

DEVELOPMENT OF A SAMPLE PROBLEM SUITE FOR VALIDATION AND VERIFICATION OF CINDER'90 AND SCRIPTING TOOLS

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A collaboration of four laboratories (Argonne, Oak Ridge, Los Alamos, and the Paul Scherrer Institute) has written a set of scripting tools to serve as an easy user interface to the CINDER'90 transmutation code, which is developed by Los Alamos. The script enables simpler and thus more accurate operation of the CINDER'90 code system than was possible using the suite of pre-processor codes previously employed. As part of this development, we generated a set of example problems that reflect common radioactivation problems in and around accelerator facilities. The test problems are used both to illustrate the use of CINDER'90 and the scripting tools in addressing accelerator activation problems, and to test features of the scripting tools for accuracy and usefulness. We describe the test problems and share our experience in validation and verification activities using several different FORTRAN language compilers to compile the individual codes that are part of the CINDER'90 package.

I. INTRODUCTION

The combination of radiation transport codes such as MCNPX [1] and MCNP5 [2] with radionuclide transmutation codes such as CINDER'90 [3] provides powerful and well-accepted tools for analysis of nuclear system performance. However, utilization of the stand-alone version of CINDER'90 is made difficult by its lack of a formal release or a comprehensive user manual. CINDER'90 is being integrated directly into MCNPX (via use of a BURN card) so that transmutation processes can be considered in an integrated manner with the particle transport. While the reactor community is well served by these efforts, the much smaller accelerator community cannot take advantage of these improvements since the MCNPX BURN feature is only accessible in eigenvalue calculations of fissile systems.

In a side meeting at ICANS-XVII, a group of CINDER'90 users from various US and European laboratories met to share their experience with the code. We decided to collaborate with the LANL code developers to both construct a better CINDER'90 user interface and to work towards a public release of the CINDER'90 code.

The approach taken was to develop scripts in the Perl programming language that simplify the process of preparing and running activation calculations and also allow preparation of decay photon source descriptions for subsequent transport analyses in MCNP5 or MCNPX. Details of these scripts can be found in the literature [4,5]. The complete packaged system will be submitted to RSICC for public release in the near future. Besides the Perl scripts, this package will include pre-compiled executables for the codes CINDER, TABCODE, and ALLCODE, sample problems, and a user manual.

The sample problems to be included in the CINDER'90 distribution are designed to guide the user in running both the CINDER'90 code package and the Perl scripts. The test problems reflect common radioactivation problems in and around accelerator facilities. They both illustrate the use of CINDER'90 and the scripting tools, and also test features of the scripting tools for accuracy and usefulness. We describe the test problems and share our experience in validation and verification activities using several different FORTRAN language compilers.

II. CINDER'90 AND SCRIPTING FRAMEWORK

With the currently available version of CINDER'90 (although not an official release), a set of ancillary codes is used to prepare the CINDER'90 input files. These codes were originally developed for use with LAHET transport results, and as CINDER'90 became used with MCNPX additional codes were developed to translate the MCNPX results into the LAHET format. As a result the process of preparing input for CINDER'90 became rather

convoluted, which makes it difficult for the casual user to prepare and execute a full activation calculation. We developed the Perl scripting tools as a means of correcting this problem.

The operation of the activation script and its relationship to the various codes are illustrated in Figure 1. The activation script provides the interface between MCNP/X and the transmutation codes CINDER'90, SP-FISPACT [6], and ORIHET-3 [7]. An input file (activation_inp) identifies the proper MCNPX output files and cells for analysis, describes the operating history of the system being studied, and sets the values of other parameters. The script extracts the material compositions and neutron flux spectra for the specified cell(s) from the MCNPX OUTP file. The physics-model-driven isotope production and destruction rates are obtained by using the HTAPE3X code (distributed with MCNPX) to post-process the MCNPX HISTP file, which contains information on secondary particle production and residual nuclei produced by the high-energy event generators. The activation script generates the necessary input files, executes the HTAPE3X code, and extracts the nuclide production and destruction rates from the HTAPE3X output files. We also run a special version of MCNPX which includes a patch [8] that tallies directly the model-based isotope production and destruction rates, in which case the script reads these quantities directly from the MCNPX output.

