ICANS XIX,
19th Meeting on Collaboration of Advanced Neutron Sources
March 8 – 12, 2010
Grindelwald, Switzerland

THE CINDER'90 TRANSMUTATION CODE PACKAGE FOR USE IN ACCELERATOR APPLICATIONS IN COMBINATION WITH MCNPX

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ABSTRACT

CINDER'90, a nuclear inventory code originated at the Bettis Atomic Power Laboratory for reactor irradiation calculations and extended for use of in accelerator driven systems and high-energy applications at Los Alamos National Laboratory, has been released as a code package for distribution through the Radiation Safety Information Computational Center (RSICC). The code package and its updated data libraries come with several scripts that allow calculations of multi-cell problems in combination with the radiation transport code MCNPX. A script was developed that manages all the pre-processing steps extracting the necessary information from MCNPX output or from one input file, and that runs the CINDER'90 code for a requested list of MCNPX cells and for a requested time history. A second script was developed that extracts the decay photon sources from CINDER'90 output for a requested list of cells and for a requested irradiation or decay time step and builds source deck for subsequent MCNPX calculations. Since the package release, improvements to CINDER'90 are underway in algorithms, libraries, and interfaces to transport codes.

1. Introduction

The CINDER'90 code has its roots in the CINDER code originally developed at the Bettis Atomic Power Laboratory for reactor irradiation calculations in the 1960's[1]. CINDER'90[2] involved an upgrade of the code to allow the spontaneous tracking of chains based upon the significant density or passby of a nuclide, where passby represents the density of a nuclide transforming to other nuclides.

Being originally developed for the reactor physics community, the code today spans applications ranging from reactor burnup over accelerator driven transmutation to accelerator activation and to astrophysics in the evolution of elements and isotopes since the birth of the universe. For this reason the data library has been extended from the traditional fission product and actinide region down to lower mass nuclides, and from the neutron-rich unstable elements populated by the fission processes and neutron activation to the proton-rich elements generated by high-energy particle bombardment.

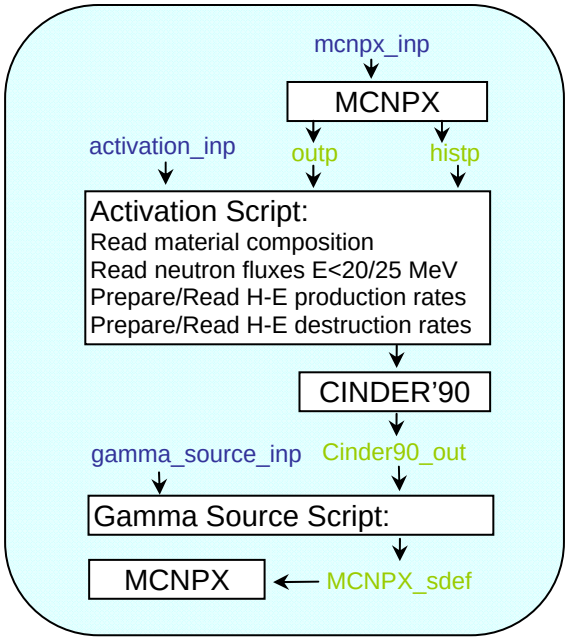

Figure 1: Flow diagram of an activation analysis employing the activation script and the gamma source script with the radiation transport code MCNPX and the transmutation code CINDER'90. Input and output files are printed in blue and green font, respectively.

As the heart of the CINDER'90 code package, the CINDER'90 code predicts the evolution of nuclide densities of a radioactive material, or a material being exposed to neutron fields, or a system with constant radionuclide production and destruction terms, or a combination of these aforementioned source terms. The later feature allows the code to describe nuclide inventories of nuclear systems being exposed to hadronic beams, where nuclide production and destruction terms and neutron fluxes are pre-calculated by transport codes.

With the CINDER'90 code package comes ancillary scripts that provide an interface into the output files of the multi-particle transport code MCNPX[3]. The inter-relation of the scripts and the CINDER'90 and MCNPX codes is outlined in Figure 1. One script, the ACTIVATION script, drives activation calculations of multi-region problems preparing CINDER'90 input files and executing CINDER'90 with minimal user input. Another script, the GAMMASOURCE script, prepares decay gamma source decks that can be directly fed back into MCNPX calculation of gamma-ray radiation filed arising from activation products.

