

Installation and Benchmark Tests of CINDER'90 Activation Code

Oyeon Kum*, Seung Uk Heo, and Sunju Oh

Korea Heavy Ion Accelerator Project, Korea Institute of Radiological and Medical Sciences,
75 Nowon-ro, Nowon-gu, Seoul, 139-706, Korea

*Corresponding author: okum1211@gmail.com

1. Introduction

Accurate analysis of nuclear systems is essential for high energy heavy ion accelerator facilities. Specifically, induced radio-active isotope analysis in complex nuclear system is very important and one of the more difficult problems [1]. Thus, many powerful analysis tools such as CINDER [2] and FLUKA [3] codes are provided. One of the authors recently obtained the license of CINDER'90 code [4] which provides powerful and well-accepted method for analyzing the radionuclide transmutation phenomena.

For the reactor community, CINDER'90 is now integrated directly into MCNPX [5] so that the transmutation processes can be considered in an integrated manner with the particle transport by using the "BURN" option card. However, the much smaller accelerator community cannot take advantage of these improvements because the BURN option card of MCNPX is only accessible in eigenvalue calculations of radioactive systems. In this study, we introduce preliminary results in activation calculations with the CINDER'90 code by using previously approved benchmarking problems.

2. Methods and Results

In this section, the governing equations of the nuclear transmutation and how the CINDER'90 code calculates the nuclide inventory are described. Several benchmarking results are shown to prove the correct code installation and usages.

2.1 Governing equations of the nuclear transmutation

In general, the three parameters such as the number of protons, Z , mass number, A , and energy state, S , specify a nuclide completely [6]. The rate of change of a nuclide density is calculated by the sum of the loss and gain rates and is represented by the differential equation describing the time change in the atom density, $N_m(t)$, of a nuclide m as follows [7]:

$$\frac{dN_m(t)}{dt} = -N_m(t)\beta_m + \bar{Y}_m + \sum_{k \neq m} N_k(t)\gamma_{k \rightarrow m},$$

where $\gamma_{k \rightarrow m}$ is the probability of nuclide k decaying or absorbing to nuclide m and β_m is the total transmutation probability of nuclide m defined as,

$$\beta_m = \lambda^m + \phi\sigma_a^m$$

Here ϕ is the energy integrated neutron flux, σ_a^m is the flux weighted average cross section for neutron absorption by nuclide m , and λ^m is the total decay constant of nuclide m . "Absorption" reactions of σ_a^m are all of those with residual nuclides other than nuclide m and thus include only inelastic scattering to states other than that of nuclide m . The underlying assumption of the governing equation is that the transmutation probabilities β_m and $\gamma_{k \rightarrow m}$, and thus the flux ϕ are constant for the time interval for which the solution is desired. In some applications, there can be significant particle production (or depletion) due to neutrons with energies above these thresholds. Such high energy reactions are accounted for by an additional constant, \bar{Y}_m , in the governing differential equation.

2.2 Solution method of CINDER'90 code

The CINDER'90 code requires no predefined set of sequential nuclides or linear chains as expected in solving linear chain differential equations. CINDER constructs the sequences to be calculated by testing each transmutation step for significance. The CINDER algorithm simply propagated the initial density and constant production rate of only the first nuclide in the chain to limit the length of the following chains. In this way, the total inventory of all nuclides in the system of chains beginning with the first nuclide is effectively calculated.

All paths are followed until insignificant or insufficiently accurate nuclear data is reached. The quantity, called "pass-by," is used to quantify the transmutation of nuclide n in a sequence and determine the significance of the subsequent elements of the path. The pass-by of nuclide n is the number of atoms of nuclide n transmuted during the time-step, which calculated by the time-step integration of the transmutation of the nuclide n . This quantity is very nearly equal to the number of atoms residing in all yet-to-be-examined paths emanating from nuclide n (i.e.,

equality broken by transmutations yielding more than one nuclide).

