# Example of connection calculation between PHITS and DCHAIN

## 1. Overview

Calculation of residual radioactivity is necessary for the radiation shielding design at accelerator facilities and the evaluation of secondary exposure for medical workers. For these purposes, its time evolution, (for example, time evolution of residual radioactivity concerning about irradiation time and its intensity and cooling time) should be considered. We therefore implemented a new tally called [T-Dchain], which automatically creates input files for DCHAIN from the PHITS simulation. The source and executable files of DCHAIN as well as its data libraries are also included in the PHITS package. Using these items, PHITS users can easily calculate the time evolution of residual radioactivities. This document supplies the usage of connection calculation between PHITS and DCHAIN. After the PHITS3.14, DCHAIN was improved in the following two respects: (1) several neutron activation libraries and decay-data libraries have been developed based on the latest evaluated data, and (2) statistical uncertainties of the induced activities can be evaluated considering those of the production yields calculated by PHITS.

## 2. Procedure for connection calculation between PHITS and DCHAIN

Figure 1 shows the flowchart of the connection calculation between PHITS and DCHAIN. PHITS creates the neutron energy spectrum with 1968-energy-group-structure, nuclear production yield, and the basic input file for DCHAIN. DCHAIN creates output files including production yield, radioactivity, decay heat, and gamma-ray spectrum at specified timing.

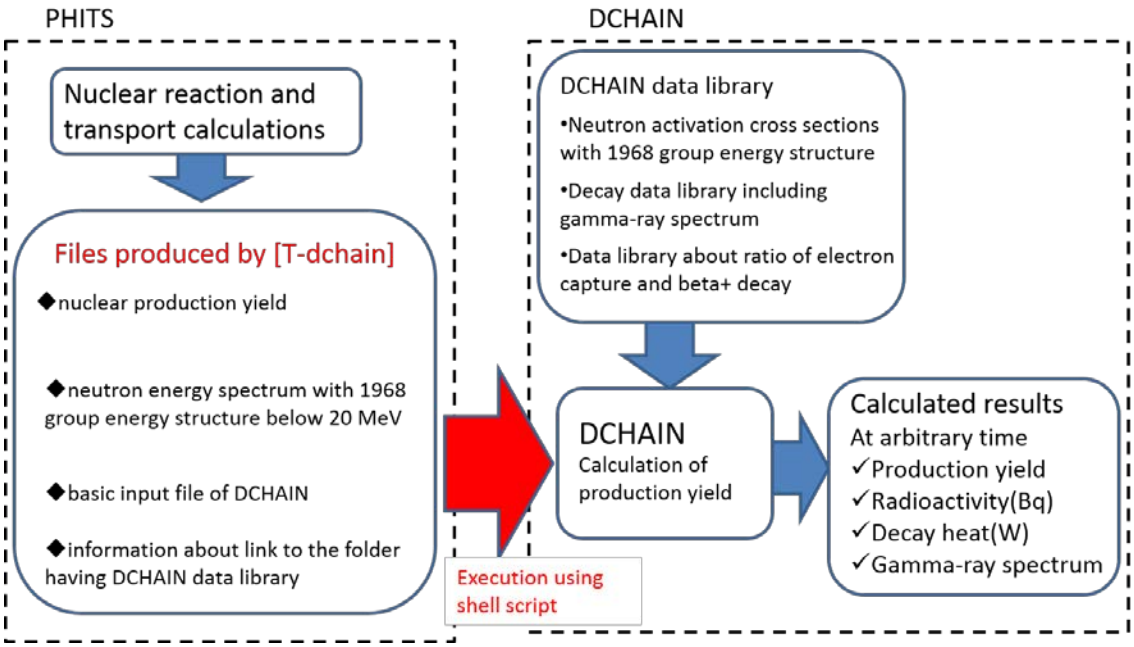


Figure 1 Flowchart of the connection calculation between PHITS and DCHAIN.

