AN ENVIRONMENT USING NUCLEAR INVENTORY CODES IN COMBINATION WITH THE RADIATION TRANSPORT CODE MCNPX FOR ACCELERATOR ACTIVATION PROBLEMS

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We have written and tested a scripting tool which extracts cell-based material, neutron fluxes and spallation product information from MCNPX output files and drives transmutation calculations using the CINDER'90 code in accelerator-driven systems. This tool was later extended to also drive the alternative transmutation codes ORIHET3 and SP-FISPACT. Another scripting tool was generated for extracting decay gamma spectra and preparing MCNP(X) source decks for remnant decay gamma field calculations. The emphasis of this development effort was put on minimizing the need for user supplied input and simplifying the process of complex activation analyses. Also, an isotope production tally was implemented into MCNPX to enable feeding the transmutation codes without having to post-process the MCNPX history tape with HTAPE3.

I. INTRODUCTION

While earlier versions of CINDER'90 [1,2] are integrated into reactor core physics packages with deterministic transport codes like in DANDE [3], and with Monte Carlo codes like in MONTE-BURNS [4], the code now is being integrated directly into MCNPX [5] contributing decay processes to the particle transport scheme that traditionally only covered prompt processes. While the reactor community is well served by the integration efforts, the much smaller accelerator community cannot take advantage of these improvements as the MCNPX burnup feature is only accessible in eigenvalue calculations of fissile systems.

Over the years, some utilities were developed around the CINDER'90 code that allowed making use of the residual production information from the physics models being reported by the LAHET code [6], since activation cross sections were for a long time developed only for neutron induced reactions and to an upper energy limit of 20 MeV [7]. The CINDER'90 utilities were originally written for linking to the LAHET code system, and later extended by utilities converting MCNPX information into LAHET format to allow the use of the original utilities, which resulted in a cumbersome process preparing and performing activation calculations.

A group of CINDER'90 users from various US laboratories and European institutions formed a collaboration with the LANL CINDER'90 code developers with the charge of constructing a better CINDER'90 user interface and in working towards a public release of the CINDER'90 code.

Since then, scripts were programmed in PERL5 language that simplify the process of preparing and running activation calculations and also allow preparation of source decks of decay gamma sources for subsequent transport analyses in MCNP/MCNPX. Also, a set of sample problems was developed and exercised on different platforms.

The task of extracting isotope production rates and flux spectra from MCNPX output is the same for performing activation analyses with other transmutation codes. Therefore the scripts were extended to serve and execute also with the ORIHET3 [8] code and a modified version of the FISPACT [9] code named SP-FISPACT [10]. Providing these options enables an easy way for cross comparison of the transmutation codes since the calculations are based on exactly the same material, neutron flux and isotope production/destruction inputs.

The following sections give a detailed description of the scripts and an example comparing results of an activation analysis performed with the different transmutation codes the script serves.

II. THE CINDER'90 CODE

The primary goal of the development was to link the MCNPX and CINDER'90 codes. CINDER'90 is a code written in FORTRAN77 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 used are outlined in the manual [11] and in reference [7]. The data library covers 3400 nuclides in the range of 1≤Z≤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 [12] 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 [2] since its 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 to which a material is exposed, 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.

III. MCNP/MCNPX IN ACTIVATION ANALYSIS

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 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 a full activation calculation within an energy range from the MCNPX physics model region down to the table data region, two sources of residual nuclide production have to be considered.

To take into account the activation by neutrons with energies in the table region the user must specify an *F4:n* tally with a multigroup energy structure. 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 an isotope production tally was developed and implemented into MCNPX that allows tallying for the cell based isotope production and destruction rates directly in MCNPX. This tally is activated by the *active* card in the MCNPX input. This avoids having to write and store and post-process large event files. The standard MCNPX code has to be patched using the provided patch files to allow for the use of the *active* card. This ORNL-developed 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 remnant 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.
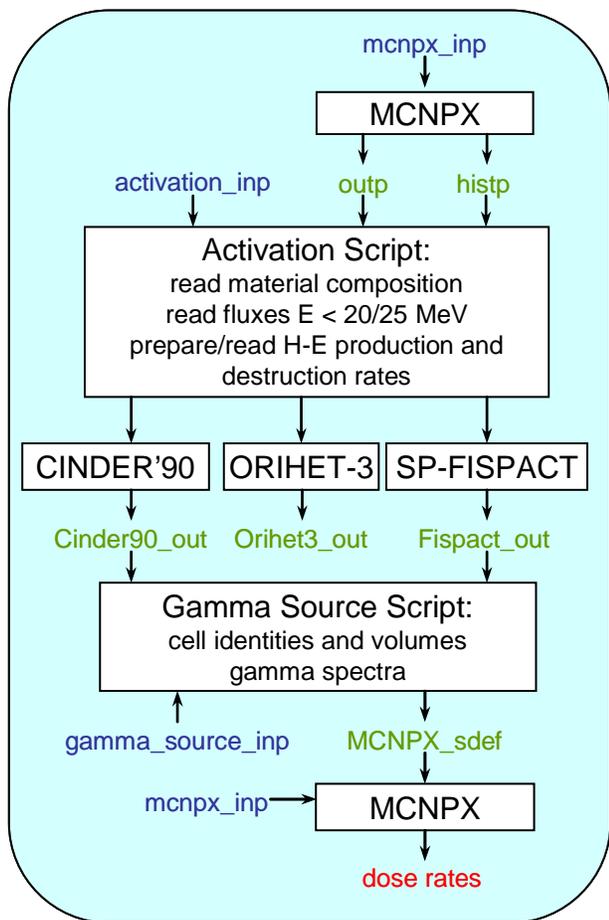
Fig. 1: Flow diagram of an activation analysis employing the activation script and the gamma source script with the radiation transport code MCNP(X) and the transmutation codes CINDER'90, ORIHET3 or SP-FISPACT. Input and output files are printed in blue and green font, respectively.