By applying the Markovian chain algorithm, the solutions are simply the summation of quantities that are different signs, which potentially results in the loss of significant figures in the sum in digital computers. Moreover, the degradation of significance in each time step must be propagated in the computations for subsequent nuclides as the sequence continues. Therefore, CINDER evaluates the number of significant figures in each atom density contribution and pass-by and the calculated pass-by is set to zero if it has less than two significant figures. If an atom density contribution with less than two significant figures is set to zero, the chain is terminated. The pass-by values are accumulated as "Losses" and listed at the end of each time interval in the primary cinder output. The details of the CINDER computing algorithms appear in CINDER manual booklet.

2.3 Combination with MCNPX code

CINDER code is not a standalone code. By the combination of MCNPX transport code, it provides powerful and well-accepted tool for analysis of nuclear system performance. However, because the use of the standalone version of CINDER'90 is very difficult due to its lack of formal release or a comprehensive user manual, the Perl scripting tools [8, 9] are developed to prepare and execute a full activation calculation. Besides the Perl scripts, CINDER code will work with TABCODE and ALLCODE which format the output results in easily readable forms. The operation of the three principle codes and input and output cascades is illustrated in Figure 1. The operation of the activation script and the interface between MCNP/X and the CINDER'90 are illustrated in Figure 2.

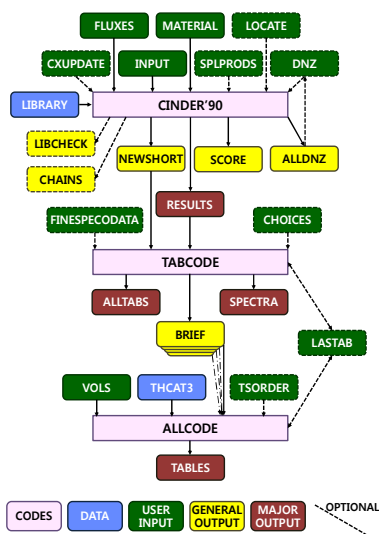


Fig. 1. The principle codes of CINDER90, TABCODE, and ALLCODE and their input and output relationships [4].

The Perl script extracts the material compositions and neutron flux spectra for the specified cell(s) from the MCNPX OUTP file. The HTAPE3X code which is distributed with MCNPX code calculates the physics-model-driven isotope production and destruction rates by processing the MCNPX HISTP file, which has information on secondary particle production and residual nuclei produced by the high-energy event generators. The gamma source script identifies the gamma sources in the problem if any.

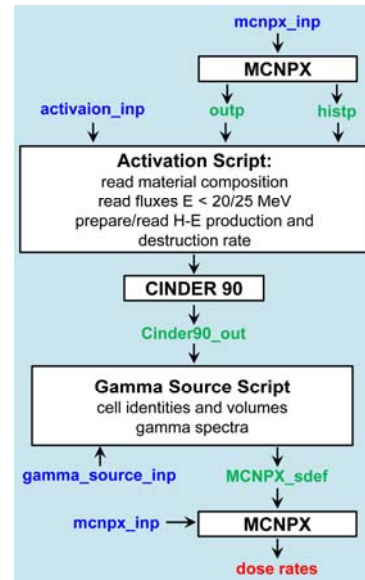


Fig. 2. Flow diagram of an activation analysis employing the activation script and the gamma script with the radiation transport code MCNPX and the transmutation code CINDER'90.

2.4 Selected benchmark problems

The well-known benchmark problems for CINDER'90 code are ubiquitous [10]. In this study, we select three of them which can be applied to many other areas with a small modification: (1) Weapons neutron research facility; (2) ^{252}Cf spontaneous fission problem; (3) Heat pipe of reactor power system.

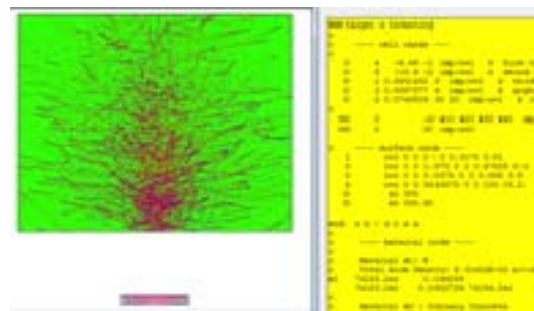


Fig. 3. Weapons Neutron Research facility targets (left) and their geometry descriptions (right). Beam trajectories are shown.

