RECENT IMPROVEMENTS TO CINDER2008 AND ACTIVATION ANALYSIS TOOLS

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ABSTRACT

CINDER2008 is a transmutation code that calculates induced radioactivity for either reactor- or accelerator-driven radiation sources. Several Perl scripts have been developed to treat multi-cell problems in combination with either the radiation transport code MCNPX or a special version of MCNPX that writes residual nuclide tallies from model-based physics directly in the MCNPX output file. These scripts simplify the preparation of CINDER input, and can use CINDER output to prepare the source term for a subsequent MCNPX run to calculate dose rates due to activated material. In addition, these scripts support calculations with the transmutation codes SP-FISPACT and ORIHET-3. A number of improvements have been made to CINDER, its data libraries, and the Perl scripts, including (1) substantial corrections to the data libraries, (2) inclusion of recent revisions to USDOE HC-2/HC-3 thresholds and the corresponding thresholds for regulatory bodies in other countries, (3) the ability to run the CINDER accident analysis tool through the script input file, and (4) an easier way to write the script input file when treating a large number of cells. Some features of running CINDER and a number of example problems are discussed.

KEYWORDS
CINDER, activation, accelerators

1. INTRODUCTION

CINDER [1] is a transmutation code, developed originally at the Bettis Atomic Power Laboratory, which calculates induced radioactivity due to either reactor or accelerator-driven radiation sources. The code and its associated data libraries were expanded and improved over the years at Los Alamos National Laboratory. CINDER refers to either the transmutation code itself or to one of the packages (CINDER90 or CINDER2008) containing CINDER and its auxiliary codes. The meaning is generally clear from the context. CINDER2008 [2-4] is a modern implementation of the CINDER code package. The most notable improvements to CINDER are (1) the use of modern programming language and methods, (2) new

algorithms to solve the underlying differential equations more accurately, (3) integrated post-processing capabilities, (4) accident analysis tools for estimating dose, (5) NAMELIST input options, and (6) a constant-power approximation that allows the user to specify the fission power in W/cm^3.

Beginning with CINDER90, an *activation* Perl script [5] has been used in combination with the radiation transport code MCNPX [6] to simplify preparation of the necessary CINDER input files. This script can also be used with the codes SP-FISPACT [7] and ORIHET-3 [8]. A *gamma_source* script [9] uses the results of calculations from one of these codes to create MCNPX source cards for decay gammas in the irradiated material. These scripting tools were updated to support the execution of CINDER2008. CINDER2008 and these Perl scripts have been combined in a package named AARE (Activation in Accelerator Radiation Environments). Although the Perl scripts in AARE support the use of SP-FISPACT and ORIHET-3, these codes are not distributed as part of the AARE package.

Figure 1 shows the flow of a typical calculation using these scripts. The user prepares a script input file that identifies the proper MCNPX output files and cells for analysis, describes the irradiation history, chooses the appropriate CINDER reaction library, and sets the values of other parameters specific to the problem. A similar function is performed when using SP-FISPACT or ORIHET-3. The script manages all the pre-processing steps and then reads the MCNPX output to extract the material compositions, neutron fluxes, and model-based isotope production and destruction rates for the specified cells. The script then prepares the input files for and executes the selected transmutation code. Another input file directs the *gamma_source* script to prepare SDEF cards for a subsequent calculation using activation gammas in the irradiated regions. CINDER2008, through use of these scripts, can also use neutron fluxes calculated by either MCNP5 [10] or MCNP6 [11], which is useful for problems that do not require the extended particle capabilities of MCNPX and do not require particle energies outside of the tabular physics regime.