After preparing the necessary files from the MCNPX output, the script executes the selected transmutation code. The script allows calculations involving multiple cells, handling each cell individually or merged into a region. Problems involving only neutrons in the tabular physics range can be treated by turning off use of the high-energy induced isotope production/destruction. This allows outputs from the MCNP code to be used as basis for transmutation studies. Further details on execution of the activation script can be found in Reference 4.

III. DESCRIPTION OF SAMPLE PROBLEMS

Problems illustrating the use of CINDER'90 and the activation script were developed for several purposes. Initially, some members of the group developed one or more problems based on typical applications at their facility as a means of learning how to use the tools that we were developing. Other problems were developed as a means of testing various features in CINDER'90 or the scripting tools to insure proper operation. In general, we have tried to keep the sample problems simple to illustrate only the basic features of each problem, thus making it easier to interpret the input and output files. In particular, geometric descriptions are simplified as much as possible, a small number of histories are used to minimize running time, and smaller cross section libraries are usually invoked to reduce storage requirements.

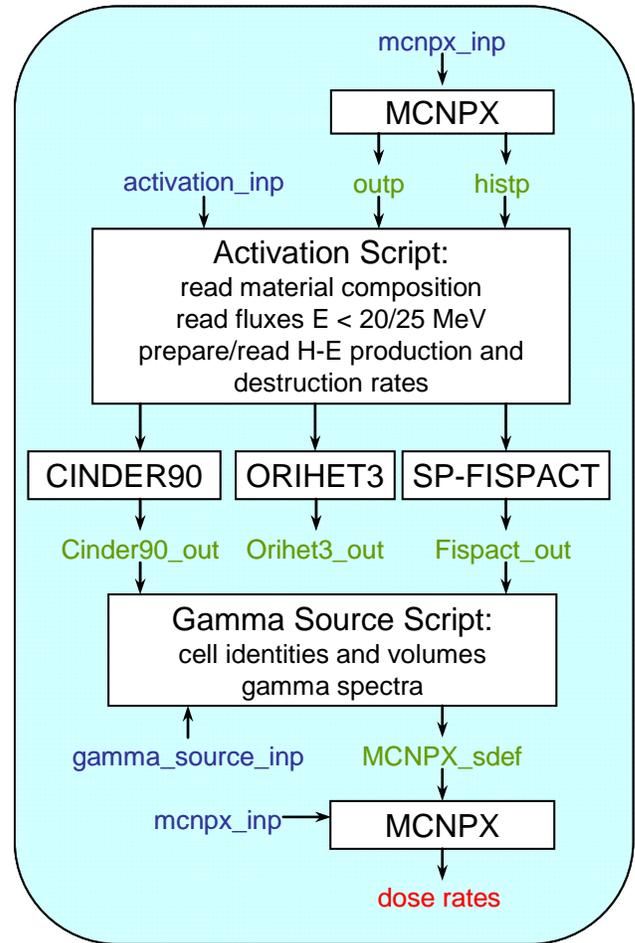


Fig. 1. Flow diagram of an activation analysis employing the activation script and the gamma source script with the radiation transport code MCNPX and the transmutation codes CINDER'90, ORIHET3 or SP-FISPACT. Input and output files are printed in blue and green font, respectively.

The sample problems also serve another important function. Each time the script is updated to add new features or to address issues, the sample test suite is run to verify that the script continues to give the correct results.

The sample problems include input for both MCNPX (for the radiation transport portion of each problem) and for the Perl scripts. All test cases were run using the CINDER'90 and associated executable codes on Linux and 32-bit Windows platforms using the transmutation codes available to each member of the collaboration (not all members are licensed to run all of the transmutation codes). Comparisons were also made between single-precision and double-precision versions of CINDER'90. The sample output files provided with the code package were obtained by running the sample inputs using the pre-compiled version of MCNPX and HTAPE3X available in

the most recent RSICC distribution of MCNPX (currently version 2.5.0) and the precompiled executables of CINDER'90 and TABCODE provided with the CINDER'90 distribution.

III.A. LANL 'Blue Room' Target Stack

The 'Blue Room' is a target area at the Weapons Neutron Research facility that produces fast neutrons for neutron irradiation research. This sample problem features a stack of air-cooled target blocks of different materials and thicknesses with a range of atomic numbers from carbon to tungsten (see Figure 2). Activation script features tested in this problem include the ability to consider physics in only the tabular or the model regime, rebinning neutron fluxes according to the CINDER'90 group structure, and combining cells containing different materials (though the user must be careful of erroneous results in doing this in real problems). This test problem will be extended in the future to compare the results of using the Bertini [9], ISABEL [10], CEM [11], and INCL4 intranuclear cascade models at intermediate energies.

