R to allow input buffering to be used on the HET low-energy neutron tape (NEUTP). The only restriction is that the FORTRAN I/ $\emptyset$  data definition card for NEUTP used in the HET card deck must conform to the following specifications:

1) RECFM = VBS (or VB)

2) 40 < LRECL < 3600

3) 44 < BLKSIZE < 3604

As a general rule, a choice of 40 for LRECL and 804 for BLKSIZE is recommended. A FORTRAN record, 36 bytes in length, is written in HET for each low-energy neutron produced. Thus a choice of 40 for LRECL and 804 for BLKSIZE would allow each physical record to contain the data for 20 lowenergy neutrons.

In order to request buffering on NEUTP, the value of NEUTP input to \$5R must be between 58 and 99 inclusive. Each tape to be used must be defined by a buffer tape data-definition card and, for each tape after the first, the logical unit number must be incremented by one.

In the event that a tape error is detected during an input buffering operation on NEUTP, a special record (NCØLL = 99) will be written on the Ø5R output collision tape. The information contained within the physical record on which the error occurred will not be used. Processing will continue with the contents of the next physical record. If tape errors persist on subsequent records, the run will be terminated.

3.3.2 The Ø5R Collision Tape

With the introduction of two new subroutines, BUF#5R and BFIN, it is now possible to input data, via the buffering package, from an #5R collision tape (NHISTR) created with FORTRAN write statements. In order to be acceptable for input buffering, the DCB field of the FORTRAN datadefinition card used for NHISTR in the #5R card deck must adhere to the following specifications:

- 1) RECFM = VBS (or VB)
- 2)  $1024 \leq LRECL \leq 10240$
- 3) 1028 < BLKSIZE < 10244

For most cases, a choice of 1024 for LRECL and 10244 for BLKSIZE is recommended.

To incorporate the buffering option in existing ØSR analysis codes which use FORTRAN I/Ø, the following statements, or their equivalent, should be inserted before the first executable statement in subroutine REDØSR:

IF (NHISTR.LT.58) GØ TØ 1001

CALL BUFØ5R (NHISTR, NHISMX, NTYPE, NWPCØL)

RETURN

1001 CONTINUE

Subroutine BUFØ5R will expect the value of NHISTR to be between 58 and 99 inclusive and the value of NHISMX to be the logical unit number of the last continuation tape to be used for NHISTR. For example, if three collision tapes were written in Ø5R, NHISTR could be input as 60 and NHISMX as 62. If only one reel of tape is to be used, NHISMX should be equal to NHISTR. The logical unit number on the buffer tape DD card for each continuation tape should be incremented by one.

In BUFØ5R, there are two methods available for the handling of tape errors. An integer variable, IERRØR, governs the path to be taken in BUFØ5R if a tape error occurs. If IERRØR is any nonzero value, only the contents of the physical record on which the error occurred will be omitted. Processing will continue with the contents of the next physical record.

In the alternate procedure (IERR@R = 0), the results from the entire batch(s) in which the error occurred will be omitted. Depending on the blocking factors used in the corresponding Ø5R run, a single physical record could contain information from more than one batch. If IET2@R is equal to zero, subroutine BUFØ5R will set NTYPE (the third variable in the argument list)

to the negative of the number of affected batches when a tape error has occurred or when an NCØLL of 99 has been encountered on the collision tape. The calling program should then zero out any results calculated only for the current batch without adding these data to the cumulative results for the entire run. Upon the next call to BUFØ5R, the first record in the next batch to be considered will be returned. An internal batch counter should be kept for normalization purposes but should not be incremented when a negative value for NTYPE is returned.

The value of IERRØR is determined by a data statement in BUFØSR. With either of the two procedures, NTYPE will be set to 3, signalling "End of Run," if tape errors occur on several consecutive records.