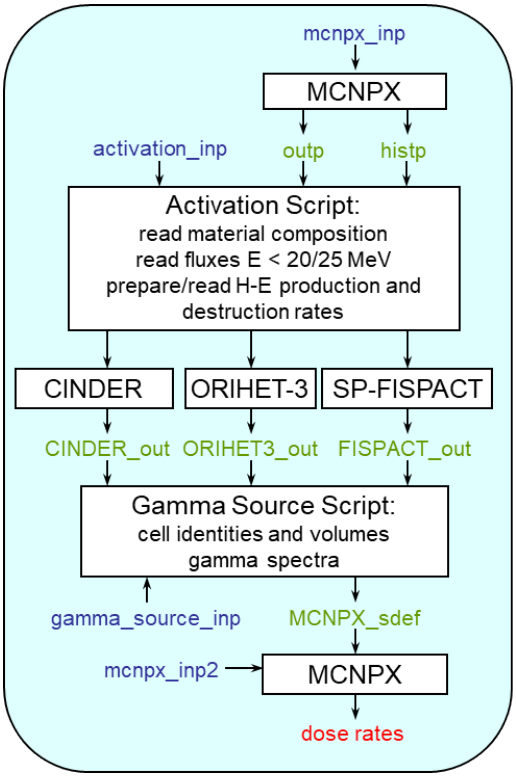

Figure 1. Use of the activation and gamma_source scripts with MCNPX and CINDER, ORIHET-3, and SP-FISPACT. Input and output file names are printed in blue and green, respectively [4].

2. UPDATES AND IMPROVEMENTS TO CINDER

2.1. EAF-2010-derived Reaction Data Libraries

CINDER2008 has three reaction data libraries, each providing the same information in a slightly different format. A 66-group library was collapsed from pointwise data using a thermal+fission spectrum. The group structure is the same as the 63-group library of CINDER90, except that the lowest-energy group from the 63-group set was replaced by four groups to provide a better estimate of neutron capture reactions in cold neutron sources. A 175-group library in the VITAMIN-J group structure was collapsed from pointwise data using a thermal+fusion energy spectrum. This library has few groups at low energy (the lowest group covers the entire range below 0.1 eV) and is best used for problems in which the neutron energy spectrum is well represented by a fusion neutron spectrum. Figure 2 shows the weighting functions used for the fission- and fusion-weighted libraries. Finally, a 321-group library based on the 315-group TRIPOLI group structure was collapsed from pointwise data using a constant weighting function. This library is expected to give the best results overall due to its fine group structure. The cross section data in each of the libraries were taken from ENDF-VII [12], EAF-2010 [13], and JENDL-3.1 and -4.0 [14]. Table I shows the sources of data in the CINDER2008 libraries. The files without reaction data are useful in decay-only calculations such as calculating the decay products from a ^{252}Cf source.

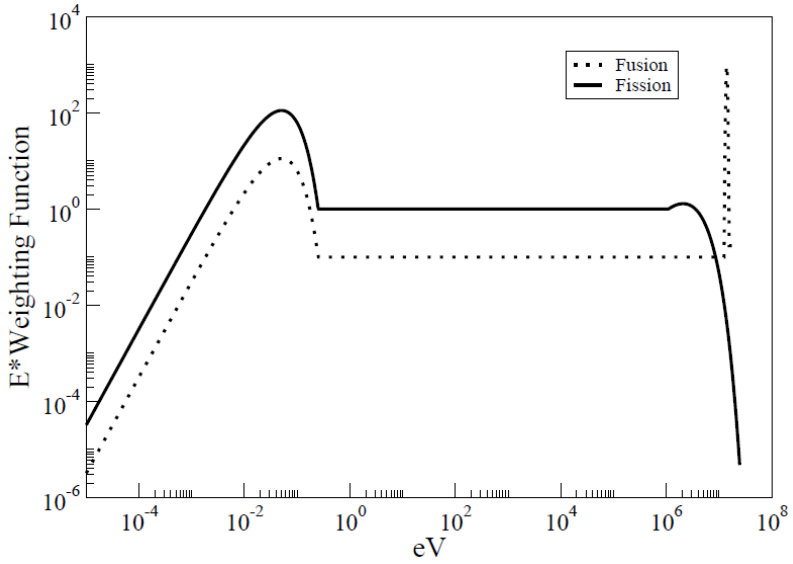

Figure 2. Spectral weighting functions for CINDER data libraries [2].