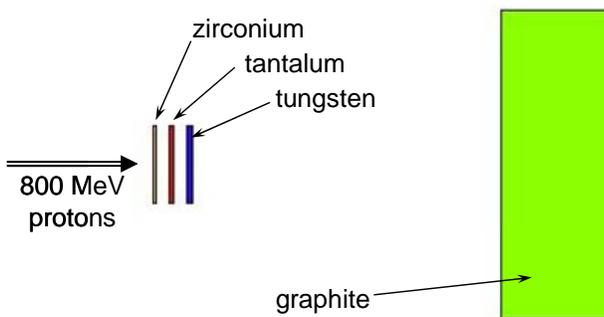


Figure 2. Schematic MCNPX model of the Blue Room target.

III.B. IPNS Depleted Uranium Target

The Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory is a pulsed spallation source that generates neutrons by accelerating protons to 450 MeV and directing them onto a target composed of light-water-cooled depleted uranium disks. The disks are clad with Zircaloy-2 to prevent corrosion and contained in a Type 304 stainless steel target shell.

In this problem, a simplified model of the IPNS target/moderator/reflector system (Figure 3) is used to estimate radionuclide inventory in the depleted uranium target disks and the stainless steel shell. The target undergoes several periods of irradiation followed by time for decay. This is a good test for CINDER and the script as the high-energy proton interactions in the target create spallation products, fission products, activation products,

and transuranic elements (through neutron absorption). The problem also includes neutron-induced activation in the stainless steel target housing.

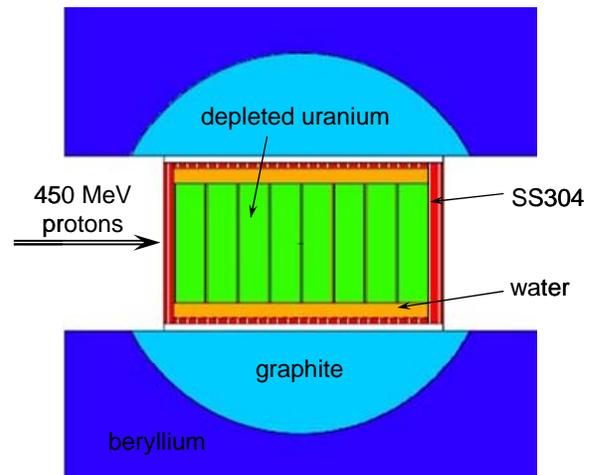


Figure 3. Simplified MCNPX model of the IPNS target and reflector assembly.

III.C. Simplified ATW Sub-Critical Core

This problem features a subcritical assembly typical of an Accelerator Transmutation of Waste (ATW) facility. ATW is intended to reduce the long-term heat load and toxicity of radioactive materials stored in a repository. To achieve this, long-lived fission products and transuranics would be 'burned' using neutrons produced by a high-power accelerator and a heavy metal target, multiplied in a subcritical blanket composed of spent and fresh fuel, structural material, and coolant. In the model problem (see Figure 4), there are three fuel regions which contain a PWR-type fuel mixture with structure and lead-bismuth eutectic (LBE) coolant included in a homogenous mixture, with the fuel being shuffled between regions in a fuel management campaign to optimize the burnup of the undesired nuclides. The proton beam target is also LBE. The system operates at a nominal power level of 2 GW, and heat from the system can be used to generate electricity.

III.D. ²⁵²Cf Spontaneous Fission Source

This problem involves the shielding of a ²⁵²Cf spontaneous fission neutron source (Figure 5). The source capsule has radius 0.5 cm, and is enclosed in a steel capsule of radius 1.0 cm and a polyethylene shield of radius 10 cm. Neutron absorption in the shield creates activation products during the operational lifetime which might complicate operations involving the shield when the source is removed and the shield material must

eventually be disposed of as waste. The neutron source for this problem has energies in the tabular regime, so that the same input file can be used with MCNP5. To run this problem with MCNPX, one must turn off the model physics but not the tabular physics in the activation script.