IV. THE ACTIVATION SCRIPT

The activation script provides the interface between MCNPX and the transmutation codes CINDER'90, ORIHET3 and SP-FISPACT as sketched in Fig. 1. The activation script operates from an input file that provides all necessary user supplied information for an activation run. The input is structured into the 10 blocks *codes, title_lines, files, run_options, cinder_options, fispact_options, orihet_options, normalization, history* and *cell_list*, which contain following information:

- *codes:* specifies the executable code names of CINDER'90, ORIHET3, SP-FISPACT, HTAPE3X and the auxiliary codes TABCODE (from the CINDER]90 package), and GROUPIE (for generating multigroup activation cross sections from pointwise data) for the use with

ORIHET3;
- *title_lines:* allows the user to define descriptive text to be placed into the result files;
- *files:* provides the file names of the MCNPX output and histp files, and a file of isotopic abundances by element;
- *run_options:* provides directory names for storing the activation calculation input and output files, and switches to turn on/off spallation product and neutron activation based production terms in the activation analysis
- *cinder_options, fispact_options, orihet_options:* set parameters like choices of activation cross section data libraries, group structures, choice of weighting spectra for flux regrouping, output options and cutoff settings specific to the transmutation code to be used;
- *normalization:* provides a normalization factor for scaling the activation calculation to the desired beam power;
- *history:* provide irradiation and decay history in sub-blocks of time steps and relative power levels;
- *cell_list:* provide a single MCNPX cell number or a list of MCNPX cell number for which an activation calculations is requested. Multiple cell numbers trigger a calculation for a merged cell conglomerate.

After reading a *cell_list* block, the script extracts the material data, neutron flux spectra, and model-driven isotope production and destruction rates for a specified material cell or for a list of cells from MCNPX outputs. The material and flux information is directly accessible from the regular MCNPX output. The radio-nuclide production and destruction rates become available only by post-processing the MCNPX histp file, which contains records of secondary particle production and residual nuclei produced by the high-energy event generators, with the HTAPE3X code from the MCNPX package. The activation script executes the HTAPE3X code after generating the necessary input files, and extracts the nuclide production and destruction rates from the HTAPE3X output files. In case the MCNPX output file was produced by the MCNPX version extended by the isotope production tally, the script reads the model-based isotope production and destruction rates directly from the MCNPX output. Up to this point the execution is the same for all three transmutation codes.

On the user request of CINDER'90 or SP-FISPACT, the script generates the appropriate material, flux and input-parameter files and executes the transmutation codes. Because ORIHET3 does not make use of neutron fluxes, on the request of ORIHET3, the script performs the folding of neutron fluxes with activation cross sections for the given material composition internally

applying either FENDL [13] or EAF [14] library cross sections and provides the overall production rates (sum of neutron-induced and high-energy parts) to ORIHET3. Also, an ORIHET3 input file is created containing parameters and the irradiation history.

Upon completion of writing the input files, the script executes the transmutation codes. The script allows multi-cell calculations, handling each cell individually or merged into a region. Neutron only problems can be treated by turning off use of the high-energy induced isotope/destruction production, which allows outputs from the MCNP [15] code to also be used as basis for transmutation studies.

The script allows stacking together calculations for different cells, or list of cells, and/or calculations with the three different transmutation codes or calculations with different transmutation code option and run-option settings.

For documentation reasons a listing of the calculations performed is maintained showing the cell list, directories of input and result files, summed volume and averaged density of the cell list.

A post-processing script has been written that allows extracting decay gamma distributions from the transmutation code result files and preparing gamma source definitions for subsequent MCNPX analyses. This script and applications of the script are in detail described in a separate contribution of this conference [16].