Some of the reaction data in the original CINDER2008 libraries, dated March 2011, were truncated in the fusion- and constant-weighted sets, so that cross section values were not included for the entire energy range. This affected only the data taken from the EAF-2010 file. A preliminary version of the EAF-2010 file was used for those original CINDER2008 libraries, and there may have been an incompatibility between the format of that data file and the CINDER2008 *library_maker* tool [15]. A new version of EAF-2010 was obtained, and the data were processed with the GROUPR module of NJOY99 [16]. The data in the fission-weighted library, though unaffected by this problem, were also updated since there were some differences in cross sections between the preliminary EAF-2010 file and the more recent one. The updated CINDER2008 libraries are dated September 2016. Figure 3 shows an example of the truncated data for the neutron capture reaction ^{18}O(n,γ), and Figure 4 shows the updated cross sections. Ref. [17] contains a full list of the nuclides and reactions affected. These were primarily radioactive nuclides, with some exceptions that include ^{18}O and isotopes of C, Ne, Pt, and Tl.

Table 1. Sources of Data in CINDER Cross Section Libraries.

xsec library	number of nuclides
none (decay only)	3265
EAF-2010	386
ENDF VII	162
JENDL 4.0	138
mixed libraries	113
JENDL 3.1	20

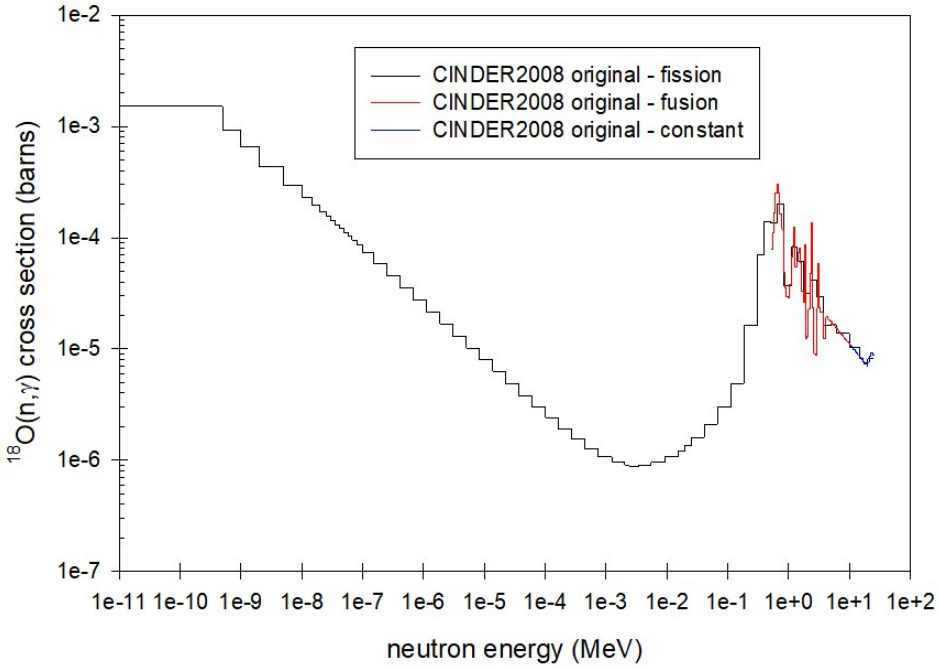

Figure 3. Cross sections for the ^{18}O(n,γ) reaction in the original CINDER2008 libraries.

2.2. Revised USDOE HazCat-3 Thresholds

One common use of CINDER is to evaluate a facility's radionuclide inventory to determine its hazard classification so that the proper regulatory approach can be applied. Threshold values have been established for each radionuclide to determine whether a facility should be considered a radiological facility or a nuclear facility. In addition, there are several grades of nuclear facility, with Hazard Category 3 (HC-3) being the lowest classification, and a separate set of threshold values applies to each. If multiple nuclides are present, a quantity called the sum of fractions (*SOF*) is calculated with the equation $SOF = \sum_i (A_i/TV_i)$, where A_i is the activity of each nuclide and TV_i is its threshold value. If the threshold values for HC-3 are used, a facility is considered a nuclear facility if $SOF \geq 1.0$, and a radiological facility if $SOF < 1.0$. In the CINDER90 code package, the HC-3 sum-of-fractions was calculated in ALLCODE using HC-3 values from a file supplied by the user. For CINDER2008, this calculation takes place in the POST code, and the HC-3 threshold values are included in the reaction data libraries.