#### 4. **AET INPUT DESCRIPTION**

4.1 Order of Input

The order of the input for HET is as follows:

- 1. The primary HET input data (described in Section 4.2);
- 2. Elastic scattering input data, if any (described in Section 4.3);
- 3. The geometry input data (described in Section 4.4);

4. Any input required by subroutine SØRS (described in Section 4.5).

#### 4.2 Primary HET Input Description

A description of the cards composing the primary HET input data is given below. Most of the input is the same as for NMT. As mentioned in Section 2, the variable ANDIT (card F of NMT input) is omitted from the HET input, and an input value of 0. for CTØFE has a different meaning in the HET input from that in the NMT input. The other differences between the HET and NMT inputs are underlined in the description below.

Cards A and B: FØRMAT (20A4)

80 columns each of Hollerith identification for the printed output. Card C: FØRMAT (324)

RANDØM: Hexadecimal representation of initial random number to be used in the generation of random numbers. Should be positive and end in 1, 3, or 5. Card D: FØRMAT (E10.4, E10.4, E10.4, I10, I10, I10, I10)

- a. EMAX: The maximum energy of particles being transported in MeV. For source muons EMAX is arbitrary. However, if source muon data are to be obtained from a previously produced nucleon-pion history tape, then by conservation of energy EMAX should not be less than  $E_{\pi,max} + m_{\pi} - m_{\mu} = E_{\pi,max} + 33$ , where  $E_{\pi,max}$  is the value of EMAX which was input for the nucleon-pion calculation,  $m_{\pi}$  is the charged-pion rest mass, and  $m_{\mu}$  is the muon rest mass.
- b. ELØP: The cutoff energy in MeV for transporting protons.
   The code computes the cutoff energy for pions as
   (pion rest mass/proton rest mass) × ELØP = 0.1488 × ELOP,

and for muons as

(muon rest mass/proton rest mass) ×  $EL \phi P = 0.1129 \times EL \phi P$ .

- c. ELØN: The cutoff energy in MeV for transporting neutrons. Normally ELØN will be chosen equal to ELØP. For muon transport ELØN is irrelevant.
- d. MXMAT: The number of different media, exclusive of voids, appearing in the system. 0 < MXMAT < 16.
- e. MAXCAS: The number of source particles to be started in each batch.
- f. MAXBCH: The number of batches to be run with the present set of input data. The total number of source particles initiated with the present input will be MAXCAS\*MAXBCH. For muon transport using a previously produced nucleonpion history tape, both MAXCAS and MAXBCH are calculated in subroutine MFPD; hence input values for these quantities are not used although they are written on the muon collision tape.
- g. N1CØL: If N1CØL > 0, each cascade history will be computed only through the second generation, that is, only through the immediate descendants of source particles. If N1CØL  $\leq$  0, all generations will be computed. Normally N1CØL is input as 0 or left blank. N1CØL is irrelevant for muon transport.

Card E: FØRMAT (110, 110, 110, 110, 110, 110)

- a. NQUIT: The number of runs with the present set of input data. Normally NQUIT will be input as 1. At the end of each run, signaled by NCØL = -4, subroutine USER (NCØL) is called. The standard version of this routine is a dummy. The user may provide his own version of USER to output specified variables or to change certain input quantities before the code calculates the next run, if any. In both cases, it will usually be necessary to include a labeled common called CØMØN. USER is also called at the end of each batch.
- b. <u>NEUTP</u>: If nucleons and pions are to be transported, NEUTP is the logical number for the tape on which descriptions of neutrons appearing below ELØN are written. If <u>NEUTP  $\leq 0$ </u>, <u>the low-energy neutron tape will not be written</u>. If the transport is for muons and source muons are to be obtained from a previously produced nucleon-pion history tape, then NEUTP is the logical number of the nucleonpion history tape. If  $58 \leq \text{NEUTP} \leq 99$ , tape buffering will be used to input data from the nucleon-pion history tape.
- c. <u>NBERTP</u>: The logical number of the tape containing the data needed in the intranuclear-cascade and evaporation calculations. If a calculation is to be made for muons only, NBERTP should be input as 0. <u>If muons are to be transported in the same</u> <u>run as nucleons and pions, NBERTP should be input as the</u> <u>negative of the logical number of the tape</u>.

