Code Package for Ion Transport in Materials: BRICE, E-DEP, HERAD, MARLOWE, TRIM

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December 1982

UWFDM-497

FUSION TECHNOLOGY INSTITUTE

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1. Introduction

This report describes briefly the use of the computer programs BRICE,[1,2] E-DEP,[3] HERAD,[4] MARLOWE,[5] and TRIM[6] on the NMFECC (National Magnetic Fusion Energy Computer Center). The computer codes BRICE and HERAD have been described in more detail in Refs. 2 and 4 respectively, and these references should be consulted for the use of both codes. All files mentioned in this report should be read by "FILEM" from the CRAY computers.

2. BRICE[1,2]

2.1 Input

See Ref. 2.

2.2 Availability

The directory "c-brice" contains the "lib" file "lbrice", which contains the source "sbrice", the controllee "xbrice", and the interactive program "xhelpbr" which can prepare the input for BRICE and run it. The directory "c-brice" also contains the input and the output for a test case. The input file for this test case is "irprt", and the output file is "orprtØØ".

3. E-DEP[3]

3.1 Input

The input for E-DEP consists of three namelist records and one title card. These input records are as follows:

a-$inlix:

This namelist record contains only the control array "lix" whose elements have the following functions:

lix(1)	default (Ø):	if lix(1) ≠ Ø the program terminates.
lix(2)	default (Ø):	if lix(2) ≠ Ø only range data will be output.
lix(3)	default (1Ø):	if lix(3) ≠ Ø range and damage will be output.

b-title: 1 to 8Ø characters.

c-$inone:

This namelist record contains the following input variables:

ebeam	default (none): incident ion energy in MeV.
emax	default (none): about 100% larger than the largest "ebeam" that will be used (in MeV).
cutoff	default (none): cutoff energy in eV.
zone	default (none): atomic number of incident ion.
atwo	default (none): atomic weight of incident ion (amu).
ntwo	default (none): number of components in the target; maximum of six, but this limit could be changed by changing the parameter "kp" at line 1Ø in the source and by precompiling, compiling, and loading the code.
ztwo(i)	default (none): atomic number of ith component.
atwo(i)	default (none): atomic weight of ith component (amu).
akstop(i)	default (Ø): the electronic stopping parameter for the ion with the ith component.

The density of the target can be supplied by one and only one of the following:

i-alat	default (Ø): the cube root of the volume of a unit cell of the target in angstroms.
nform(i)	default (none): the number of atoms of the ith component in the unit cell of the target.
ii-alatd	default (Ø): the density of the target in g/cc.
nform(i)	default (none): the weight fraction of the ith component.
iii-alata	default (Ø): the atomic density of the target in atoms/cc.

nform(i) default (none): the atomic fraction of the ith component.

iv-dens(i) default (Ø): the atomic density of the ith component in atoms/cc.

d-$intwo:

This namelist record contains the following input variables:

ebeam default (none): incident ion energy in MeV.

delta default (Ø): spacing in microns for which the energy deposition distribution is calculated. If delta=Ø the program will supply it.

The program, after reading "$intwo" and completing the calculations for the beam energy "ebeam", expects to read another "$intwo" record to do the calculations for a different value of "ebeam". This cycle stops when the input value of "ebeam" is negative. In this case the program starts to read the namelist record "$inlix", which might, according to the values in the array "lix", stop or start a new case. Thus the sequence of the input should be as follows:

(i) $inlix

stop if lix(1) ≠ Ø

(ii) title

(iii) $inone

(iv) $intwo

go to (i) if ebeam < Ø.

go to (iv) if ebeam > Ø.

3.2 Availability

The directory "c-edp" of user number 14225 contains the following files:

a. "sedpl" : the source of E-DEP.

b. "xedp1" : the controllee.

c. "sorqedp" : the original source of E-DEP.

d. "iedp" : input for a test case.

e. "oedpØØ" : output for the test case.

4. HERAD[4]

4.1 Input

See Ref. 4.

4.2 Availability

The directory "c-herad" of user number 14225 contains the source, the controllee, and input and output for a test case. See Ref. 4 for more details.

5. MARLOWE[5]

5.1 Input

The file "prologue" contains a complete description of the input and the program structure. To obtain this file type (from either the C or the D machine):

```
filem rds 14225 .c-marl prologue
```

5.2 Availability

The directory "c-marl" of user 14225 contains the following files:

a. "smarl" : the source of MARLOWE. This source contains all the modifications that were received from M. Robinson up to bulletin number 8 (8 April 1981).

b. "xmarl" : the controllee.

c. "icase1" : input for a test case.

d. "icase2" : input for a test case.

e. "icase3" : input for a test case.

f. "icase4" : input for a test case.

g. "prologue" : the user's guide.

h. "lorgcdc" : a "lib" file which contains the original CDC version of MARLOWE and related files.

i. "lorgibm" : a "lib" file which contains the IBM versions of MARLOWE.

6. TRIM(6)

6.1 Input

The input for TRIM consists of one title card and two namelist records. These records are:

a-title: 1 to 8Ø characters. If the first 8 characters contain the word "end", the program terminates.

b-$indata: this namelist record has the following input variables:

z1	default (none): atomic number of the ion.
m1	default (none): atomic weight of the ion (amu).
z2	default (none): atomic number of the target.
m2	default (none): atomic weight of the target (amu).
tt	default (1.e99): target thickness (Å).
ed	default (25): displacement energy (eV).
ck	default (1.): correction factor for LSS electronic stopping power.
eØØ	default (none): incident ion energy in keV.
ef	default (1Ø): ion cutoff energy in eV.
xØ	default (Ø.): initial ion position (Å).
alpha	default (Ø.): initial ion direction with respect to the target normal (degree).

lfx — default (Ø.): if "lfx" < Ø, the initial mean free path between collisions will be $n^{-1/3}$, where n is the target atomic density. If "lfx" > Ø the initial mean free path will be "lfx" in angstroms.

cw — default (none): channel width of the output depth distributions (Å).

hn — default (none): number of histories.

istp — default (Ø): if "istp" > Ø and < hn, range statistics could be output every "istp" histories.

iseed — default (-1)-lost: if "iseed"=-1, the initial seed of the random number generator will be Ø. If "iseed" > Ø the initial seed will be "iseed". Use "iseed"=-1 to reset the seed for different cases in the same run.

The density could be entered by using one of the following:

i-alat — default (Ø.): cube root of the volume of a unit cell of the target (Å).

natom — default(Ø): number of atoms in the unit cell.

ii-alata — default (Ø): atomic density of the target (atoms/cc).

iii-alatd — default (Ø): target density (g/cc).

or

rho — default (Ø): target density (g/cc).

c-$inrange: this namelist record has the following input variables:

boxd — default (25): the initial channel width of the depth distribution (Å).

boxp — default (25): the initial channel width of the path distribution (Å).

6.2 Availability

TRIM's files are in the directory "c-trim" in filem under user number 14225. There are in this directory an input file for a test case "itheni", and the controllee "xtrim".

7. Running the Programs

All the controllees could be run by typing:

"controllee name" i="input file name" /t v

The time required "t" depends on the program and its input. An estimate of the time required by each program was made in Ref. 7.

Acknowledgement

Support for this work has been provided by the U.S. Department of Energy.

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