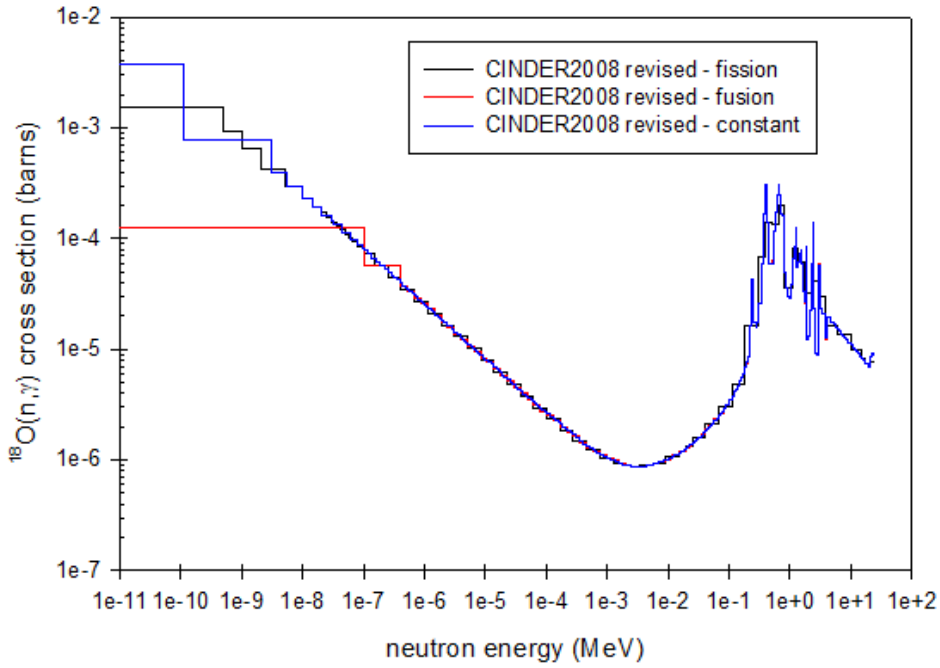

Figure 4. Cross sections for the ^{18}O(n,γ) reaction in the revised CINDER2008 libraries.

In 2014, the USDOE revised the HC-3 threshold values to be consistent with current radionuclide decay data, biokinetic models, and dosimetry. These revised values are contained in Ref [18], and Table II shows the original and revised HC-3 values for a few selected nuclides important in accelerator activation problems. An option in POST allows the use of user-supplied HC-3 threshold values by including a file named *thcat3* in the directory in which POST will run. This feature can also be activated in the *activation* script input. Figure 5 shows an application of this feature. If the user specifies a file name for the variable *thcat3* in the **post_options** data block, that file is copied into the directory in which POST runs. This file contains a nuclide identifier ZAS and the HC-3 threshold value in Curies for each nuclide. For those nuclides without HC-3 values specified in the given file, POST will use the HC-3 values in the CINDER data library. In this way, the user can update all or only a few HC-3 values and use the values in the CINDER data library for the remaining nuclides. Similarly, the user may apply threshold values used by regulatory bodies in other countries. A file with the complete revised HC-3 threshold values from Ref. [18] is included with the AARE package. Example problem #8 for the activation script [19] includes an example of the use of the *thcat3* file.

