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ANALYSIS SUBROUTINES FOR THE NUCLEON-MESON TRANSPORT CODE NMTC

T. W. Armstrong
K. C. Chandler

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

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*Mathematics Division.

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ANALYSIS SUBROUTINES FOR THE NUCLEON-MESON TRANSPORT CODE NMTC

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

Abstract

Several subroutines for analyzing the transport data generated by the nucleon-meson transport code NMTC are described. The principal subroutines compute: (a) flux and current from boundary crossings, (b) flux from collision densities, (c) residual nuclei distributions, and (d) star densities in emulsions. Various auxiliary subroutines are also described.

*Mathematics Division.

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I. INTRODUCTION

The principal output from the nucleon-meson transport code NMTC[1] consists of one or more magnetic tapes containing a series description of each of the events that took place during the transport calculation. The programs to read and process the data on these tapes must be written by the user to obtain the results of interest for his particular problem. Although it is impractical to attempt to write a general analysis program that would be applicable for all problems, there are certain quantities (flux, dose, etc.) that are frequently required in NMT analyses. The purpose of this report is to describe a set of subroutines that have been written to calculate some of these more commonly required quantities. It is hoped that by making these subroutines available some duplication of effort on the part of NMT users will be eliminated. Although the subroutines are somewhat specialized, especially in terms of allowable geometries, nevertheless they should be useful in providing a starting point for modifications necessary to arrive at analysis programs for particular problems.

The principal subroutines described here are:

(1) BCEST, which computes flux and current from particle boundary crossings,

(2) CDF, which computes flux from collision densities,

(3) BCDØSE, which computes dose using boundary-crossing fluxes and flux-to-dose conversion factors,

(4) RND, which computes residual nuclei distributions, and

(5) EMSTAR, which computes star densities in emulsions.

Although subroutine EMSTAR is quite specialized, it is included because the star-production cross sections in EMSTAR can readily be changed to obtain other flux-weighted quantities of interest.

Subroutines BCEST, BCDØSE, CDF, and RND compute the spatial distribution of the results in either the z direction or the r direction, where r is the perpendicular distance from the z axis. EMSTAR computes two-dimensional r-z distributions.

Subroutines BCEST and BCDØSE compute quantities based on boundary crossings, and therefore results can be obtained only at boundary positions that have been specified in the NMT geometry input. These subroutines compute z distributions from boundary crossings at all x and y coordinates at the specified z and r distributions from boundary crossings at all z at the specified r.

Subroutines CDF, RND, and EMSTAR compute quantities based on collisions in regions defined by boundaries input to the analysis subroutines. For CDF and EMSTAR these boundaries must include those used in the NMT geometry, but additional boundaries may also be specified in the analysis. The boundaries used for RND are independent of those used in the NMT geometry input.

Subroutines BCEST and BCDØSE are applicable for NMT nucleon-pion, NMT muon, and Ø5R analyses. Subroutines CDF, RND, and EMSTAR are applicable for only NMT nucleon-pion analyses.

In Section II some of the details of these subroutines are given and the input is described. The principal subroutines mentioned above call numerous other subroutines, and these secondary subroutines are also described. A main program (NMTA) has been written to illustrate the calling procedure for the subroutines, and this main program is described.

The information on the NMT collision tape is read by subroutine REDNMT (see Section II) and made available to the analysis subroutines through common LABEL. The definition of the variables contained in LABEL are given

in the NMTC manual.[1] The labeled common MISC is used for communication between the main program (NMTA) and various subroutines, and the definition of the variables in MISC is given in Section II with the description of NMTA.

Source decks for the main program and the subroutines, as well as input and output for a sample problem, may be obtained from the Radiation Shielding Information Center of the Oak Ridge National Laboratory. The sample problem is the same as that described in the NMTC manual.[1]

II. INPUT AND DESCRIPTION

Input specifications and brief descriptions of the routines are given in this section in the following order: main program (NMTA), principal subroutines (BCEST, BCDØSE, CDF, EMSTAR, and RND), and, alphabetically, the secondary subroutines used by the principal subroutines.

The answers in the printed output from the principal subroutines are normalized to one source particle; i.e., the sum of the contributions to the answer of interest is divided by MAXCAS*BCHS, where MAXCAS is the number of cascades per batch, which is specified in the NMT input, and BCHS is the number of batches to be analyzed, which is specified in the NMTA input. An exception to this normalization is that some of the printed output give the number of events that contribute to the answer. This number of events is not divided by MAXCAS*BCHS and, furthermore, does not account for the statistical weight of the particles.

The bookkeeping procedure for computing statistics and answers of interest is the same for all of the subroutines and is illustrated below:

A. At start of run

```
S = 0.
SA = 0.
SE = 0.
```

B. At event of interest

```
S = S + SCØRE
```

C. At end of batch

```
SA = SA + S
SE = SE + S*S
S = 0.
```

D. At end of run

```
SA = SA/(BCHS*PBCH)
CALL STAT(SA,BCHS,PBCH,SE,FSD,EL,EH)
```

Definitions:

SCØRE = the contribution to the answer of interest by a single event;

S = the sum of contributions over a batch;

SA = the variable that eventually becomes the grand mean, i.e., the mean value of SCØRE over all batches;

SE = the sum over all batches of the square of the contributions (needed for computing statistics);

BCHS = the number of batches;

PBCH = MAXCAS = the number of cascades per batch.

Subroutine STAT (see page 55) computes FSD (the fraction standard deviation of SA in percent), EL (SA minus one standard deviation), and EH (SA plus one standard deviation).

Main Program

Program Name:	NMTA (MAIN)
Subroutines Called:	BCDØSE, RND, BCEST, EMSTAR, REDNMT, CDF
Labeled Common:	LABEL, MISC
Length (decimal bytes):	1,838
Function:	Basically, NMTA calls REDNMT to read an event from the nucleon-pion or muon collision tape and then (optionally) calls BCEST, BCDØSE, CDF, RND, and EMSTAR according to the type of event read.
Definition of Variables in Common MISC:	Certain variables needed by the analysis subroutines are set in NMTA and communicated through the labeled common MISC. The variables are:

a. IGØM*, the geometry indicator,

b. 15, the logical tape number for card input (set internally in NMTA as 5),

c. 16, the logical tape number for printed output (set internally in NMTA as 6),

d. XX*, the normalization factor,

e. BCHS*, the number of batches to be analyzed,

f. PBCH, the number of source particles per batch (the value for PBCH is taken from the NMT collision tape).