The Weapons Neutron Research facility at LANL produces fast neutrons for neutron irradiation research. This benchmark problem shows a stack of air-cooled target blocks of different materials and thicknesses with a range of atomic numbers from carbon to tungsten (see Figure 3). This problem can easily be modified to the accelerator activation problem because accelerator system contains typical targets of steel, iron, and copper. Activation script tested in this problem includes the ability to consider physics in only the tabular or the model regime, re-binning neutron fluxes according to the CINDER'90 group structure, and combining cells containing different materials although the user must be careful of erroneous results in real problems.

The shielding of a ^{252}Cf spontaneous fission neutron source shows a typical gamma source problem (see Figure 4). The source capsule with radius of 0.5 cm is enclosed in a steel capsule of radius 1.0 cm and a polyethylene shield of radius 10 cm. Activation products are produced by neutron absorption in the shield materials during the operational lifetime. The shield materials must eventually be disposed of as waste when the source is removed. This problem can be calculated with MCNP5 because the neutron source has energies in the tabular regime. To run this problem with MCNPX, one must turn off the model physics but not the tabular physics in the activation script

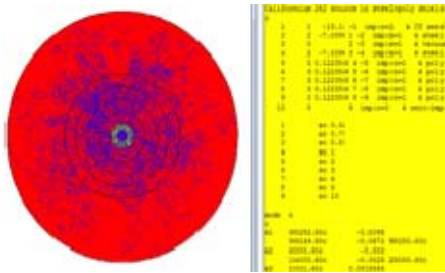


Fig. 4. Cf-252 target and surrounding shields (left) and its geometry input data (right). Beam trajectories are shown in blue color.

The heat pipe of reactor power system is a sample problem with an earlier version of CINDER. Since the neutron source for this problem has energies solely in the tabular regime and the MCNP5 code can be used, an MCNPX input file was solely constructed to test the activation script operation. Figure 5 shows horizontal and vertical views through the MCNPX model. This problem calculates the irradiation of ~97% enriched uranium to confirm the proper tracking of ^{235}U and ^{235}mU in CINDER'90 simulations.

2.5 Tabular results of three benchmark problems

Benchmark tests were performed on Windows 7 and Linux operating systems. The results were the same on both systems. As shown in Figure 1, the outputs of CINDER'90 code are the following four files and two additional edit files will be written if requested:

RESULTS which is the ascii file and includes all results of the calculation including the initial nuclide inventory, the final nuclide and total atom density activity for each time step, the delayed neutron production rate as well as time step integrated fissions from SF and (n; f), burn up information where fission is present; *ALLDNZ* which is a binary file giving the atom densities of all nuclides present initially or produced in the time intervals of the calculation; *NEWSHORT* which is a binary file giving the data of library utilized during the calculation with flux-integrated reaction data; *SCORE* which is a table showing the tally of tests resulting in chain terminations in the calculation. Two additional edit files are the following: *LIBCHECK* which is an optional file summarizing (for *klib=1*) the data of library as applied to the problem including flux-integrated reaction data and associated flux-weighted-average cross sections; *CHAINS* which is an optional file listing (for *kchn=1*) the density and pass-by of each nuclide contribution, pertinent adjustments to beta, and chain terminations.

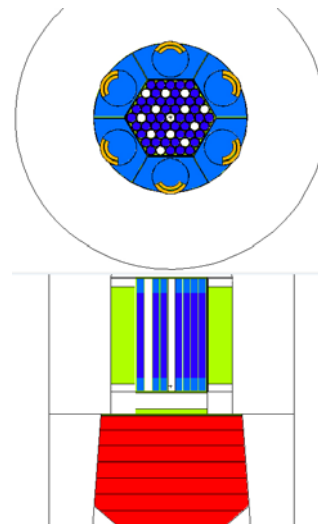


Fig. 5. Horizontal and vertical cuts through a MCNPX model of a heat pipe power system.