- d. NPØWR2: NGRØUP =  $2^{NPØWR2}$ . NGRØUP is the number of energy groups used in computing the range and energy tables. NPØWR2  $\leq$  11. Normally a value of 10 or 11 should be input.
- e. NPIDK: If NPIDK is positive, x<sup>-</sup> mesons reaching the x energy cutoff (= .1488 ELØP) will be assumed to decay at the spatial point where the cutoff has been reached. For NPIDK ≤ 0,
   x<sup>-</sup> mesons reaching their energy cutoff will be forced to interact via the intranuclear-cascade subroutine. NPIDK is irrelevant for muon transport.
- f. <u>NHSTP</u>: The logical tape number of the nucleon-pion or muon history tape. If NHSTP is input as 0, it is assumed that the user will not write a history tape but will provide his own version of subroutine ANALYZ which normally writes the history tape. If NHSTP is input between 58 and 99 inclusive, tape buffering will be used in producing the history tape.
- g. <u>MXHIST</u>: <u>The maximum number of buffered history tapes that may be</u> <u>filled. MXHIST is irrelevant if tape buffering is not</u> <u>being used on NHSTP</u>.

Card F: FØRMAT (10X, E10.4, 110, 110, 110, 110)

Quantities a and b on this card are irrelevant when transporting muons only.

a. CTØFE: A signal to indicate the cutoff energy to be used in the intranuclear-cascade calculations. Normally CTØFE should be input as 0.

- NEXITE: EX, the excitation of the residual nucleus immediately ь. following an intranuclear cascade is determined by an energy balance involving the incident-particle kinctic energy, the escaping particle kinetic energies, and the average binding energy of the most loosely bound nucleon in the nucleus (taken as a constant = 7 MeV). EREC, the kinetic energy of the recoiling nucleus prior to evaporation, is computed from a momentum balance involving the incident and escaping-particle momenta. If NEXITE > 0, the code executes the FØRTRAN statement EX = EX - EREC, and this new value of EX is used as input to the evaporation calculation. If NEXITE  $\leq 0$ , EREC is not subtracted from the value of EX that is computed initially. In this case, the values determined for EX will be conservatively high since the kinetic energy of the nucleus is not taken into account. Conversely, setting NEXITE > 0 will occasionally result in a negative value for EX since the scheme for calculating EX, and then EREC, does not yield a precise conservation of energy and momentum. When a negative value of EX occurs, the evaporation calculation is bypassed.
- c. <u>NSPRED</u>: <u>If NSPRED > 0</u>, <u>small-angle multiple Coulomb scattering</u> will be computed for primary charged particles only. <u>If NSPRED < 0</u>, <u>multiple Coulomb scattering is neglected</u> <u>in the entire calculation</u>.

- d. NWSPRD: If NWSPRD > 0, collision records for each Coulomb scattering (NCØL = 8) vill be written on the HET history tape. If NWSPRD ≤ 0, no collision records will be written for Coulomb scattering. If NSPRED ≤ 0, the value of NWSPRD is irrelevant. Normally NWSPRD should be input as 0.
- e. NSEUD#: If NSEUD# > 0, all pseudo collision records in all media, including internal voids, will be included on the history tape. For NSEUD# < 0, all of these records will be excluded. A contribution to the muon source is made at all pion collisions. It follows that in a nucleon-pion calculation pseudo collision records should be written (NSEUD# > 0) if muon source data are to be read from the nucleon-pion history tape.

a b c d Card G: FØRMAT (E10.3, 110, 110, 110)

- a. ELAS: The energy (MeV) above which elastic scattering of neutrons with nuclei other than hydrogen is ignored (< 100 MeV).</li>
- b. NØELAS: The total number (i.e., for all media) of different nuclide types for which elastic scattering is to be considered (excluding hydrogen).
- c. NELSTP: The logical number of the BCD tape containing the elastic scattering data for NØELAS nuclides. If NELSTP is the logical number of the standard input, the code expects all of the elastic scattering data to be input on cards after the primary NMT input data and before the geometry input data.
- d. NLEDIT: An elastic scattering data edit signal:
  - = 0: no edit,
  - # 0: print an edit of all the elastic scattering data on the standard output unit.