*Values for these variables are input to NMTA.

Input:

Card A: Format (I10)[a]

a. NHSTP: Logical number of NMT collision tape

Card B: Format (I5[a],5X,2F10.2[b-c])

a. IGØM: Geometry indicator

IGØM = 1: slab geometry (one dimensional in z direction)

IGØM = 2: cylindrical geometry (one dimensional in radial direction)

b. XX: All answers multiplied by this number (normally, XX = 1.0)

c. BCHS: Number of batches to be analyzed (may be less than the number of batches on the collision tape)

Card C: Format (7I5)[a-g]

a-g. (IDØ(I),I=1,7), an array of integers used to determine the information to be calculated:

IDØ(I) > 0: calculate

IDØ(I) ≤ 0: don't calculate

a. IDØ(1): Residual nuclei information

b. IDØ(2): Flux and/or current at boundaries

c. IDØ(3): Flux by collision density

d. IDØ(4): Irrelevant

e. IDØ(5): Irrelevant

f. IDØ(6): Star densities in emulsion

g. IDØ(7): Boundary-crossing dose

Subroutine BCEST

Subroutine Name: BCEST (NKEY,IP,XP,YP,ZP,ALP,BET,GAM,WATE)

Calling Program: MAIN

Subroutines Called: STAT, BCFLX, GETIE

Labeled Common: MISC, EGRID, BCESTA

Length (decimal bytes): 186,054

Definition of Calling Arguments:

NKEY = the index for path to be taken in BCEST

= 1 - start of run

= 2 - score

= 3 - end of batch

= 4 - end of run

IP = the particle type index

= 1 - primary proton

= 2 - secondary proton

= 3 - neutron

= 4 - π^+

= 5 - π^-

= 7 - μ^+ or μ^-

XP,YP,ZP = position coordinates (cm)

ALP,BET,GAM = direction cosines with respect to x, y, and z axes, respectively

E = particle energy (MeV)

WATE = statistical weight of particle

Function: BCEST computes particle fluxes and/or currents from boundary crossings. The following flux- and current-related quantities may be requested in the BCEST input:

a. $J_{oik}(d) = \dfrac{\sum_j W_{ij}(d,\mu,E)}{N\ A\ \Delta E_k}$, $\quad -1 \le \mu \le +1$, $E \in \Delta E_k$

b. $\phi_{oik}(d) = J_{oik}(d)/|\mu|$

c. $J_{oi}(d) = \sum_k J_{oik}(d)\ \Delta E_k$

d. $\phi_{oi}(d) = J_{oi}(d)/|\mu|$

e. $J_{fik}(d) = \dfrac{\sum_j W_{ij}(d,\mu,E)}{N\ A\ \Delta E_k}$, $\quad \mu > 0$, $E \in \Delta E_k$

f. $\phi_{fik}(d) = J_{fik}(d)/\mu$

g. $J_{fi}(d) = \sum_k J_{fik}(d)\ \Delta E_k$

h. $\phi_{fi}(d) = J_{fi}(d)/\mu$

where

$J_{oik}(d)$ = the omnidirectional current spectrum at position d for particle of type i

$\phi_{oik}(d)$ = the omnidirectional flux spectrum at position d for particle of type i

$J_{oi}(d)$ = the omnidirectional current

$\phi_{oi}(d)$ = the omnidirectional flux

$J_{fik}(d)$ = the forward current spectrum

$\phi_{fik}(d)$ = the forward flux spectrum

$J_{fi}(d)$ = the forward current

$\phi_{fi}(d)$ = the forward flux

i = the particle type index

= 1 - primary protons

= 2 - all protons

= 3 - neutrons

= 4 - π^+

= 5 - π^-

= 6 - π^+ plus π^-

= 7 - μ^+ plus μ^-

d = depth z or radius r

$\mu = \vec{n} \cdot \vec{\Omega}$

$\vec{\Omega}$ = the unit vector along particle direction

$\vec{n}$ = the unit vector along positive z direction for slab case, or the unit vector along positive r direction for cylindrical case

$W_{ij}(d,\mu,E)$ = the statistical weight of particle of ith type making jth crossing of boundary at position d with direction μ and energy E

N = the number of source particles, MAXCAS*BCHS

MAXCAS = the number of cascades per batch specified in NMT input

BCHS = the number of batches analyzed, specified in NMTA input

A = area (cm^2)

= 1.0 for slab case

= $2\pi r$ for cylindrical case

In the slab geometry case, contributions to the flux and current at depth z are made by particles that cross, at any x and z, a plane perpendicular to the z axis at z. In the cylindrical geometry case, contributions at radius r are made by particles crossing, at any z, the boundary at r.

BCEST calls subroutine BCFLX to compute μ. Special provisions are made to prevent the possibility of extremely large contributions to the flux when $\mu \approx 0$ (see subroutine BCFLX). The energy grid for calculating the current and flux spectra is defined in subroutine GETIE.

The time unit in the printed output is seconds; i.e., it is assumed that N is on a per-second basis.

Input: (no input if ID$\emptyset$(2) $\leq$ 0 in main program)

Card A: Format $(\overset{a-f}{6I5})$

a. IJ$\emptyset$B:

IJ$\emptyset$B = 1: NMT nucleon-pion analysis

IJ$\emptyset$B = 2: NMT muon analysis

IJ$\emptyset$B = 3: $\emptyset$5R analysis

b-f. (IA$\emptyset$P(I),I=1,5)

IA$\emptyset$P(I) > 0: Calculate corresponding flux and/or current at specified boundaries

IA$\emptyset$P(I) $\leq$ 0: Don't calculate above

b. IA$\emptyset$P(1): Omnidirectional flux

c. IA$\emptyset$P(2): Flux in forward direction

d. IA$\emptyset$P(3): Omnidirectional current

e. IA$\emptyset$P(4): Current in forward direction

f. IA$\emptyset$P(5): Neutron flux (< 25 MeV) in various energy groups

Card B: Format ($I5^{a}$)

a. IBMX: Number of boundaries at which flux and/or current to be calculated (≤ 50)

Cards C: Format ($8F10.2^{a}$)

a. (BND(I),I=1,IBMX)

Boundaries (cm) at which total flux and/or current to be calculated. These must coincide with boundaries used in NMT (or Ø5R) geometry input, although all boundaries need not be included.