The paper gives an overview of the different components of the CINDER'90 code package and demonstrates its use in re-calculating the radionuclide inventories measured in a benchmark experiment.

2. The CINDER'90 code

CINDER'90 is a code written in FORTRAN90, which calculates the inventory of isotopes in a material over time based on initial material composition, isotope production and destruction rates, and exposure to neutron fluxes varying in time and energy. Details of the algorithms are outlined in the manual [4]. The data library contains 3400 nuclides in the range of $1 \leq Z \leq 103$ including about 600 meta-stable states. These data include decay constants, branching ratios, average decay energies, activation cross sections, fission product yields (thermal, epithermal, and fast), and gamma production spectra. The data library entries are fine-tuned [5] with the nuclear data library PHTLIB used by the MCNPX code for the gamma-deexcitation step of the residual nuclei resulting from the

high-energy reaction models and determining its isomeric state. All production cross sections are provided in multi-group form (63 groups for activation cross sections, and 25 groups for gamma production) and have been collected from many sources since the start of compilation. The CINDER'90 code execution assumes four input files: a file for execution parameters and power history, a file for initial material composition, a file for averaged neutron spectra a material is exposed to, and a file for explicit radionuclide production and destruction rates. Outputs of the CINDER'90 calculations include nuclide concentrations for requested time steps, activity, thermal decay power, decay gamma spectra, and delayed neutron production rates. The post-processing code TABCODE produces easy to read tables from the CINDER'90 output, the ALLCODE utility merges results from several regions.

3. The ACTIVATION Script

The Activation Script reads most of the problem information like cell properties, material compositions and neutron fluxes from the MCNPX output file. For it to perform properly, the script hunts for key strings of tables and tallies in the MCNPX output. The cell information is read from MCNPX print table 60, the material information from the reported input cards, and the neutron fluxes including the cell volumes from tally 4. The MCNPX input has to be instrumented accordingly. To perform an activation calculation within a full energy range from the MCNPX physics model region down to the table data region, two sources of residual nuclide production have to be considered:

the isotope production and destruction rates explicitely calculated in MCNPX by the physics models and the production and destruction rates due to neutron-induced reactions in the table region, for which MCNPX calculates only neutron fluxes.

To take into account the activation by neutrons with energies in the table region an *F4:n* tally with a multigroup energy structure has to be specified. Tally multipliers (*EM4* or *EM0* cards) are not allowed; a *FQ* card for the *F4* tally for rearranging the output format is not permitted either. Although the Activation Script works with any multigroup structure and re-bins the fluxes into the energy structure the activation code needs; it uses user-provided typical energy functions to achieve a best match.

Isotope production and destruction rates from interactions described by the MCNPX physics models region are reported by MCNPX on an event file using the *histp* card. The HTAPE3X code is able to evaluate the *histp* file(s) for cell based isotope production and destruction rates. The ACTIVATION script prepares the necessary HTAPE3X input files, executes three HTAPE3X runs (for isotope production rates, for gas production rates, and for isotope destruction rates), and reads the necessary information from the HTAPE output.

At ORNL a MCNPX extension was developed that allows tallying for the cell based isotope production and destruction rates directly in MCNPX, which is activated by the *active* card. This avoids the need to post-process large event files with HTAPE3X. The standard MCNPX code has to be patched using the provided patch files to allow for the use of the *active* card. This ORNL MCNPX extension also provides a cell location and dimensions tally, which is a listing of minimum and maximum x, y, and z coordinates encountered in the particle tracking. This tally is useful for setting up gamma decay sources for remanent dose rate analyses.

The use of a mix of neutron cross sections with different upper energy limits, as well as the use of tabulated proton cross sections, is not yet supported. This restricts the use of tabulated cross sections for neutron transport to 20-25 MeV and forces the use of the reaction models with protons, ions, and mesons.

4. The GAMMASOURCE Script

Besides the information of radionuclide densities, activities, decay heat and associated tables, CINDER'90 also reports the decay gamma spectra for each time step of the calculation. This piece of information is useful for assessing the residual dose rates in the vicinity of radioactive material and for analyses of the decay gamma energy deposition in nuclear systems but requires the transport of the decay gammas.