The following cards, H and I M,1,..., H M,NEL(M) are input for each medium:

Card H. : FØRMAT (E10.4, 110, 110)

- a. DENH(M): The density (atoms/cm<sup>3</sup>) of hydrogen in medium M multiplied by  $10^{-24}$ .
- b. NEL(M): The number of nuclide types other than hydrogen in in medium M.  $1 \le \text{NEL(M)} \le 10$ .
- c. NØEL(M): The number of nuclide types (other than hydrogen) for which elastic scattering is to be considered in medium M.  $0 \le NØEL(M) \le NEL(M)$ .

a b c d Card(s) I. FØRMAT (E10.4, E10.4, E10.4, I10)

a. ZZ(N,M): The charge number of the Nth nuclide in the Mth medium.

- b. A(N,M): The mass number of the Nth nuclide in the Mth medium; A(N,M) > 1.
- c. DEN(N,M): The atom density (atoms/cm<sup>3</sup>) of the Nth nuclide other than hydrogen in the Mth medium multiplied by  $10^{-24}$ .
- d. ID(N,M): Identifier for the Nth elastic scattering nuclide in the Mth medium.  $0 \le ID(N,M) \le MPELAS$ . ID specifies the position of the elastic scattering data cards for nuclide (N,M) in the elastic scattering input data.

The order of the  $I_{M,N}$  cards for a given medium must be such that all nuclide types that are elastic scatterers are listed first; i.e., the first NØEL(M) nuclide types should be elastic scatterers with ID(N,M) > 0. If elastic scattering is not desired for a particular nuclide, then ID(N,M) for this nuclide should be 0. If elastic scattering is not used for any nuclide, then ELAS, NØELAS, NELSTP, NLEDIT, MØEL(M), and ID(N,M) should all be zero.

The media numbers selected must start at 1 and run consecutively through MXMAT.

The order of the H<sub>M</sub> and I<sub>M,N</sub> cards is: H<sub>1</sub>, I<sub>1,1</sub>, I<sub>1,2</sub>,..., I<sub>1,NEL(1), H<sub>2</sub>, I<sub>2,1</sub>, I<sub>2,2</sub>,..., I<sub>2,NEL(2</sub>,..., H<sub>MXMAT</sub>, I<sub>MXMAT,1</sub>, I<sub>MXMAT,2</sub>,..., I<sub>MXMAT,NEL(MXMAT</sub>).</sub> 4.3 Elastic-Scattering Input<sup>\*\*</sup>

If so specified on cards G,  $H_{H}$ , and  $I_{H,N}$  above, HET will treat the elastic scattering of neutrons with nuclei other than hydrogen in the energy range from ELAN to ELAS. The neutron direction after scattering is chosen from the linearly anisotropic distribution  $P(\mu) = (1 + 3f_1\mu)/2$ , where  $\mu$  is the cosine of the scattering angle. The elastic-scattering cross sections and  $f_1$  values at various energy points from ELAN through ELAS are required as input by HET.

The input format for the elastic-scattering data is given below. It will be assumed that NELSTP on Card G is specified as the logical number of the standard input so that card input is used for the elastic-scattering data. Card J: FØRMAT (I5, I5, I5, I5, F10.5, 5A6)

- a. IDT(1): Element identifier [conventionally, equal to (the charge number) × 1000 + (mass number), with mass number equal to zero for elements having natural isotopic composition].
- b. IDT(2): Cross section identifier (conventionally, 2 for elasticscattering cross sections, 71 for f, values).
- c. IDT(3): May be left blank.
- d. IDT(3): Number of following cards K which contain elasticscattering cross sections.
- e. FMAS: Atomic mass of element.
- f. Thirty characters of Hollerith input.