Card D: Format ($I5^{a}$,$I5^{b}$)

a. IBSMX: Number of boundaries at which current or flux (omnidirectional and forward) spectra to be calculated (≤ 15)

b. ISØP

ISØP ≤ 0: Calculate flux spectrum

ISØP > 0: Calculate current spectrum

Card E: Format ($16I5^{a}$)

a. (IBSØP(I),I=1,IBSMX)

Indices of boundaries at which current or flux spectra to be calculated

IBSØP(I) = K: Calculate spectrum at kth boundary input on Card C, i.e., at BND(K) cm

Subroutine BCDØSE

Subroutine Name: BCDØSE (NKEY,IP,XP,YP,ZP,ALP,BET,GAM,E,WATE)

Calling Program: MAIN

Subroutines Called: BCFLX, STAT, NEUFTD, MUFTD, PIFTD, PRØFTD

Labeled Common: MISC

Length (decimal bytes): 38,016

Definition of Parameters in Argument List: Definitions same as given previously for BCEST.

Function: BCDØSE computes the absorbed dose and dose equivalent at specified boundaries using boundary-crossing fluxes and flux-to-dose conversion factors. The output from BCDØSE is

$$D_i(d) = \int_{\text{all } E} \phi_i(d,E)\, C_i(E)\, dE \ ,$$

where $D_i(d)$ is the dose at position d due to ith particle type (primary protons, all protons, i.e., primary plus secondary protons, neutrons, π^+, π^-, π^+ plus π^-, and μ^+ plus μ^-), $\phi_i(d,E)$ is the flux spectrum, and $C_i(E)$ is the flux-to-dose conversion factor. BCDØSE also outputs the dose from all particle types, $\sum_i D_i(d)$.

BCDØSE calls PRØFTD, NEUFTD, PIFTD, and MUFTD to obtain C_i for protons, neutrons, charged pions, and muons, respectively, and the values used for C_i are discussed in the description of these subroutines. All of the flux-to-dose conversion factors pertain to the maximum dose in a 30-cm slab of tissue.

BCDØSE contains (in a DATA statement) the variable FWD which denotes the manner in which the dose is to be calculated. For

FWD > 0, D_i is calculated using the forward ($\vec{\Omega} \cdot \vec{n} > 0$) flux spectrum, and for FWD ≤ 0 D_i is calculated using the omnidirectional flux spectrum. In the standard version of BCDØSE, FWD = 1.0.

Input: (no input if IDØ(7) ≤ 0; see NMTA input)

Card A: Format ($F\overset{a}{10}.0,I\overset{b}{10},I\overset{c}{10}$)

a. TYMFAC:

D_i is multiplied by TYMFAC to obtain the desired units for the dose rate. Since C_i has units (rad or rem)/particle/cm^2), the time unit for ϕ_i depends on the time unit assumed for the source particles in NMT and on the value input for TYMFAC. Allowable values for TYMFAC are 1.0, 3600. (sec/hour) and 3.154×10^7 (sec/year).

b. KJØB:

KJØB = 1: NMT nucleon-pion analysis
KJØB = 2: NMT muon analysis
KJØB = 3: Ø5R analysis

c. IBMX: The number of B values (≤ 50)

Cards B: Format ($8F\overset{a}{10}.0$)

a. (B(I),I=1,IBMX)

Boundaries (cm) at which the dose is to be calculated.

Subroutine CDF

Subroutine Name: CDF

Calling Program: MAIN

Subroutines Called: GETIE, STAT

Labeled Common: LABEL, MISC, EGRID, CDFA

Length (decimal bytes): 93,298

Function: CDF computes by collision density the omnidirectional flux and flux spectra in specified regions for one-dimensional (in z) slab geometry or one-dimensional (in r) cylindrical geometry. The regions are defined by an input r or z grid. This grid does not have to be the same as that used in the NMT geometry. However, the boundaries used in NMT must be included in defining the regions for CDF since no region can contain more than one medium composition.

The flux spectra and flux are computed by

$$\phi_{ijk} = \frac{\sum_{\ell} W_{ijk\ell}}{N \, \Delta V_i \, \Sigma_{ij} \, \Delta E_k}$$

and

$$\phi_{ij} = \sum_{k} \phi_{ijk} \, \Delta E_k \, ,$$

where

i = the region index

j = the particle type index

k = the energy interval index

$W_{ijk\ell}$ = the statistical weight of jth type particle with energy in kth interval upon entering its ℓth collision in region i

N = the number of source particles

ΔV_i = the volume of ith region

$= z_{i+1} - z_i$ for slab geometry

$= \pi(r_{i+1}^2 - r_i^2)$ for cylindrical geometry

Σ_{ij} = the maximum cross section for jth type particle in region i

$\Delta E_k = E_{k+1} - E_k$

Σ corresponds to the maximum transport cross section used in NMT. Therefore, contributions to the flux are made at real nuclear collisions, pseudo nuclear collisions, and decay collisions. CDF will (optionally) output the flux spectra on tape.

Input: (no input if ID$\emptyset$(3) $\leq$ 0 in input of main program)

Card A: Format (I5)[a]

a. IST:

IST > 0: logical number of output tape for spectra

IST $\leq$ 0: don't output spectra on tape

Card B: Format (I5[a],I5[b])

a. IBMX: the number of boundaries defining spatial regions in which flux is to be calculated ($\leq$ 50)

b. IRSMX: the number of regions in which flux spectra are to be calculated ($\leq$ 49)

Card C: Format (8F10.2)[a]

a. (BND(I),I = 1,IBMX): Boundaries (cm) defining the spatial regions for which flux by collision density to be calculated. For slab geometry, these boundaries correspond to z values of planes along the z axis; for cylindrical geometry, these boundaries correspond to radii. For either geometry, the boundaries must

be in increasing order with the first boundary at 0.0. The Ith region is defined by BND(I)→BND(I+1). All boundaries used in NMT geometry input must be included since no region can contain more than one medium.