To obtain more easily readable tabular format of files, post processing is performed and the first step is to run TABCODE and the second step ALLCODE. The required input files and out files for both codes are shown in Figure 1. Among them, *ALLTABS* is the most important file which contains all requested tables (59 tables) generated by the TABCODE. However, the tables can be grouped by three classes, specific quantity by nuclide, total by element, and total by nuclide mass A. For simplicity purpose, we present activity densities (unit: curies/cc) for each benchmark problem in this paper.

Tables 1-3 summarize the specific activity in Zr, Ta, and W targets, respectively in the Weapons neutron research laboratory test problem (see Figure 3). The results are shown by nuclide but, because a number of isotopes are too many, only the summaries are partially presented in this paper.

Table 4 shows the fission properties of Cf-252 and the generation of gamma sources is shown in Figure 6. The gamma sources [9] are used in turn for the MCNPX source definition for the calculation of the dose rate due to the fission sources.

Table 1. Summary of specific activity in Zr target.

| NUCLIDE | UP | DOWN | UP | DOWN | DOWN |
|----------|-----------|-----------|-----------|-----------|-----------|
| | 1.00E+00S | 3.00E+01S | 1.00E+00S | 4.50E+00Y | 4.67E+00Y |
| A<66 | 9.694E-07 | 9.682E-07 | 1.938E-06 | 1.601E-09 | 1.580E-09 |
| 65<A<173 | 3.866E-02 | 1.162E-03 | 3.979E-02 | 1.132E-10 | 9.616E-11 |
| 172<A | 0.000E+0 | 0.000E+0 | 0.000E+0 | 0.000E+0 | 0.000E+0 |
| Total | 3.866E-02 | 1.163E-03 | 3.979E-02 | 1.714E-09 | 1.676E-09 |

Table 2. Summary of specific activity in Ta target.

| NUCLIDE | UP | DOWN | UP | DOWN | DOWN |
|----------|-----------|-----------|-----------|-----------|-----------|
| | 1.00E+00S | 3.00E+01S | 1.00E+00S | 4.50E+00Y | 4.67E+00Y |
| A<66 | 5.094E-10 | 5.094E-10 | 1.019E-09 | 4.791E-09 | 4.745E-09 |
| 65<A<173 | 2.183E-02 | 2.166E-03 | 2.396E-02 | 2.550E-09 | 2.388E-09 |
| 172<A | 8.279E-05 | 8.057E-05 | 1.633E-04 | 3.887E-09 | 3.628E-09 |
| Total | 2.191E-02 | 2.247E-03 | 2.413E-02 | 1.123E-08 | 1.076E-08 |

Table 3. Summary of specific activity in W target.

| NUCLIDE | UP | DOWN | UP | DOWN | DOWN |
|----------|-----------|-----------|-----------|-----------|-----------|
| | 1.00E+00S | 3.00E+01S | 1.00E+00S | 4.50E+00Y | 4.67E+00Y |
| A<66 | 4.659E-10 | 4.659E-10 | 9.318E-10 | 4.382E-09 | 4.340E-09 |
| 65<A<173 | 2.238E-02 | 2.176E-03 | 2.454E-02 | 3.801E-09 | 3.565E-09 |
| 172<A | 7.962E-03 | 4.621E-04 | 8.415E-03 | 3.736E-09 | 3.472E-09 |
| Total | 3.034E-02 | 2.638E-03 | 3.295E-02 | 1.192E-08 | 1.138E-08 |

Table 4. Specific activity of Cf-252 fission source after 30 days irradiation.