\*A method of obtaining elastic-scattering data from the O5R/MHTC master cross-section tape in the format required for HET is described in the NHTC manual.<sup>1</sup>

The input format for the elastic-scattering data in HET is identical to the format used in NMT.

The only number on Card J which is used internally by HET is IDT(4); all other input is for identification purposes only.

Cards K: FØRMAT (E15.5, E15.5)

a. ES: Energy, in eV, for the elastic-scattering cross section.
b. SIGE: Elastic-scattering cross section, in barns, at energy ES.
Card L: Blank card.

Card M: This card has the same format as Card J and should contain the same information except that IDT(4) now refers to the number of Cards N containing f values.

Cards N: P#RMAT (815.5, 815.5)

a. EF: Energy, in eV, for the f, values.

b. F1: f<sub>1</sub> value at energy EF.

Card **\$:** Blank card.

The series of K and H cards must be arranged in order of decreasing energy, and the highest energy value must be  $\geq$  ELAS and the lowest value must be  $\leq$  ELMM. There must be NMELAS sets of cards J through é, and the order of these sets must be correlated with ID(N,M) on card I<sub>M,K</sub>. To illustrate, consider a material configuration containing two media with medium 1 composed of hydrogen, oxygen, and aluminum and medium 2 composed of oxygen and lead. Suppose that neutron elastic scattering is desired for all nuclides except lead and that oxygen is listed as the first nuclide on card I<sub>M,N</sub>. Then NMELAS = 2, NMEL(1) = 2, ID(1,1) = 1, ID(2,1) = 2, NMEL(2) = 1, ID(1,2) = 1, and ID(2,2) = 0. Thus, the elastic-scattering data for oxygen would be input first and followed by the data for aluminum.

> I I

#### 4.4 HET Geometry Input<sup>\*</sup>

The geometry routines in HET are identical to those used in OSR.<sup>13</sup> However, internal voids in HET <u>must</u> be designated by medium number 6666 in the geometry input, whereas in the OSR geometry input internal voids are designated by medium number 1000. Particles in HET may undergo pseudo collisions in medium 6666. The statistical weight of a pion or muon is reduced at these collisions to account for decay. For nucleons, the total cross section in medium 6666, which is equal to the pseudo cross section, is arbitrarily set equal to the maximum pion decay cross section.

A rather detailed description of the geometry routines and geometry input restrictions is given in the 05R manual.<sup>13</sup> For convenience, the format for the geometry input given in the 05R manual is repeated below.

4.4.1 <u>Geometry Input Format</u>. (All alphabetic input must be leftadjusted.)

Card A: \*\* FORMAT (15)

a. An index which indicates whether or not region geometry is to be considered. A 1 specifies that both material media and statistical region geometry are considered; a 2 indicates that only material media are pertinent.

\*The geometry routines used in HET are the same as those used in NMT.

\*\*HET is not programmed for statistical regions. Thus, only an index value of 2 is allowed.

Card B: FØRMAT [A11,5(E10.5,A1)]

This card lists the zone boundaries in increasing order along the X axis, including the boundaries of the parallelepiped enclosing the entire system. Since the number of boundaries depends upon the problem, commas in the Al fields separating the boundaries are used to indicate that the list continues, while the absence of a comma following the last boundary indicates that the list has ended. The Ali field is for the programmer's convenience and will be ignored by the code.

Card(s) B': FØRMAT [6(E10.5,A1)]

If the number of boundaries exceeds the five allowed by the format of card B, the list is continued on as many cards B' as are required.

Card C: FØRMAT [A11,5(E10.5,A1)]

Identical with card B except that the listing is of the zone boundaries in order along the Y axis.