Cards D: Format (16I5)[a]

a. (IAMED(I),I=1,IREGMX) where IREGMX = IBMX-1: Medium number of the Ith region as defined in NMT input

Cards E: Format (16I5)[a]

a. (IRSØP(I),I=1,IRSMX): Region indices for which spectra are to be calculated

IRSØP(I) = K: Calculate spectra in Kth region, i.e., between BND(K) and BND(K+1)

Subroutine EMSTAR

Subroutine Name: EMSTAR

Calling Program: MAIN

Subroutines Called: STAT, GETZR3, SPACER

Labeled Common: LABEL, MISC, SGRID3

Length (decimal bytes): 63,752

Function: The purpose of EMSTAR is to estimate the density of nuclear stars produced in emulsion; i.e.,

$$S(\vec{r}) = \int dE\ \phi(\vec{r},E)\ \Sigma^*(E)\ ,$$

where $S(\vec{r})$ is the star density at position $\vec{r}$ and $\Sigma^*(E)$ is the macroscopic cross section for the production of stars having two or more prongs.[2] $\phi(\vec{r},E)$ is the flux spectrum in the transport medium used in NMT; i.e., the emulsion is not included in the NMT transport calculation. Calculating the star density in this manner assumes, therefore, that the flux perturbation which would occur if the emulsion was actually included in the transport calculation is small.

Emulsion star densities are not among the more common quantities of interest in NMT analyses, and therefore EMSTAR is expected to be of only very limited value to NMT users. However, EMSTAR is included here because it can be readily modified to obtain other flux-weighted quantities by replacing Σ^* with the appropriate weighting function.

EMSTAR computes the star density as

$$S_{ijk} = \frac{\sum_{\ell} W_{ijk\ell}(E)\ \Sigma^*(E)}{\Delta V_{jk}\ \Sigma_{ijk}\ N}\ ,$$

where

i = the particle type index, denoting protons, neutrons, and charged pions

j = the z interval index

k = the r interval index

$W_{ijk\ell}(E)$ = the statistical weight of ith type particle with energy E upon entering its ℓth collision in spatial regions j and k

$\Sigma^*(E)$ = the macroscopic star production cross section at energy E

$\Delta V_{jk} = (z_{j+1} - z_j)\ \pi(r_{k+1}^2 - r_k^2)$

Σ_{ijk} = the collision cross section used in NMT for ith particle type in spatial regions j and k

N = the number of source particles

EMSTAR also outputs the star density integrated over all radii, $\sum_k S_{ijk}\ \pi(r_{k+1}^2 - r_k^2)$, and summed over all particle types, $\sum_i S_{ijk}$. The spatial regions are defined by an input r-z grid. The emulsion cross sections at various energy points are specified in a DATA statement. To obtain the cross section at other energies, EMSTAR calls SPACER to perform three-point Lagrangian interpolation.

Input: (no input if ID$\emptyset$(6) $\leq$ 0 in input of main program)

Card A: Format (I5)[a]

a. IZMX: The number of boundaries in z direction ($\leq$ 50)

Cards B: Format (8F10.2)[a]

a. (ZBND(I),I=1,IZMX): Boundaries (cm) in z direction. Must include the boundaries used in NMT geometry input, starting at 0.0.

Card C: Format (I5)[a]

a. IRMX: the number of boundaries in r direction (≤ 10)

Cards D: Format (8F10.2)[a]

a. (RBND(I),I=1,IRMX)

Radial boundaries (cm), starting at 0.0

Cards E: Format (16I5)[a]

a. (IAMED(I),I=1,IZMX-1)

Medium numbers for the (IZMX-1) regions defined by the z boundaries (ZBND), as defined in the NMT geometry input

Subroutine RND

Subroutine Name: RND (NKEY,QZ,QA,XP,YP,ZP,WAIT,KASE,NPART)

Calling Program: MAIN

Subroutines Called: STAT

Labeled Common: MISC

Length (decimal bytes): 189,030

Definition of Variables in Argument List:

NKEY = index for path to be taken in RND

= 1 - start of run

= 2 - score residual nucleus

= 3 - end of batch

= 4 - end of run

QZ,QA = charge and mass numbers, respectively, of residual nucleus

XP,YP,ZP = position coordinates (cm) of produced residual nucleus

WAIT = statistical weight of particle producing residual nucleus

KASE = 1 if residual nuclei distribution after intranuclear cascade only desired

= 2 if residual nuclei distribution after intranuclear cascade and evaporation desired

NPART(I) = the number of Ith type evaporated particles. NPART is obtained from CØMMØN/LABEL/ and is needed by RND only if KASE = 1.

Function: RND computes, in specified regions, the distribution of residual nuclei according to mass and charge numbers. RND also computes the spatial distribution (in r or z) of particular residual nuclei.

The NMT collision tape contains the mass and charge number (variables APR and ZPR in CØMMØN/LABEL/) of each residual nucleus after intranuclear cascade and evaporation have taken place. If the residual-nuclei distribution after the intranuclear cascade and evaporation steps is desired, RND should be called with QZ = ZPR, QA = APR, and KASE = 2. If the residual-nuclei distribution after the intranuclear cascade but before evaporation is desired, then RND should be called as above but with KASE = 1. If evaporated particles (e.g., ^{4}He, ^{3}He) are to be included in the residual-nuclei distribution, then additional calls to RND must be made with QZ and QA corresponding to the charge and mass of the evaporated particle. The listing of the main analysis program (NMTA) may be referred to for an example of the calling procedure for RND.

RND is programmed for $2 \leq QZ \leq 82$. For a given QZ, a range of QA values about the most likely QA is allowed. RND outputs counters for the number of residual nuclei that do not fall within the allowed QZ and QA ranges.

Input: (no input if ID∅(1) ≤ 0 in input of main program)

Card A: Format (I5[a],I5[b])

a. NREG1: Number of spatial regions for which residual-nuclei distribution is to be calculated (≤ 4)

b. KASE: = 1 if residual-nuclei distribution after intra-nuclear cascade only desired

= 2 if residual-nuclei distribution after intra-nuclear cascade and evaporation desired

Cards B: Format (8F10.2[a])

a. (BND1(I),I=1,NREG1+1): Boundaries (in cm) defining the NREG1 spatial regions. For slab geometry, these boundaries correspond to the position of planes along the z axis; for cylindrical geometry, boundaries correspond to radii.
For either geometry, these boundaries must be in increasing order with the first boundary at 0.0.