The procedure for the connection calculation between PHITS and DCHAIN is described below:

1. Define [T-Dchain] tally in PHITS input files. : see PHITS manual.
2. Execute PHITS → Input files of DCHAIN are created
3. Execute DCHAIN using the created input file

**How to execute DCHAIN**

For Windows: Right-click the basic input file of DCHAIN → send to → "DCHAIN"

For Linux and Mac: use the shell script "dchain.sh". You have to change its status using the command:

>chmod u+x dchain.sh

Then execute it

>./dchain.sh 150MeVH2O.out

For Linux, you have to compile DCHAIN by yourself, using Makefile in phits/dchain-sp/src. You have to select the appropriate machine environment from the list written in the file.

**Output file of DCHAIN**

*.lst : Input echo and the summary file for DCHAIN calculation.

*.act: Output file of residual radioactivities, decay heat, dose contribution factor and gamma-ray spectra based on radioactivities of each elapsed time in a region.

*.yld: Output file of nuclear production in each region at the end of irradiation and cooling.

*.gsd: Output file of gamma spectra based on radioactivities at the specified time with the MCNP/MCNPX input style of a source (SDEF card).

*.gso: Output file of origin of nuclei for gamma spectra based on radioactivities at the specified time in a region and its contribution ratio (%).

*.alr: Output file of radioactivities and decay heat at the specified time over all region. The number of nuclei is up to 30.

*.pht: Output file of gamma spectra based on radioactivities at the specified time in a region with the PHITS input style for the [source] section. Note that users should change the range of a region (x0, x1, y0, y1, z0, z1) so as to fit it to each region.

*.ang: Output file of radioactivities, decay heat and dose contribution factor at the specified time. (Output file for eps production by ANGEL)

*.dcs: Output file which, for each region and calculation time step (a convolution of the irradiation/cooling and output times), lists the change in inventory for each nuclide and the decay schemes of the relevant linear decay chains contributing to that change.

**3. Instruction of the sample input "dchain.inp"**

"dchian.inp" is a sample input file of PHITS, which is made for calculating time dependence of radioactivity and gamma spectrum in water blocks bombarded with 150 MeV protons. Its usage is given below:

### 3.1 PHITS execution

At first, you have to execute PHITS using "dchain.inp". In this file, [T-Track] tally is defined to output the behavior of protons and neutrons in water blocks. Figure 2 shows the 2-dimensional distribution of calculated neutron and proton tracks.

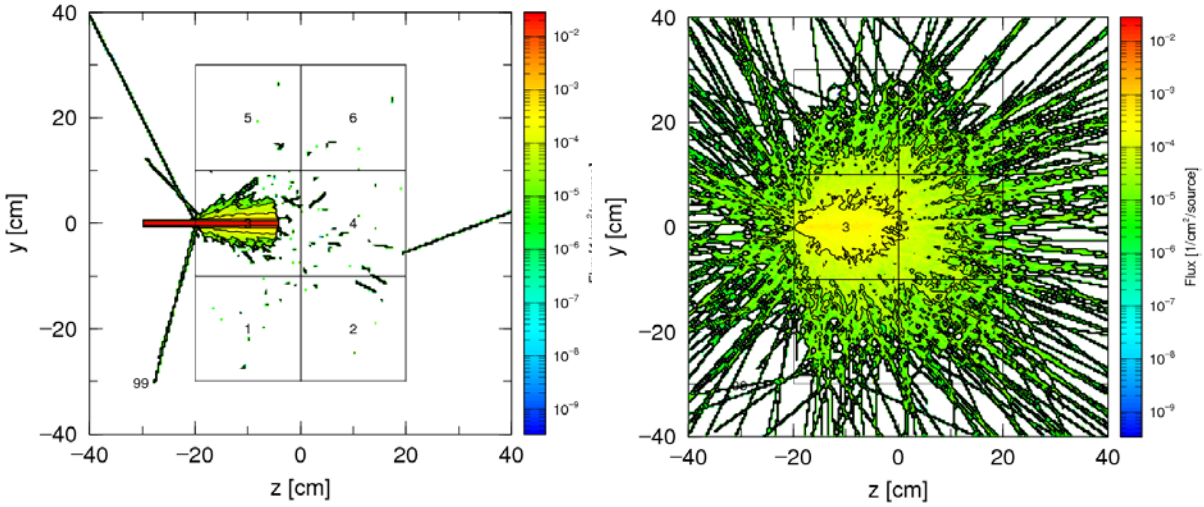


Figure 2 Tracks of protons (left) and neutrons (right) calculated by [T-Track] in "dchain.inp"

Protons stop at approximately 15 cm depths in region 3, and many neutrons are created along with their trajectories.