Card C': FØRMAT [6(E10.5,A1)]

Identical with card B' but continues the Y axis zone boundaries.

Card D: FØRMAT [A11,5(E10.5,A1)]

Identical with card B except that the listing is of the zone boundaries in order along the Z axis.

Card D': FØRMAT [6(E10.5,A1)]

Identical with card B' but continues the Z axis zone boundaries.

Cards E through P: Constitute a complete zone description. This set of cards must be included once for each zone. Card E: FØRMAT (A6, 15, 15, 15)

a. The word ZONE.

L, m, n: Each zone is located in the system by three integers:

k, m, and n. These specify the zone as being the 1th in the X direction, the mth in the Y direction, and the nth in the Z direction. The integers l, m, and n run from 1 to the maximum number of zones in each direction.

Card F: FØRMAT [A11,5(E10.5,A1)]

This card lists the block boundaries in this zone in increasing order along the X axis, including the boundaries of the zone.

Card(s) 7': F#EMAT [6(E10.5,A1)]

This is a block list continuation card similar to card B' of the zone listing.

Cards G, G':

The same as cards F and F' except that the block boundaries along the Y axis are listed.

Cards H, H':

The same as cards F and F' except that the block boundaries along the Z axis are listed.

Cards J through P constitute a complete block description. This set of cards must be included once for each block in the zone.

Card J: PORMAT (A6, I5, I5, I5)

a. The word BLOCK.

1,m,n: Each block is located in the zone by three integers: 1, m, and n. These specify the block as being the 1th in the X direction, the mth in the Y direction, and the nth in the Z direction. The integers 1, m, and n run from 1 to the maximum number of blocks in each direction.

Card K: FØRMAT [A12,10(15,A1)]

- a. The word MEDIA.
- b. A list of the media, sector by sector, in the block. As with other lists, a comma in the Al field indicates that the list continues; its termination is indicated by the absence of the comma.

Cord(s) K': F#RMAT [12(15,A1)]

The continuation, if required, of the medium list.

Card L: FURMAT [A12,10(15,A1)]

- a. The word SURFACES.
- b. A list of the quadric surfaces appearing in the block. Commas in the Al field indicate that the list continues; a blank indicates the end of the list. The numbers appearing in this list derive from the order in which the surfaces are mathematically described on card R, which will be described later in the input.

Card L': FØRMAT [8(15,A1)]

The continuation, if needed, of the list begun on card L. Card M: FØRMAT (A6, 1813)

- a. The word SECTØR.
- b. The designation of each sector with reference to its position relative to the quadric surfaces. For every sector in the block there must be a card M, which will have as many references as there are surfaces in the block. The status of the sector is listed according to the following key:

+1: The sector is on the positive side of the surface.

-1: The sector is on the negative side of the surface.

0: The surface is not needed in the definition of the sector. The order in which each reference to a quadric surface appears on each card M must correspond to the order in which the quadric surfaces are listed on card L.

If there is only one sector in a block, cards L and M should be omitted. Cards N, Ø, and P:

Specify the region geometry in the block. If there is no region geometry, these cards are omitted.

Card N: FURMAT [A12,10(15,A1)]

a. The word REGIMES.

b. A list of the regions, sector by sector, in each block. As with other lists, a comma in the Al field indicates continuation, a blank in the Al field ends the list. It should be recalled that the region sectors do not have to be the same as the media sectors.

Card N': P\$RMAT [12(15,A1)]

A continuation, if required, of the region list. Card #: F#RMAT [Al2,10(I5,Al)]

a. The word SURFACES.

b. A list of the quadric surfaces in the block. The treatment is the same as for card L.

Card #': F#RMAT [8,(15,A1)]

A continuation of the SURFACES list.

Card P: F#EMAT (A6, 1813)

- a. The word SECTOR.
- b. The definition of each region sector, in the same fashion that media sectors were defined on card M.