Card C: Format (I5[a])

a. NREG2: Number of regions for calculating spatial distribution of specific residual nuclei (≤ 50)

*Cards D: Format (8F10.2[a])

a. (BND2(I),I=1,NREG2+1): Boundaries defining NREG2 regions (see Cards B above)

*Card E: Format (I5[a])

a. N∅NUC: Number of nuclei for which spatial distribution is to be calculated (≤ 25)

*Cards F: Format (8F10.2[a])

a. (RCHG(I),RMAS(I),I=1,N∅NUC): Residual charge and mass numbers of nuclei for which spatial distribution is to be calculated

*Omit Cards D, E, and F if NREG2 ≤ 0.

Subroutine FUNCTIØN ALAG

Subroutine Name: FUNCTIØN ALAG (XØ,X1,X2,X3,Y1,Y2,Y3)

Calling Program: SPACER

Subroutines Called: None

Labeled Common: None

Length (decimal bytes): 636

Definition of Calling Parameters:

XØ = value of independent variable at which value of dependent variable desired

X1,X2,X3 = values of independent variable to be used in the interpolation

Y1,Y2,Y3 = values of dependent variable corresponding to X1, X2, and X3, respectively

Function: ALAG is called by SPACER to perform three-point Lagrangian interpolation for the value of the dependent variable at XØ.

Subroutine GETIE

Subroutine Name: GETIE (IJØB,E,IE)

Calling Program: BCEST, CDF

Subroutines Called: None

Labeled Common: EGRID

Length (decimal bytes): 1,138

Definition of Calling Parameters:

IJØB = 1 - NMT nucleon-pion analysis

= 2 - NMT muon analysis

= 3 - Ø5R analysis

E = energy (MeV)

IE = energy index

Function: The first time GETIE is entered the energy grid, EG(I), and other variables used by BCEST and CDF for computing the flux and current spectra are defined and placed in the labeled common EGRID. For the first and all subsequent entrances, GETIE is called with E defined and the value of IE such that $EG(IE) \leq E \leq EG(IE+1)$ is returned.

Subroutine BCFLX

Subroutine Name: BCFLX (JGØM,X,Y,Z,U,V,W,WATE,XMU,FLX)

Calling Program: BCEST, BCDØSE

Subroutines Called: None

Labeled Common: None

Length (decimal bytes): 540

Definition of Calling Parameters:

JGØM = geometry indicator

X,Y,Z = position coordinates (cm) of boundary crossing

U,V,W = direction cosines at boundary crossing with respect to x, y, and z axes, respectively

WATE = statistical weight of particle

XMU = cosine of angle between particle direction and boundary normal

FLX = flux contribution

Function: BCFLX computes the contribution to the flux (FLX) at a boundary due to a particle crossing the boundary. The flux is computed as

$$FLX = WATE/|XMU| ,$$

where $|XMU|$ is the absolute value of the cosine of the angle between the particle direction and the boundary normal. For JGØM = 1, the boundary is assumed to be normal to the z axis and XMU = W. For JGØM = 2, the boundary is assumed to be a radial boundary about the z axis and

$$XMU = (V*X + V*Y)/(X^2 + Y^2)^{\frac{1}{2}} .$$

To eliminate the possibility of extremely large contributions to the flux for grazing angles (see ref. 3) BCFLX scores the flux

contribution for $|XMU| < \mu_c$ as if the angular distribution of the flux were isotropic. Thus, for $|XMU| < \mu_c$

$$FLX = WATE/(\mu_c/2)$$

for either geometry. μ_c is set to 0.0349, which corresponds to 2°.

Subroutine DEDXDØ

Subroutine Name: DEDXDØ (IP,FLUX,E,RAD,REM)

Calling Program: MUFTD

Subroutines Called: SPACER

Labeled Common: None

Length (decimal bytes): 874

Definition of Calling Parameters:

IP = particle type index
= 1 - protons
= 2 - charged pions
= 3 - muons

FLUX = particle flux

E = particle energy (MeV)

RAD = rad dose

REM = rem dose

Function: DEDXDØ evaluates the stopping power, S(E), for protons, charged pions, or muons and returns the absorbed dose (RAD = FLUX*S(E)) and dose equivalent (REM = RAD*QF(E)), where QF is the quality factor. (In computing dose using BCDØSE, DEDXDØ is used only for muons.) For $1 \leq E \leq 100$ MeV, the stopping power of tissue for protons given by Turner *et al.*[4] is used, and for $E > 100$ MeV the stopping power of water for protons based on the calculational method described in ref. 5 is used. The stopping power for charged pions and muons is calculated from the proton stopping power; i.e.,

$$S_\pi(E) = S_p(m_p\ E/m_\pi)$$

and

$$S_\mu(E) = S_p(m_p\ E/m_\mu)\ ,$$

where m_p, m_π, and m_μ are the rest masses of protons, charged pions, and muons, respectively.

The energy-dependent quality factor for protons, $QF_p(E)$, from Turner *et al.*[4] is used, and the quality factor for charged pions and muons is calculated from the proton quality factor; i.e.,

$$QF_\pi(E) = QF_p(m_p\ E/m_\pi)\ ,$$

$$QF_\mu(E) = QF_p(m_p\ E/m_\mu)\ .$$

DEDXDØ calls subroutine SPACER to obtain S and QF at E by three-point Lagrangian interpolation from tabulated values of S and QF at various energy points.

Subroutine GETZR3

Subroutine Name: GETZR3 (X,Y,Z,IR,IZ)

Calling Program: EMSTAR

Subroutines Called: None

Labeled Common: SGRID3

Length (decimal bytes): 574

Definition of Calling Parameters: X,Y,Z = position coordinates (cm) of interaction

IR,IZ = radial and depth indices

Function: GETZR3 is called to determine IZ such that ZBND(IZ) $\leq$ Z < ZBND(IZ+1) and to determine IR such that RBND(IR) $\leq$ R < RBND(IR+1), where R = $(X*X + Y*Y)^{\frac{1}{2}}$. The Z and R boundaries, ZBND and RBND, are communicated to GETZR3 from EMSTAR through labeled common SGRID3. If Z is greater than the largest ZBND value, then IZ = -1 is returned. If R is greater than the largest RBND value, then IR = -1 is returned.