| NUCLIDE | HALFLIFE,S | UP |
|----------|------------|------------|
| | | 3.00E+01 D |
| H-3 | 3.888E+08 | 2.750E-16 |
| Sc-47 | 2.894E+05 | 1.017E-119 |
| Ti-51 | 3.456E+02 | 3.630E-63 |
| V-49 | 2.920E+07 | 7.692E-103 |
| V-52 | 2.246E+02 | 5.275E-56 |
| V-54 | 4.980E+01 | 3.651E-51 |
| V-66 | 2.000E-02 | 4.013E-15 |
| V-67 | 1.900E-02 | 9.224E-16 |
| V-68 | 1.000E-02 | 1.198E-20 |
| Cr-51 | 2.394E+06 | 5.110E-85 |
| | | |
| Cf-247 | 1.120E+04 | 1.153E-08 |
| Cf-248 | 2.881E+07 | 1.384E-08 |
| Cf-249 | 1.106E+10 | 4.372E+00 |
| Cf-250 | 4.128E+08 | 7.541E+01 |
| Cf-251 | 2.834E+10 | 7.409E-01 |
| Cf-252 | 8.347E+07 | 6.755E+03 |
| Cf-253 | 1.539E+06 | 4.546E-06 |
| Cf-254 | 5.227E+06 | 7.886E-17 |
| Es-253 | 1.769E+06 | 1.960E-06 |
| Es-254 | 2.380E+07 | 1.076E-17 |
| A<66 | | 1.782E-09 |
| 65<A<173 | | 1.179E+03 |
| 172<A | | 6.835E+03 |
| TOTAL | | 8.015E+03 |

Table 5 shows a partial summary of specific activity of the heat pipe power system after 30 days irradiation. Total number of bench mark problems were 12 but only are selected presented in this paper. The answers were supplied in the package and we confirmed the successful installation and benchmark tests by comparing out results with them.

Table 5. Specific activity of heat pipe power system after 30 days irradiation.

| NUCLIDE | HALFLIFE,S | UP |
|----------|------------|------------|
| | | 3.00E+01 D |
| H-3 | 3.888E+08 | 1.894E-03 |
| Li-8 | 8.403E-01 | 2.036E-23 |
| Be-8 | 7.000E-17 | 1.115E-08 |
| Be-10 | 4.765E+13 | 9.381E-14 |
| Be-11 | 1.381E+01 | 4.921E-08 |
| C-14 | 1.799E+11 | 6.078E-04 |
| C-15 | 2.449E+00 | 1.884E-10 |
| N-13 | 5.979E+02 | 2.906E-04 |
| N-16 | 7.130E+00 | 1.744E-10 |
| Ca-45 | 1.406E+07 | 1.578E-72 |
| | | |
| Np-240 | 3.714E+03 | 4.314E-06 |
| Np-240* | 4.332E+02 | 1.938E-06 |
| Pu-236 | 9.152E+07 | 4.347E-10 |
| Pu-237 | 3.903E+06 | 1.121E-08 |
| Pu-238 | 2.768E+09 | 2.287E-07 |
| Pu-239 | 7.608E+11 | 1.153E-05 |
| Pu-240 | 2.071E+11 | 1.485E-08 |
| Pu-241 | 4.528E+08 | 3.383E-09 |
| Pu-242 | 1.179E+13 | 2.790E-18 |
| Am-241 | 1.366E+10 | 1.797E-13 |
| A<66 | | 2.792E-03 |
| 65<A<173 | | 6.548E+02 |
| 172<A | | 1.173E+02 |
| TOTAL | | 7.721E+02 |

```

c SDEF card produced with Version 1.0 of the Gamma Source perl script
c Production date of sdef card: 2/27/2014
sdef par=p cel=d1 erp=foel d2 s=foel d3 y=foel d4 s=foel d5
eff=le-5 wgt=3.91898E+013
#s1 l 1
sp1 D 3.91898E+013
#b1 1.0
dm1 S 4
dm2 S 7
dm3 S 0
dm4 S 8
dm5 S 9
c
c CELL 1
c
#s6
1.00e-3
1.00000E-002 3.00000E-002 4.00000E-002 1.00000E-001 2.00000E-001
3.00000E-001 5.00000E-001 5.25000E-001 7.50000E-001 1.00000E+000
1.33000E+000 1.64000E+000 2.00000E+000 2.50000E+000 3.00000E+000
4.00000E+000 5.00000E+000 6.00000E+000 7.00000E+000 8.00000E+000
9.00000E+000 1.00000E+001 1.20000E+001 1.70000E+001 3.00000E+001
0.00000
5.12947E+011 1.03408E+013 1.79433E+012 9.09511E+011 2.73127E+012
2.77320E+012 5.52133E+012 4.61221E+011 4.48290E+012 2.97227E+012
2.18620E+012 1.47414E+012 8.21734E+011 1.02668E+012 7.02608E+011
3.99821E+011 5.04285E+010 1.00081E+010 1.98635E+009 1.91464E+008
3.46351E+007 8.01357E+004 2.27828E+006 6.46948E+004 0.00000E+000
#s7
0.0 1.0
#s8
-5.00000E-001 5.00000E-001
0.0 1.0
#s9
-5.00000E-001 5.00000E-001
0.0 1.0
#p9
0.0 1.0