The GAMMASOURCE script picks up the decay gamma spectra for a user defined list of cells and a user defined time step and prepares a MCNPX source deck in the SDEF general source format. In addition the script prepares the spatial distributions of the sources either from user-provided information of a Cartesian box envelope for each requested region/cell or from the above mentioned cell location and dimensions tally. It is assumed that the source is homogenously distributed in the region/cell. In cases when this does not hold, the user is advised to subdivide the region/cell and redo the activation calculation.

5. The CINDER'90 Package

The CINDER'90 code version 7.4.2 with its libraries and table generation utilities TABCODE and ALLCODE, and the Perl scripts ACTIVATION and GAMMASOURCE and their respective user manuals were combined to the code package CCC-755, which is now available through RSICC. The code package comes also with installers for the LINUX and WINDOWS platforms, and a list of 12 test problems that are exercised upon request in the installation process.

Since its release, the development group is working on improvements to the CINDER code (next stable version CINDER-2008[6]), modernizing the CINDER activation cross section library, formalizing an extension of the library and the algorithms to more particle types.

6. Comparisons to Experimental Measurements

A number of comparisons have been made to experimental measurements as part of the developers' work with CINDER'90 and the ACTIVATION and GAMMSOURCE scripts. One of these comparisons is for the depleted uranium target NSU-2 at the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory. The IPNS was a pulsed spallation source that generated neutrons by accelerating protons to 450 MeV and directing them onto a light-water-cooled neutron production target. The IPNS accelerator system produced a time-averaged current of 15 μA in 70-ns pulses at a rate of 30 Hz. The neutron production target consisted of eight disks of thickness 2.54 cm and diameter 10.16 cm. Figure 2 shows the IPNS accelerator system and a cutaway view of the IPNS target, reflector, and moderators.

In target NSU-2, the first seven disks were composed of depleted uranium and the eighth disk was type 304 stainless steel. The depleted uranium material was a composition referred to as 'Springfield alloy', which contains 450 ppm carbon, 250 ppm iron, and 350 ppm silicon. The target disks were clad with Zircaloy II having a thickness of 0.5 mm on the faces and 1.25 mm on the edges. A shell composed of type 304 stainless steel surrounded the target.

Radiation dose measurements were made of the IPNS targets during target handling operations, both as a means of benchmarking the radionuclide inventory calculations and to obtain operational data on the targets in support of future target handling. Measurements

were made with a RO-20 ion chamber for far-field measurements and a RO-7 ion chamber equipped with a high-range probe for near-field measurements. Target NSU-2 has been handled more often than the other targets and provided the most opportunities for measurement and comparison. Table 1 shows the results of these measurements. Calculations for NSU-2 far from the unshielded target agree well with the measurements, while those near the unshielded target overestimate the measurements by 60-80%. In general, calculations made for locations far from the targets, or for shielded configurations, agree better with the measured dose rates than the calculations for locations near the bare target.

Comparisons have also been made with measurements of long-lived activation products from irradiation of a thick lead target with 660-MeV protons [7]. Figure 3 shows results of total activity over the entire target using the MCNPX default nuclear models and each of the three activation codes, and for CINDER'90 using selected nuclear models in MCNPX. For the radionuclides considered, there is a greater dependence on the nuclear model used in MCNPX than there is on the activation code used. In nearly all cases the calculation and measurement agree within a factor of two. However, the production of certain metastable states is significantly underpredicted by the calculation, most likely due to deficiencies in the nuclear models or the underlying nuclear data such as branching ratios between metastable and ground states.