Card Q: F#RMAT (15, 11A6)

a. The total number of quadric surfaces in <u>the entire system</u>. The alphabetic data in the A6 fields is ignored by the code.
 Card R: F#EMAT [4(E10.5,A5,A1)]

Each quadric surface is described by writing the quadratic function whose zeros define the surface, in a fixed field format resembling the normal manner of writing functions. Each term in the function is specified by:

- a. The coefficient of the term.
- b. May be XSQ, YSQ, ZSQ (used for  $x^2$ ,  $y^2$ , and  $z^2$ ), XZ, YX, YZ, XY, ZX, YZ, X, Y, Z, or blank.
- c. A comblank character in this field indicates the end of the function. The next function must start on a new card.

#### 4.5 Source-Particle Description

 $2_{-} = \pi^{+}$ 

 $3_{-} = 1^{0}$ 

 $4. = \pi^{-}$ 

 $5_{-} = \mu^{+}$ 

 $6. = u^{-}$ 

The source-particle data required by HET are as follows:

E(1) = the source-particle kinetic energy in MeV; X(1) = the source-particle x position coordinate in cm; Y(1) = the source-particle y position coordinate in cm; Z(1) = the source-particle z position coordinate in cm; U(1) = the source-particle x <u>direction cosine</u>; V(1) = the source-particle y <u>direction cosine</u>; W(1) = the source-particle z <u>direction cosine</u>; W(1) = the source-particle z <u>direction cosine</u>; W(1) = the source-particle statistical weight; TIP(1)<sup>±</sup> = the source-particle type: 0. = proton 1. = neutron

The above source-particle data must be furnished in subroutine SØRS (NCØL), which is written by the user. SØRS is called when NCØL = -1 (start of run), NCØL = 1 (source particle), and NCØL = -4 (end of run). Any input required by SØRS should be read in when SØRS is called with NCØL = -1.

\*The source-particle type should never be assigned a value of 3 since  $\pi^0$  particles are not transported.

Since the parameters E(1) through TIP(1) are stored in labeled common CMMMMN, this common must be included in subroutine SMRS. Common CMMMN should appear in subroutine SMRS as:

COMMON/COMMIA(10,17), ALPHA(60), APR, ARG(17), BETA(40), BJ 40), COSKS, COSPHI, COSTH, D, DELSIG, DEN(10,17), DENH(17), DKNT, E(3000), EA(40), EB(40), EC(3000), EIGN(10,17), EMAX, EMIN(7), EP(60), EPART(100,2), SREC, EX, GAM(60), HEVSUM, HSIGG(5,17), HSIG, IBERT, ITYP, KIND(60), LELEM, MAT, MAXBCH, MAXCAS, MXMAT, N, NABGV, MAMAX, NAME(3000), NAMEA(40), NBELØ, NBERTP, NDØGUS, NEGEX, NEL(17), NEUTNØ, NEUTP, NGRØUP, NPIDK, IMED(3000), NØ, NØBCH, NØCAS, NØMAX, NØPART, NPART(6), NQUIT, ØLDWT, SIGG(10,17), SIGNX(7,17), SINKS, SINPHI, SINTH, TIP(3000), TIPA(40), TIPB(40), U(3000), UA(40), UB(40), UMAX, UU, V(3000), VA(40), VB(40), W(3000), WA(40), VB(40), WT (3000), JC(3000), ZC(3000), ZZ(10,17), ZPR

The user should choose values for TIP(1) that are in accordance with the value of NBERTP. If NBERTP < 0, any legitimate value may be used for TIP(1), whereas 0 < NBERTP indicates that all source particles are either nucleons or pions. For NBERTP = 0, it is assumed that all source particles are muons. When much source data are to be read from a previously produced nucleon-pion history tape, subroutine SØRS (NCØL) should contain the PØRTRAN statement CALL MFPD (NCØL). Subroutine MFPD reads the nucleon-pion history tape and calculates parameters E(1) through TIP(1) for each source muon. It is assumed that muons are created from pion decay that occurs isotropically with respect to the pion at rest.

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