```

Fig. 6. SDEF file produced by Gamma_source Perl script in the Cf-252 target source which is reused in MCNPX for the dose rate calculations.

3. Conclusions

Transmutation computing code, CINDER'90, which is widely used in the USA and European national laboratories, was successfully installed and benchmarked. Basic theory of atomic transmutation is introduced and three typical benchmark test problems are solved. The code works with MCNPX and is easy to use with the Perl script. The results are well summarized in a tabular format by using a post processing code, TABCODE. The cross benchmark tests with FLUKA are underway and the results will be presented in the near future. On the other hand, creating a new integrated activation code (MCNPX + CINDER) is now considered seriously for the more successful activation analysis.

AND VERIFICATION OF CINDER'90 AND SCRIPTING TOOLS, AccApp'07, Eighth International Topical Meeting on Nuclear Applications and Utilization of Accelerators, Pocatello, Idaho, July 29 – August 2, 2007.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIP) (No. 2014029534).

REFERENCES

- [1] O. Kum, S. Heo, S. Choi, Y. Song, S. Cho, S. Oh, and W. Jung, Radiation Protection for the First Korea Heavy-ion Medical Accelerator (KHIMA) Facility, ANS RPSD2014-18th Topical Meeting of the Radiation Protection & Shielding Division of ANS, September 14-18, 2014, Knoxville, TN.
- [2] W.B. Wilson, T. R. England, D. C. George, D. W. Muir, and P.G. Young, Recent Developments of the CINDER'90 Transmutation Code and Data Library for Actinide Transmutation Studies," Proceedings of GLOBAL'95 Int. Conf. on Evaluation of Emerging Nuclear Fuel Cycle Systems, September 11-14, 1995, Versailles, France.
- [3] A. Ferrari, P. R. Sala, A. Fass'ò, J. Ranft, Fluka: a multi-particle transport code (Program version 2011), <http://www.fluka.org>.
- [4] W. B. Wilson, S. T. Cowell, T. R. England, A. C. Hayes and P. Moller, A Manual for CINDER'90 Version 07.4 Codes and Data, LA-UR-07-8412, Los Alamos National Laboratory, NM, 2008.
- [5] D. B. Pelowitz, ed., MCNPX User's Manual, Version 2.7.0, Los Alamos National Laboratory report LA-CP-11-00438, NM, April 2011.
- [6] X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5," LAUR-03-1987, NM, April 2003.
- [7] S. T. Holloway, W. B. Wilson, Charles T. Kelsey, IV, Hannah Little, V. Mozin, A Manual for cinder2008 Codes and Data, Los Alamos National Laboratory report LA-UR 11-00006, NM, March, 2011.
- [8] F. X. Gallmeier, M. Wohlmuther, ACTIVATION SCRIPT VERSION 1.0 USER GUIDE, ORNL/TM-2008/031, OAK RIDGE NATIONAL LABORATORY, Oak Ridge, TN, August, 2008.
- [9] M. Wohlmuther and F.X. Gallmeier, User Guide for the Gamma Source Perl Script 1.0, Oak Ridge National Laboratory, Oak Ridge, TN, August, 2008.
- [10] B. J. Micklich, E. B. Iverson, F. X. Gallmeier, W. Lu, H. Trellue, C. Kelsey, and M. Wohlmuther, DEVELOPMENT OF A SAMPLE PROBLEM SUITE FOR VALIDATION