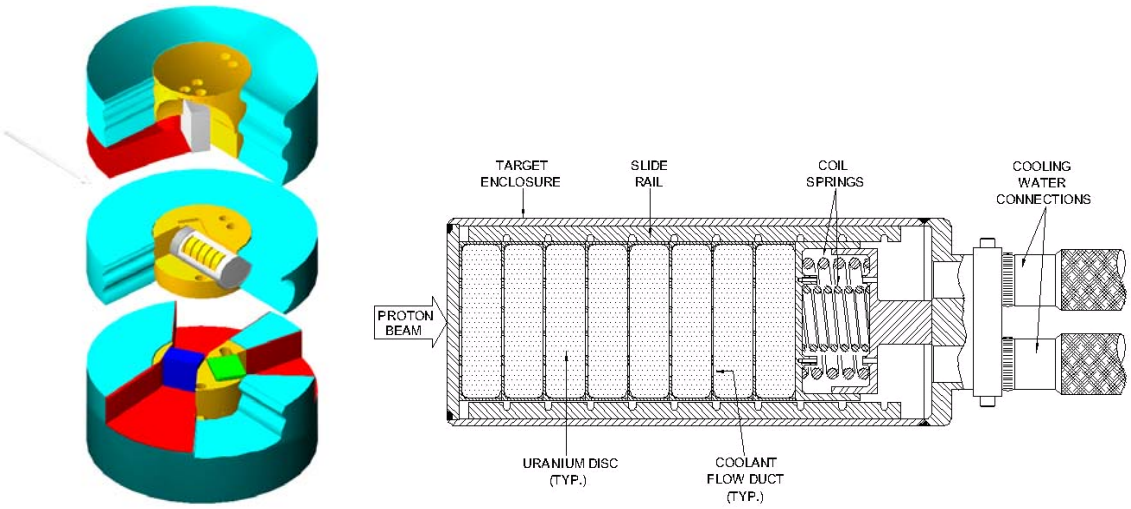

Figure 2. (left) Cutaway view of the IPNS target/moderator/reflector assembly. The proton beam is incident from the upper left. (right) Schematic picture of the IPNS neutron production target.

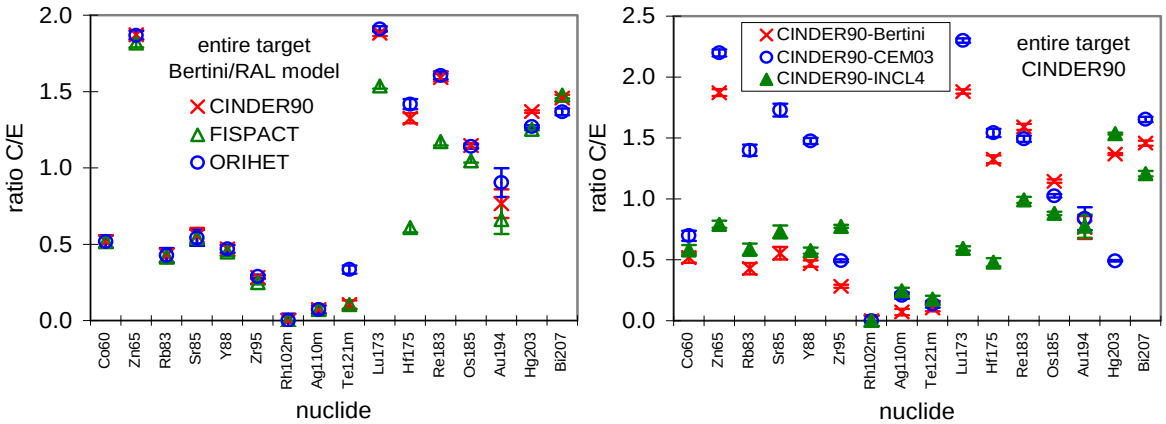

Figure 3. Ratio of calculated to measured total activity for selected nuclides in lead benchmark target: (left) as function of activation code; (right) as function of high-energy physics model used in MCNPX.

Table 1: Comparison of Measured and Calculated Dose Rates for IPNS Depleted Uranium Targets.

Target	Measurement date	Distance (m)	Calculated exposure rate (R/hr)	Measured exposure rate (R/hr)	C/E
NSU-2	31 July 2003[(a)]	contact	1.28	1.0	1.28
		1.0	0.18	0.25	0.72
	15 Dec 2004	1.524	2.50	1.4	1.79
	24 May 2005	12.19	0.038	0.045	0.84
	22 Feb 2007	1.0	3.70	2.3	1.61
		10.67	0.036	0.035	1.03
	16 July 2008	1.0	3.04	1.7	1.79
		5.0	0.128		

(a) shielded configuration; all other measurements were made in unshielded target configuration

7. Conclusion

The CINDER'90 code and data library, the ancillary codes TABCODE and ALLCODE, and the ACTIVATION and GAMMSOURCE scripts have been utilized in the institutes of the code developers for several years as a reliable tool in activation analyses of accelerator driven systems. They have been packaged together with a sample and test problem suite and installers and are available now as code package CCC-755 through RSICC.

8. References

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