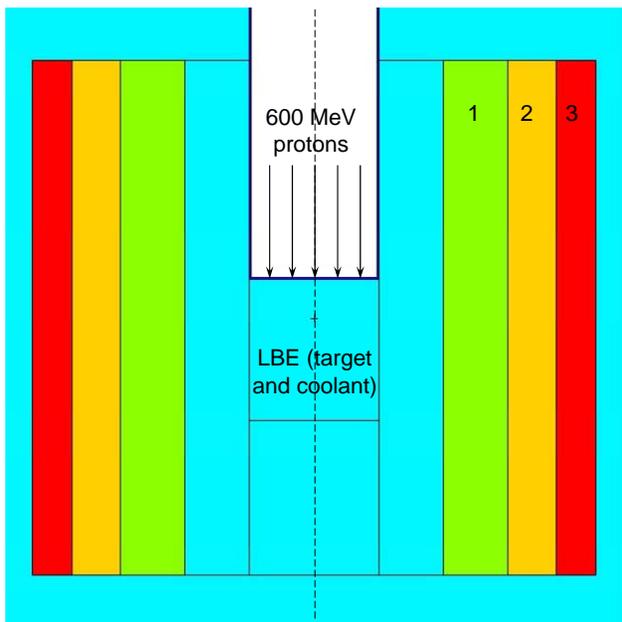


Figure 4. Simplified MCNPX model of a subcritical ATW core. The three fuel regions are identified by number. The dashed line represents an axis of rotation.

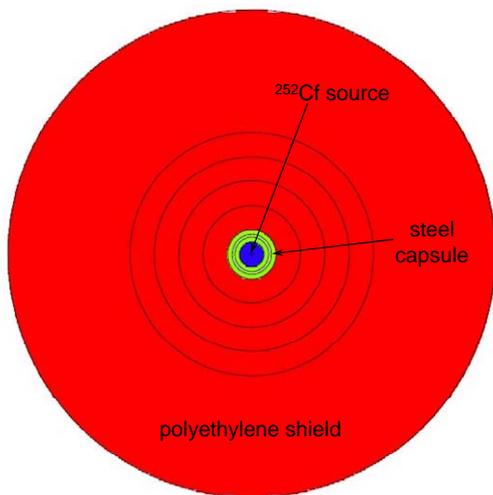


Figure 5. MCNPX model of a shielded ^{252}Cf source.

III.E. Liquid Deuterium Moderator

The preprocessor code suite used to prepare CINDER'90 input extracts the information on residual radionuclide production and on gas production separately from the HISTP file, and then combines them together. One important check for the activation script was to make sure that this was done correctly. An early version of the Perl script incorrectly handled problems that involved only gas production as defined in HTAPE3X (production of hydrogen and helium) without spallation product production. As a result we developed a simple problem analogous to a spallation target with a liquid deuterium cold neutron moderator. The simplified geometry shown in Figure 6 contains only a tungsten target and liquid ortho- D_2 moderator region.

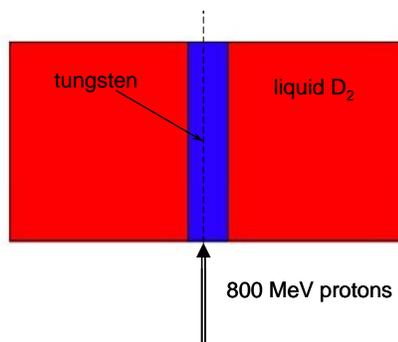


Figure 6. MCNPX model for problem of gas production in liquid deuterium. The dashed line represents an axis of rotation.

III.F. BMA Beam Dump

At the Paul Scherrer Institute in Villigen, Switzerland, negative pions were used for cancer therapy in the PIOTRON facility during the period 1980-1992. The biomedical area (BMA) was located on the western edge of the PSI West accelerator facility and used a fraction (20 μA) of the beam from the 590-MeV cyclotron. A pencil beam of protons irradiated a helium-cooled cylindrical beryllium target of radius 3 mm and approximate length 70 mm and was then deposited onto a beam dump located 40 cm behind the beryllium target. The beam dump was a water-cooled cooper block with a diameter of 8 cm and a length of 37 cm, and was surrounded by massive steel shielding. Figure 7 shows the MCNPX model geometry for this problem [12]. The beam dump was irradiated with an average current of 1.58 μA over the twelve-year period. The PIOTRON was switched off in September 1992 and decommissioned.