[T-dchain] tally written in “dchain.inp” is shown below together with its explanations.

```
[ T - D C H A I N ]
$    must section for DCHAIN
       title = 150MeV proton into water
         mesh =    reg                    ←region mesh
           reg =    1 2 3 4 5 6          ←cell number
           file = 150pH2O.out             ←file name of DCHAIN input
    timeevo =        2                   ←Number of irradiation and cooling steps
       6.0 m    1.0                      ←irradiation for 6 minutes
       50.0 m 0.0                        ←cooling for 50 minutes
    outtime =        7                   ←Number of output timing
       1.0 m                            ←1 minute later from the first irradiation start time.
       3.0 m                            ←3 minutes later from the first irradiation start time.
       6.0 m                            ←6 minutes later from the first irradiation start time.
      10.0 m                            ←10 minutes later from the first irradiation start time.
      20.0 m                            ←20 minutes later from the first irradiation start time.
      30.0 m                            ←30 minutes later from the first irradiation start time.
      40.0 m                            ←40 minutes later from the first irradiation start time.
$ beam current (nA)
set:c1[100.0]                           ←Beam current(nA).
$ beam power (source/sec)
set:c2[ c1 * 1.0e-9 / (1.602177e-19) ]  ←Unit conversion from (nA) to (protons/sec)
     amp = c2                           ←source power(source/sec)
```

The files created by this tally are:

- “150pH2O.out”: Basic input file of DCHAIN
- “150pH2O.dtrk”: Neutron energy spectrum with 1968 group energy structure below 20 MeV in regions 1 to 6
- “150pH2O.dyld”: Nuclear production yield
- “150pH2O_err.dyld”: Nuclear production yield statistical uncertainties
- “dch_link.out”: Information about link to the folder having DCHAIN data library

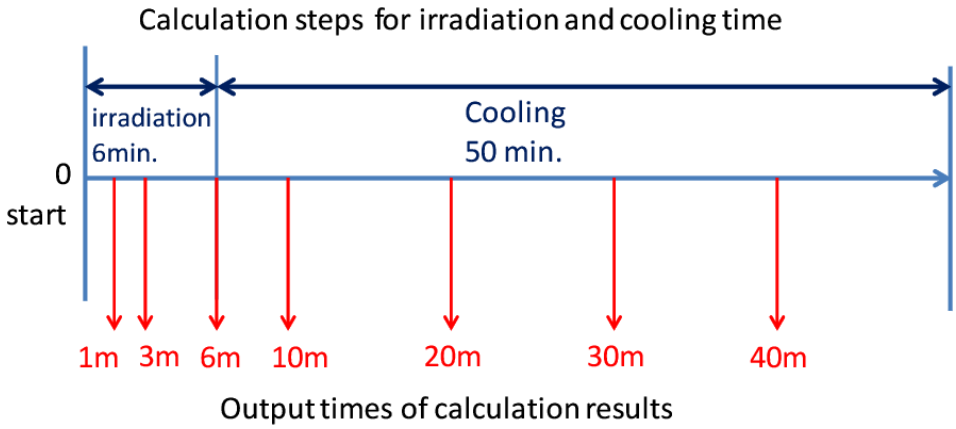


Figure 3 Time structure specified by [T-Dchain] in "dchain.inp"

The time structure specified by this tally is shown in Figure 3. Note that this time structure is used not in PHITS but in DCHAIN calculation.