Subroutine INTERP

Subroutine Name: INTERP (INTØP, X1,X2,XM,FX1,FX2,FXM)

Calling Program: NEUFTD, PIFTD

Subroutines Called: None

Labeled Common: None

Length (decimal bytes): 1,220

Definition of Calling Parameters:

INTØP = interpolation option

X1,X2,XM = independent variables

F1,F2,FXM = dependent variables

Function: INTERP interpolates between X1 and X2 and between F1 and F2 to determine FXM corresponding to XM($X1 \leq XM \leq X2$). The interpolation options are: INTØP = 1, linear between X1 and X2 and linear between F1 and F2; INTØP = 2, logarithmic between X1 and X2 and linear between F1 and F2; INTØP = 3, logarithmic between X1 and X2 and logarithmic between F1 and F2.

Subroutine SERCH

Subroutine Name: SERCH (ARRAY,IMAX,X,ILØW,IHIGH)

Calling Program: NEUFTD, PIFTD

Subroutines Called: None

Labeled Common: None

Length (decimal bytes): 502

Definition of Calling Parameters:

ARRAY = a one-dimensional array of numbers (ascending order)

IMAX = the number of values in ARRAY

X = an input value to SERCH in the range ARRAY(1) $\leq$ X $\leq$ ARRAY(IMAX)

ILØW,IHIGH = indices for values in ARRAY returned by SERCH

Function: Given ARRAY, IMAX, and X, SERCH performs a binary search to determine ILØW and IHIGH such that ARRAY(ILØW) $\leq$ X $\leq$ ARRAY(IHIGH).

Subroutine PIFTD

Subroutine Name: PIFTD (ICHG,EIN,FLUX,DØSE)

Calling Program: BCDØSE

Subroutines Called: SEARCH, INTERP

Labeled Common: None

Length (decimal bytes): 1,272

Definition of Calling Parameters:

ICHG = the parameter for denoting charge of pion (> 0 for π^+, ≤ 0 for π^-)

EIN = energy of pion (MeV)

FLUX = pion flux

DØSE(1) = rad dose

DØSE(2) = rem dose

(DØSE(3) through DØSE(6) are irrelevant.)

Function: For each charged pion crossing a boundary at which the dose is to be calculated, PIFTD is called with ICHG, EIN, and FLUX defined and DØSE(1) and DØSE(2) are computed by multiplying FLUX by the appropriate flux-to-dose factor at energy EIN.

The flux-to-dose factors are taken from the calculations of Alsmiller *et al.*[6] for pions at various energies between 10 MeV and 2000 MeV incident normally on one side of a slab of tissue 30 cm in thickness. These factors are based on the maximum dose produced in the tissue. It is important to note that for energies less than approximately 108 MeV (the energy corresponding to the pion range of 30 cm in tissue) the maximum dose was computed by Alsmiller *et al.* from average values over 1-cm spatial intervals.

Quite different values for the maximum dose might be obtained if smaller intervals were used.

If EIN < 10 MeV, PIFTD uses the flux-to-dose factor at 10 MeV; if EIN > 2000 MeV, PIFTD uses the flux-to-dose factor at 2000 MeV. The dose-vs-incident-energy relation near 108 MeV is not well defined from the calculations of Alsmiller *et al.*[6] In PIFTD, the flux-to-dose factors near 108 MeV were obtained by extrapolating the dose curves on either side of 108 MeV to 108 MeV, which results in a sharp discontinuity at 108 MeV. PIFTD calls SERCH to find the indices of the closest two energy points on either side of EIN and then calls INTERP to perform a two-point log-log interpolation to get the flux-to-dose factor at energy EIN.

Subroutine PRØFTD

Subroutine Name: PRØFTD (E,FLUX,DØSE)

Calling Program: BCDØSE

Subroutines Called: None

Labeled Common: None

Length (decimal bytes): 1,106

Definition of Calling Parameters:

E = proton energy (MeV)

FLUX = proton flux

DØSE(1) = rad dose

DØSE(2) = rem dose

(DØSE(3) through DØSE(6) are irrelevant.)

Function: For each proton crossing a boundary at which the dose is to be calculated, PRØFTD is called with E and FLUX defined, and DØSE(1) and DØSE(2) are computed by multiplying FLUX by the appropriate flux-to-dose factor at E.

The flux-to-dose factors used by PRØFTD are shown in Fig. 1. The factors refer to the maximum dose in a 30-cm slab of tissue due to an infinitely broad beam of protons incident on one face of the tissue. The factors below 60 MeV were computed for isotropic incidence using the stopping power in tissue from Turner *et al.*[4] and neglecting nuclear interactions. The quality factor vs linear energy transfer relationship, recommended in the National Bureau of Standards Handbook 59,[7] was used. Above 60 MeV, nuclear interactions were taken into account. Between 60 and 400 MeV the factors computed by Zerby and Kinney[8] for

isotropic incidence were used. Above 400 MeV, factors for isotropic incidence are not available, so the factors computed by Alsmiller *et al.*[9] in the energy range from 400 to 3000 MeV for normal incidence were used.

If E < 1 MeV, PRØFTD returns DØSE(1) = 0. and DØSE(2) = 0. If E > 3000 MeV, PRØFTD uses the flux-to-dose factor at 3000 MeV.