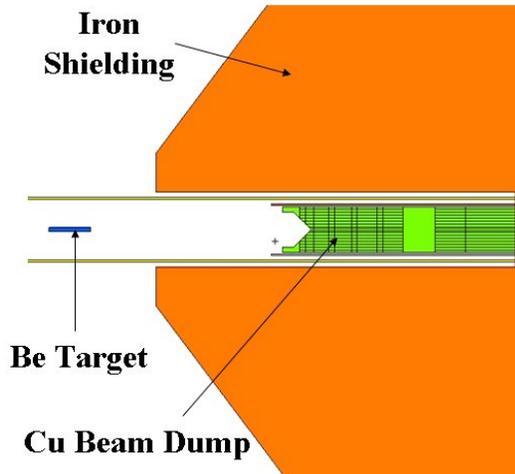


Fig. 7. Simplified MCNPX model of the BMA beam dump.

III.G. Decay of Short-Lived Isomers (Part 1)

The heat pipe power system is a reactor power system that was provided as a sample problem with an earlier version of CINDER. An MCNPX input file was constructed to test the activation script operation. Since this neutron source for this problem has energies solely in the tabular regime, the same input file can be used with MCNP5. Figure 8 shows horizontal and vertical views through the MCNPX model. Older versions of CINDER'90 contain a bug in which inelastic reactions in ^{235}U to $^{235\text{m}}\text{U}$ were not properly tracked back down to the ground state (the half-life of $^{235\text{m}}\text{U}$ is 26 minutes); they were being terminated (i.e., deleted from the chain) instead. This bug has been corrected starting in version 6.1 of CINDER'90. This problem represents irradiation of ~97% enriched uranium to assure that ^{235}U and $^{235\text{m}}\text{U}$ are properly tracked in CINDER'90.

III.H. Decay of Short-Lived Isomers (Part 2)

This problem for decay of $^{182\text{m}}\text{Ta}$ was also provided as a sample problem with an earlier version of CINDER'90. The sample MCNPX input file for this problem can also be used in MCNP5. In version 6.1 of CINDER'90, a bug was fixed so that the decay of $^{235\text{m}}\text{U}$ was properly tracked. However, a similar bug was found for the decay of $^{182\text{m}}\text{Ta}$ when decay times much longer than the half-life (15.8 minutes) were used. Thus, version 6.2 of CINDER'90 contains yet another modification. This problem tracks the decay of $^{182\text{m}}\text{Ta}$ after it is produced.

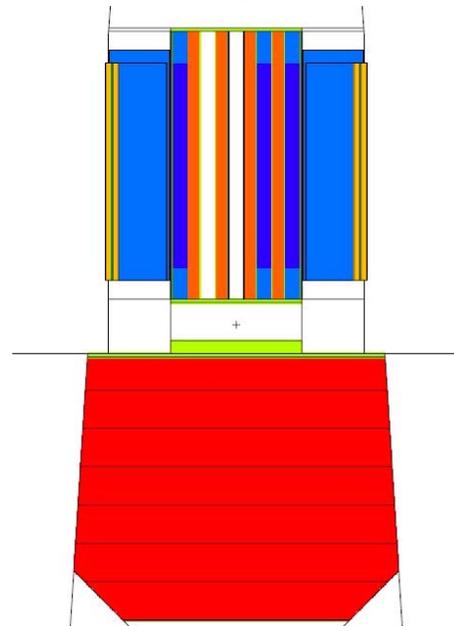
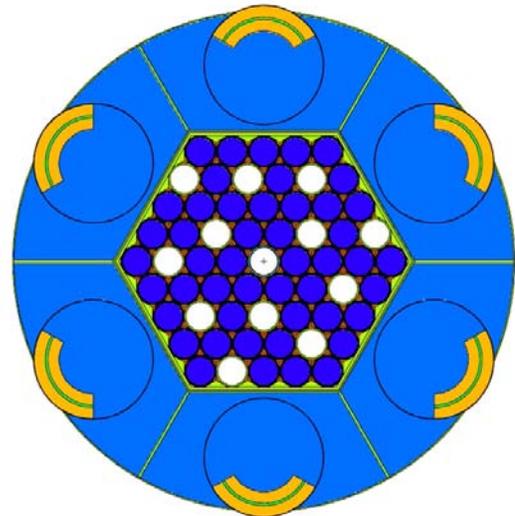


Fig. 8. Horizontal and vertical cuts through a MCNPX model of a heatpipe power system.