### 3.2 DCHAIN execution

When you execute DCHAIN using "150pH2O.out", 10 files are produced. In this example, time dependence of total activity (Bq/cc), production yield, and gamma-ray spectrum are summarized in "150pH2O.act". Please see the manual of DCHAIN in more detail.

Lines 1-11 in "150pH2O.act" show the summary of calculation.

```
<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>
 <>-<>     no.        1    regionwise calculation data        <>-<>
 <>-<>     region label : DUMMY01                                <>-<>
 <>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>-<>
beam current ......   1.0000E-04 [mA]          ←power of source, 100nA
beam energy .......   3.0000E+00 [GeV]          ←no affect to calculation
beam power ........   3.0000E-04 [MW]          ←no affect to calculation
neutron flux ......  1.2414E+07 [n/cm**2/s]    ←neutron flux at 100nA
region volume .....   8.0000E+03 [cm**3]       ←volume
irradiation time ..                6 [m]
region number .....                 1    (in nmtc yield file)
```

Lines 12-101 show the calculated results of DCHAIN (production nuclide, gamma-ray spectrum, radioactivity, decay heat, and so on) at the timing of 60 seconds. After line 102, results for different timings and regions are given.

### 3.3 Results of calculation

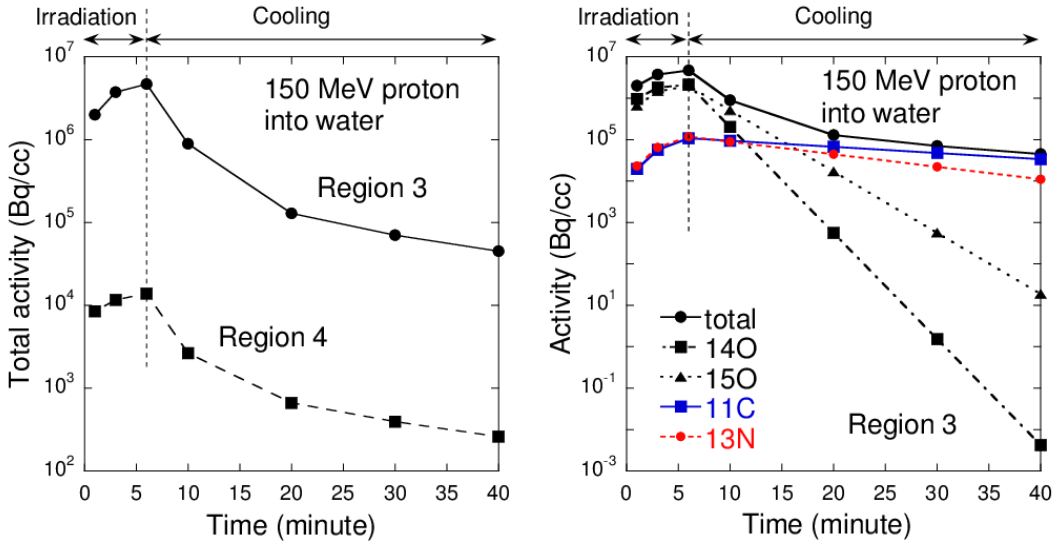


Figure 4 Time dependences of the total activities in regions 3 and 4 (left), and those of each nuclide in region 3 (right) outputted in "150pH2O.act"

Figure 4 graphically presents the time dependence of the calculated activities written in "150pH2O.act". Radioactive nuclides are produced during the beam irradiation, and radio activity decreases exponentially after beam irradiation. For region 3 in which protons hit directly, total activity is higher than that at other regions by 2 orders of magnitude. During irradiation, $^{14}$O and $^{15}$O are the dominant radioactive nuclides, while $^{11}$C and $^{13}$N becomes the dominant after the irradiation.