A series of 12 sample problems has been developed to test and describe the activation and gamma source scripts in preparation of packaging and distributing the package through appropriate channels as described in another contribution of this conference [17].

V. COMPARISON OF CINDER'90, ORIHET3 AND SP-FISPACT

For demonstration of the script and the capability of the featured transmutation codes, test problem 1 with stacked plates of tungsten, tantalum and zirconium, was run with the different available transmutation codes using the activation script. The merged isotopic activity of the zirconium and tantalum discs were compard for a one second irradiation with 800 MeV protons at 3.5 kW power. The plots in Fig. 2 show the abundance of about 370 isotopes produced separated into three isotope ranges to be able to distinguish single isotopes. For most of the isotopes all code report values of activity that are undistinguishable on the plots. But outliers exist, as a large quantity of He-5 (circled on Fig. 2a) activity reported by CINDER'90, which has no equivalent entries in the other codes, or a large quantity of Ta-182m reported by CINDER'90 with no entry in ORIHET3 and an order of magnitude lower values for SP-FISPACT

(circled in Fig. 2c), to address only the extreme cases. CINDER'90 reports the largest number of isotopes compared to the other codes, most of which are with low abundance. In some occasions ORIHET3 reports metastable states not seen by the other codes. SP-FISPACT seems to have a deficit on the neutron-poor side of the isotopes.

VI. CONCLUSIONS

Scripting tools developed to feed MCNPX output into the transmutation codes CINDER'90, ORIHET3 and SP-FISPACT have tremendously simplified activation calculations of accelerator driven systems. They contribute to the confidence in such elaborate analyses by helping reduce the error rate in input generation and by allowing easy comparisons of calculations performed by three independently developed transmutation codes.

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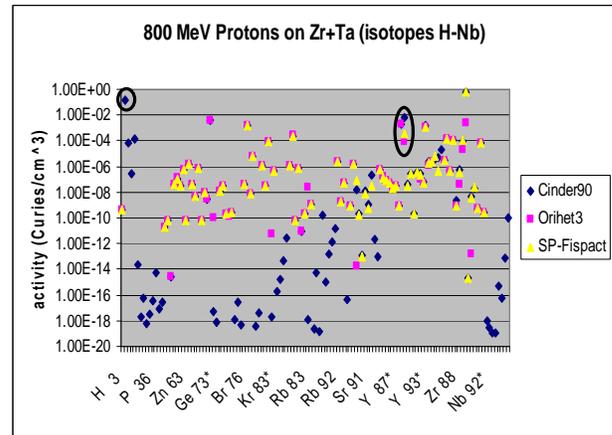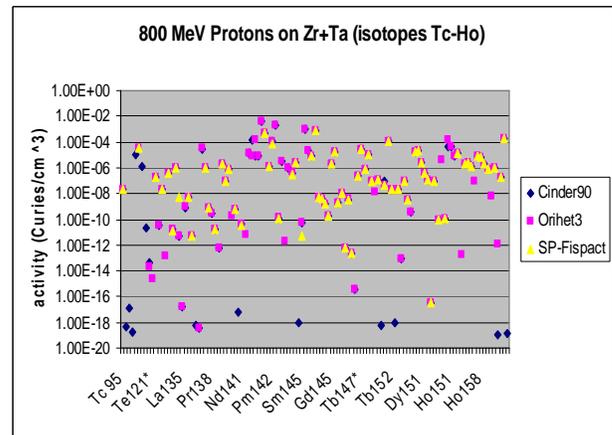
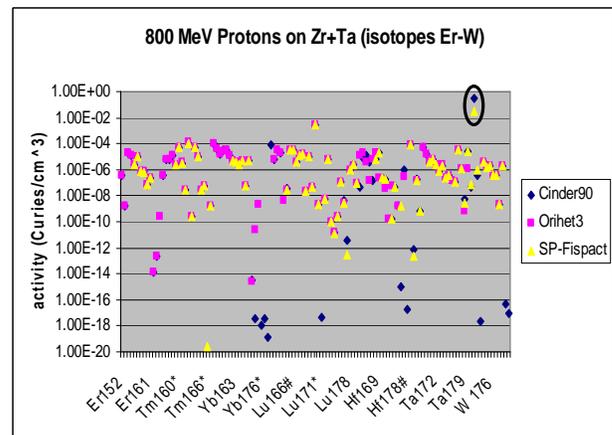Fig 2a: Elements H-Nb

Fig 2b: Elements Tc-Ho

Fig 2c: Elements Er-W

Fig. 2: Activity of isotopes in zirconium and tantalum discs irradiated for 1 second with 800 MeV protons at 3.5 kW. The circled areas are discussed in the test.