III.I. CINDER Manual Test Problem

This problem is based on the example problem in the (unreleased) CINDER manual. The problem geometry is comprised of concentric cylinders of hydrogen, helium, and lithium. However, the problem in the manual has input files FLUXES and SPLPRODS that are not the result of an actual transport calculation. For the purposes of testing the activation script and CINDER'90 codes we constructed a MCNPX input file in which the cylinders are irradiated with 100-MeV protons incident on one end of the cylinders. The problem geometry is shown in Figure 9.

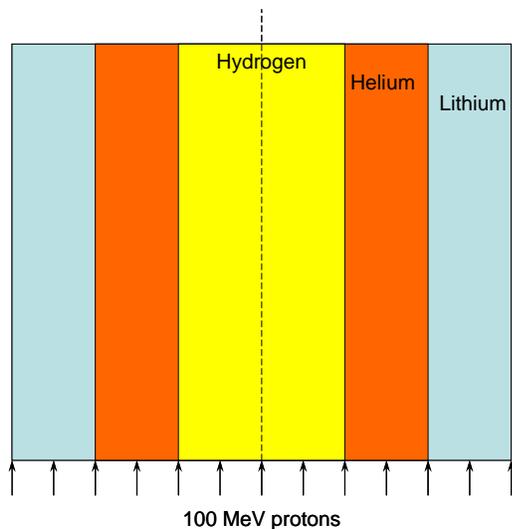


Fig. 9. Sample problem from CINDER'90 manual, with concentric cylinders of hydrogen, helium, and lithium irradiated with 100-MeV protons. The dashed line represents an axis of rotation.

III.J. 8-GeV Proton Beam

In MCNPX, hadron- and pion-induced nonelastic reactions at higher energies than 3.5 GeV and 2.5 GeV, respectively, are handed over to the FLUKA89 [13] physics model. To test how the residual products are treated by this model we have constructed a test case which has an 8 GeV proton beam (corresponding to the energy of the proposed proton driver linac at Fermilab [14]) incident on a 1-m long, 10-cm radius cylinder of graphite.

III.K. Electron Beam Irradiation of Subcritical Assembly

Subcritical assemblies can also be driven by electron accelerators, in which case the neutron source is photoneutrons released by bremsstrahlung created by electron interactions in the target. One proposal uses 200-MeV electrons incident on a water-cooled natural uranium target [15]. The MCNPX model for this system includes the target and coolant surrounded by a graphite reflector but with no fuel.

IV. FORTRAN COMPILERS

There are a variety of FORTRAN language compilers available on most computing platforms. Likewise, there are also many implementations of the Perl programming language. We did not attempt to test all FORTRAN and Perl versions available, but did test those owned by members of the collaboration. On the 32-bit Windows

platform (both XP and 2000) we used the Portland, Lahey, and Intel FORTRAN compilers, as well as the Linux-based MinGW cross-compiler suite, all with ActiveState Perl. Under Linux, we used the Portland, SilverFrost, and g77 FORTRAN compilers with the standard implementation of Perl or the ActiveState version.

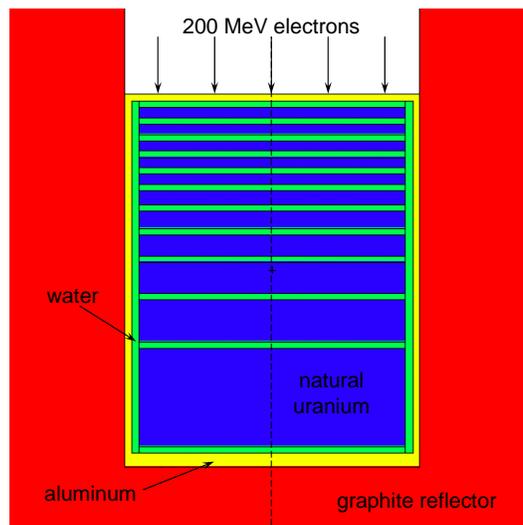


Fig. 10. Water-cooled natural uranium target irradiated with 200-MeV electrons. The dashed line represents an axis of rotation.

V. SUMMARY

The development of a sample problem suite serves several purposes. In the initial stage of code development, sample problems allow the developers a means of testing the features of the developed code, and to learn which additional features should be included. They provide users with a general idea of how to use the tools by providing examples of common applications, and also provide a valuable means of checking that changes to the code do not introduce errors.

ACKNOWLEDGMENTS

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