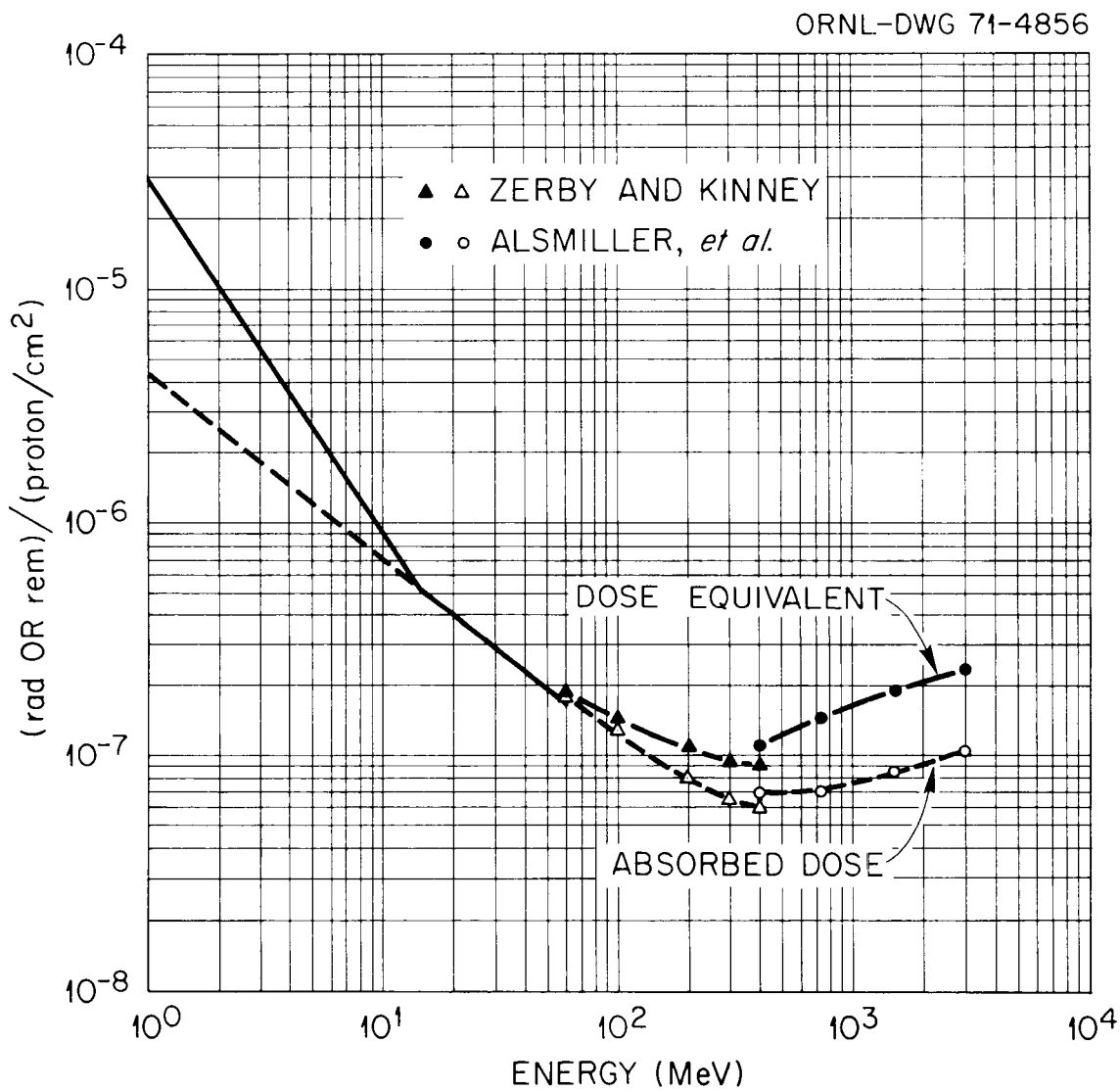

Fig. 1. Flux-to-Dose Conversion Factors for Protons.

Subroutine MUFTD

Subroutine Name: MUFTD (E,FLUX,DØSE)

Calling Program: BCDØSE

Subroutines Called: DEDXDØ

Labeled Common: None

Length (decimal bytes): 332

Definition of Calling Parameters:

E = energy of muon (MeV)

FLUX = muon flux

DØSE(1) = rad dose

DØSE(2) = rem dose

(DØSE(3) through DØSE(6) are irrelevant.)

Function: MUFTD calls DEDXDØ to determine DØSE(1) and DØSE(2) for muons at energy E.

Subroutine NEUFTD

Subroutine Name: NEUFTD (EIN,FLUX,DØSE)

Calling Program: BCDØSE

Subroutines Called: SERCH, INTERP

Labeled Common: None

Length (decimal bytes): 930

Definition of Calling Parameters:

EIN = neutron energy (MeV)

FLUX = neutron flux

DØSE(1) = rad dose

DØSE(2) = rem dose

(DØSE(3) through DØSE(6) are irrelevant.)

Function: For each neutron crossing a boundary at which the dose is to be calculated, NEUFTD is called with EIN and FLUX defined, and DØSE(1) and DØSE(2) are computed by multiplying FLUX by the appropriate flux-to-dose factor at energy EIN.

The flux-to-dose factors used for neutrons are given in Fig. 2. The factors used below 400 MeV are those recommended by the National Council on Radiation Protection and Measurements (NCRP),[10] and the factors calculated by Alsmiller *et al.*[9] are used between 400 and 3000 MeV. The small energy dependence of the factors between thermal (0.025 eV) and 0.01 MeV, which is not shown in Fig. 2, is taken into account by NEUFTD. Both sets of data in Fig. 2 correspond to the maximum dose produced in a 30-cm slab of tissue.

The Alsmiller *et al.*[9] factors are for normally incident neutrons. The NCRP factors do not strictly correspond to any particular

angular distribution since they were obtained by smoothing several sets of data for both normal and isotropic incidence.

If EIN < 0.025 eV, NEUFTD uses the flux-to-dose factor at 0.025 eV; if EIN > 3000 MeV, NEUFTD uses the flux-to-dose factor at 3000 MeV.

The flux-to-dose factors at various energy points are stored in a data statement in NEUFTD. NEUFTD calls SERCH to obtain the indices for the closest two energy points on either side of EIN and then calls INTERP to perform a two-point log-log interpolation to get the flux-to-dose factor at energy EIN.