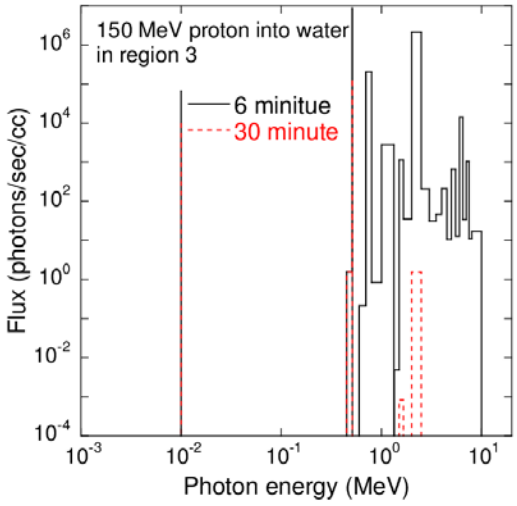


Figure 5 Gamma-ray spectra at 6 and 30 minutes after the beginning of the irradiation

Figure 5 shows gamma-ray spectra at 6 and 30 minutes after the beginning of the irradiation. A lot of high-energy gamma-rays are produced just after the irradiation (6 minutes). On the other hand,

511 keV and low-energy photons become the dominant at 30 minutes.

Figure 6 shows the output file (150pH2O.eps converted from 150pH2O.ang) for radioactivities, decay heat and dose contribution rate at the specified time. Where the number of DUMMY corresponds to the order of the region specified by “reg=” in the [t-dchain] tally.