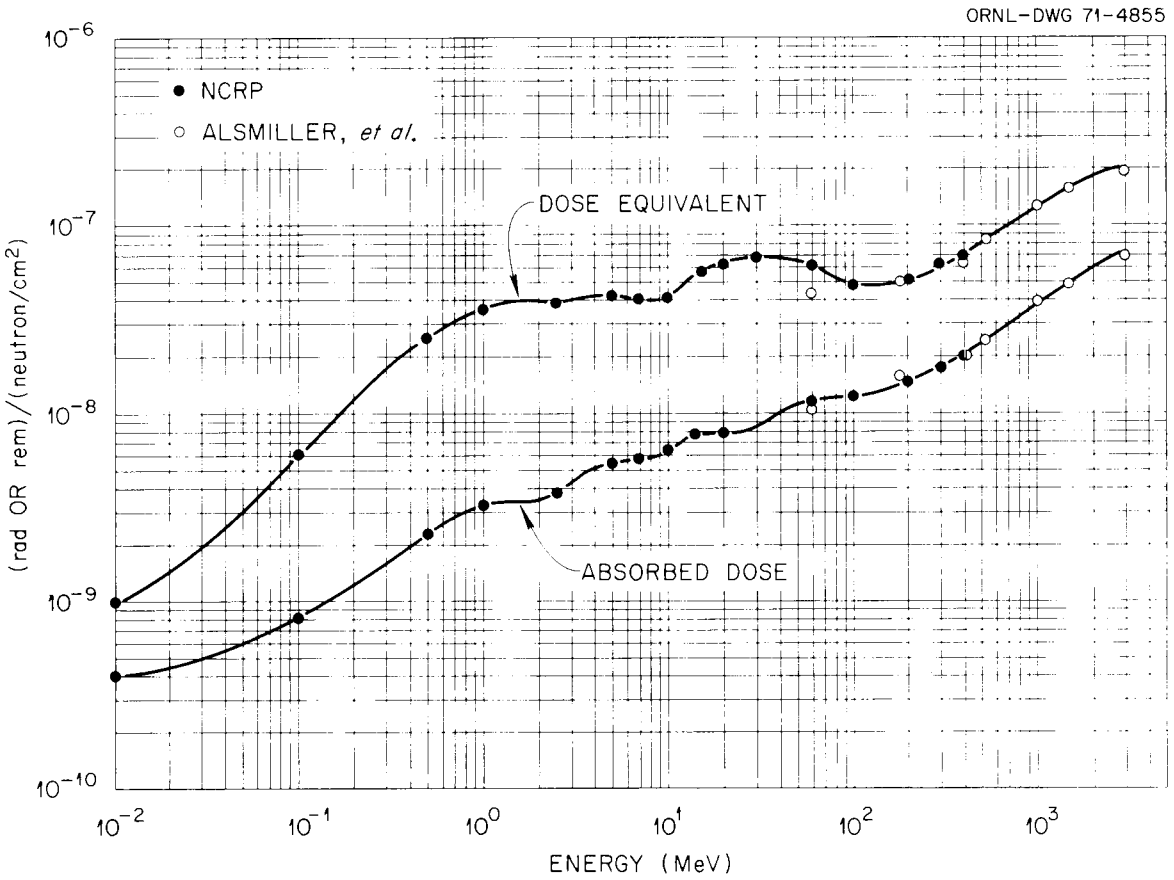

Fig. 2. Flux-to-Dose Conversion Factors for Neutrons.

Subroutine REDNMT

Subroutine Name: REDNMT

Calling Program: MAIN

Subroutines Called: None

Labeled Common: LABEL

Length (decimal bytes): 3,594

Definition of Calling Parameters: None

Function: REDNMT reads the NMT collision tape and stores the information read in common LABEL. It is through LABEL that the analysis subroutines receive the data for each event that occurs during the transport process. Definition of the variables contained in LABEL are given in the NMTC manual.[1] A separate call to REDNMT must be made for each particle event on the tape. Values for NHST (the logical number of the collision tape to be read) and IØ (the logical number of the tape for the printed output) must be set before the first call to REDNMT. These variables are contained in common LABEL.

Subroutine SPACER

Subroutine Name: SPACER (X,FX,ØX,ØFX,NX,NØX)

Calling Program: EMSTAR, DEDXDØ

Subroutines Called: FUNCTIØN ALAG

Labeled Common: None

Length (decimal bytes): 952

Definition of Calling Parameters:

X = the value of the independent variable at which the value of the dependent variable FX is desired

FX = the value of the dependent variable at X which is returned by SPACER

ØX = the array containing values for the independent variable (must be in ascending order)

ØFX = the array containing values of dependent variable

NX = the number of X values (usually one)

NØX = the number of values in ØX array

Function: SPACER interpolates in the ØX and ØFX arrays to determine FX at the specified value of X. SPACER obtains FX by calling FUNCTIØN ALAG to perform three-point Lagrangian interpolation.

Subroutine STAT

Subroutine Name: STAT (ANS,BCH,PBCH,SBS2,FSD,EL,EH)

Calling Program: EMSTAR, RND, BCEST, CDF, BCDØSE

Subroutines Called: None

Labeled Common: None

Length (decimal bytes): 512

Definition of Calling Parameters:

ANS = the grand mean

BCH = the number of batches

PBCH = the number of cascades per batch

SBS2 = the sum of the squares of the batch answers (unnormalized)

FSD = the fractional standard deviation (in percent) of the grand mean

EL = the grand mean minus one standard deviation

EH = the grand mean plus one standard deviation

Function: STAT computes batch statistics. Let

S_{ijk} = the kth "score" to the answer of interest by a particle in the jth cascade of the ith batch .

Then

$$\bar{S}_i = \sum_{j=1}^{N_c} \sum_k S_{ijk}/N_c ,$$

where $\bar{S}_i$ is the mean score for the ith batch, N_c is the number of cascades per batch (N_c is assumed to be the same for each batch), and the k summation is over all scores during the jth cascade of the ith batch.

Also,

$$\langle S \rangle = \sum_{i=1}^{N_b} \bar{S}_i / N_b \ ,$$

where $\langle S \rangle$ is the grand mean, i.e., the average score over all batches, and N_b is the number of batches.

The variance of $\langle S \rangle$ is

$$\sigma^2 = \frac{1}{N_b(N_b-1)} \sum_{i=1}^{N_b} (\bar{S}_i - \langle S \rangle)^2$$

$$= \left[\sum_{i=1}^{N_b} \left(\sum_{j=1}^{N_c} \sum_{k} S_{ijk} \right)^2 / N_c^2 \, N_b - \langle S \rangle^2 \right] \Big/ (N_b - 1) \ .$$

In terms of the calling parameters,

$$\text{ANS} = \langle S \rangle$$

$$\text{BCH} = N_b$$

$$\text{PBCH} = N_c$$

$$\text{SBS2} = \left(\sum_{j=1}^{N_c} \sum_{k} S_{ijk} \right)^2$$

$$\text{FSD} = \sigma \times 100 / \langle S \rangle$$

$$\text{EL} = \langle S \rangle - \sigma$$

$$\text{EH} = \langle S \rangle + \sigma$$

ANS, BCH, PBCH, and SBS2 must be defined upon entering STAT; FSD, EL, and EH are returned.

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