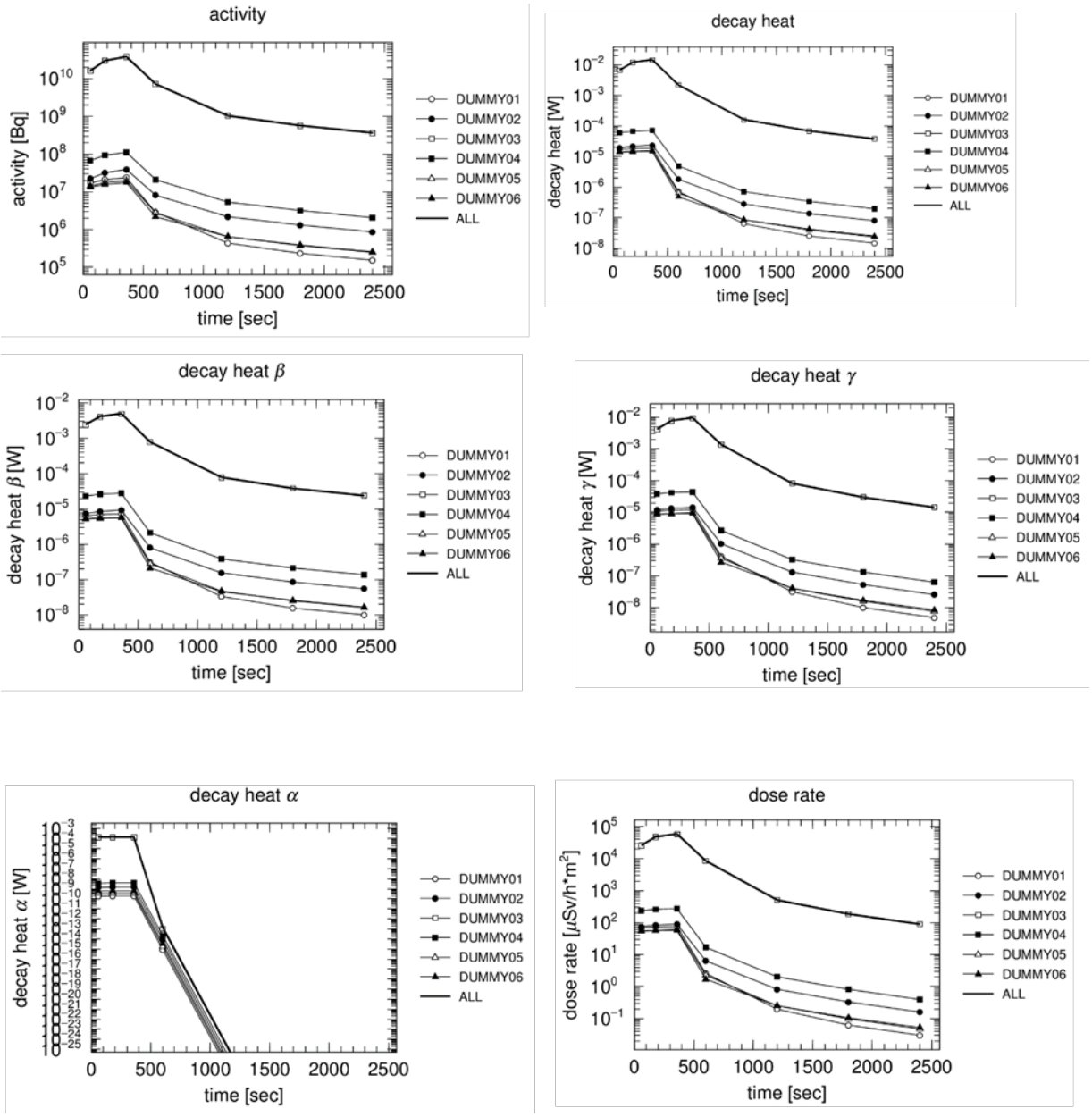


Figure 6 Output file (150pH2O.eps converted from 150pH2O.ang) for radioactivities, decay heat and dose contribution ratio at the specified time.

### 3.4 Restart calculation for DCHAIN

When you would like to change time steps for irradiation and cooling, output times, source power (source/sec), and/or the data libraries used in the calculation, you need not to execute PHITS again. All you have to do is to change the parameters written in the DCHAIN basic input file "150pH2O.out", and execute DCHAIN again. The related parameters are shown below

```
      htitle = 150MeV proton into water

! --- control parameters ---
       imode =          2
       jmode =          2

! --- calculation parameters ---
       idivs =         50
      ichain =        100
      itdecs =          0
      itdecn =          0
      isomtr =          2
      ifisyd =          0
      ifisye =          0

! --- data library parameters ---
    inxslib =          2      Specification of neutron reaction cross section library
    idcylib =          5      Specification of decay data library

! --- output parameters ---
       iyild =          2
       iggrp =          3
      ibetap =          1
       acmin =  1.0000E-20
      istabl =          0
      igsdef =          1
      igsorg =          1
    iwrtchn =          1
    chrlvth = -1.0000E+00
    iwrchdt =          0
    iwrchss =          0

! --- Proton beam current and neutron flux ---
          amp =  1.0000E-04      Source intensity converted to mA
        ebeam =  3.0000E+00
       prodnp =  1.0000E+00
```

```
! --- irradiation time ---
      itstep =          2
        6.0000E+00 m   1.0000E+00
        5.0000E+01 m   0.0000E+00
! --- output time ---
       itout =          7
        1.0000E+00 m
        3.0000E+00 m
        6.0000E+00 m
        1.0000E+01 m
        2.0000E+01 m
        3.0000E+01 m
        4.0000E+01 m

! --- irradiation condition ---
      inmtcf =          1
!   ffnmtcf =      1.0
   itdchout =          1
   hhnmtcf = 150pH2O.dyld
   iertdcho =          1
   henmtcf = 150pH2O_err.dyld

      iregon =         6
!1)HRGCMM 2)IREGS 3)ITGNCLS 4)FLUXS 5)HNFLUXS 6)VOLUMES
    DUMMY01          1      2   1.2198E+07    150pH2O.dtrk   8.0000E+03
    H-1          6.6893E-02
    O-16         3.3447E-02
!1)HRGCMM 2)IREGS 3)ITGNCLS 4)FLUXS 5)HNFLUXS 6)VOLUMES
    DUMMY02          2      2   8.4922E+06    150pH2O.dtrk   8.0000E+03
    H-1          6.6893E-02
    O-16         3.3447E-02
......
```

Number of steps for irradiation and cooling time

Normalized factor for beam intensity

ex) beam power: 100nA->0nA

normalized factor: 1.0 -> 0

Number of output times

Output times of calculation results

Total neutron number

Volume of the region