Table II. Original and revised HC-3 values for selected nuclides.

nuclide	original value		revised value	
	activity (Ci)	mass (g)	activity (Ci)	mass (g)
Na-22	2.4e+2	3.8e-2	2.54e+2	4.0e-2
Ti-44	6.2e+1	3.6e-1	9.31e+1	6.9e-1
Co-60	2.8e+2	2.5e-1	2.90e+2	2.6e-1
Zn-65	2.4e+2	2.9e-2	2.06e+2	2.4e-2
Mo-99	3.4e+3	7.1e-3	3.85e+3	8.8e-3
Cs-137	6.0e+1	6.9e-1	6.19e+1	7.0e-1
Hg-203	3.6e+2	2.6e-2	5.18e+2	1.3e-1

```
post_options
  run  1
  postdir  act08-31
  thcat3  ../data/thcat3_lanl2014_zas.dat
```

```
ZAS   HC-3 threshold
110220 2.54E+02
220440 9.31E+01
270600 2.90E+02
300650 2.06E+02
420990 3.85E+03
551370 6.19E+01
802030 5.18E+02
```

Figure 5. Example of a *thcat3* file and its use in the *activation* input file.

2.3. CL_FILE Option Block

If a large number of cells are being processed with CINDER, it can be tedious to set up all the **cell_list** data blocks in the *activation* script input. A new option, the **cl_file** option block, will automatically create the desired **cell_list** data blocks. The only entry to the **cl_file** option block is a file name that contains a list of cells to be treated. In this file, the cell numbers should be entered on a single line with the first cell beginning in column 1. A new script input file named *input_expanded_cell_list_file.inp* is created in the directory in which *activation* is run. An example of the **cl_file** data block and a corresponding cell list file, used in *activation* example problem #6, is shown in Figure 6.

cl_list data block

```
cl_file
  file  bma_cells
```

contents of file *bma_cells*

```
1 2 3 4 5 6 7 8 9 10 11 12 101
```

Figure 6. Example of cl_list option block in the activation Perl script.

2.4. CINDER2008 Accident Analysis Tool

A new feature introduced in CINDER2008 is the Accident Analysis tool, which provides an estimate of dose due to release of radioactive material. This calculation accounts for both submersion (external) and inhalation (internal) dose. In executing this feature, the user may input nuclide-specific values for many quantities, or specify global values that are used for all nuclides. CINDER does not perform an atmospheric dispersion calculation, but uses a user-specified dispersion factor, and thus has no explicit time dependence.

CINDER calculates a Total Effective Dose Equivalent (TEDE) $= T_E \cdot X \cdot [DCF_E + DCF_I \cdot BR \cdot RF]$ where

T_E = exposure time
X = radionuclide concentration (Bq/m^3)
DCF_E = external dose conversion factor (Sv/h)/(Bq/m^3)
DCF_I = internal dose conversion factor (Sv/Bq)
BR = breathing rate (m^3/h)
RF = respirable fraction

CINDER makes use of a normalized dispersion factor DF, which is the ratio of activity concentration X to release rate $\dot{Q}$. The release is assumed to be constant in time so that $\dot{Q} = ST/T_R$ and then $X = DF \cdot \dot{Q}$ $= DF \cdot (ST/T_R)$ where

T_R = release time
ST = source term (Bq) = $MAR \cdot DR \cdot ARF \cdot LPF$
MAR = material at risk (activity calculated by CINDER)
DR = damage ratio
ARF = airborne release fraction
LPF = leakage path factor

Combining these, one arrives at the equation for total dose

$$TEDE = DF \cdot ST \cdot (T_E/T_R) \cdot (DCF_E + DCF_I \cdot BR \cdot RF)$$

where (T_E/T_R) is called the time ratio, for which the user may specify a global value or nuclide-specific values. The release takes place over a time T_R, and the exposure occurs for a fraction of that time T_E/T_R.

To run the Accident Analysis tool, the user provides an input file to CINDER named *dose_input.dat* that contains the necessary parameters, or the names of the files where they are located. The user can construct the *dose_input.dat* file manually if running CINDER in a stand-alone mode, or use the *activation* Perl script through the **aat_options** block. Figure 7 shows an example of using the Accident Analysis tool in CINDER (CINDER example problem #3), and Figure 8 shows how to use the *activation* script to construct the same *dose_input.dat* file (*activation* script example problem #2).

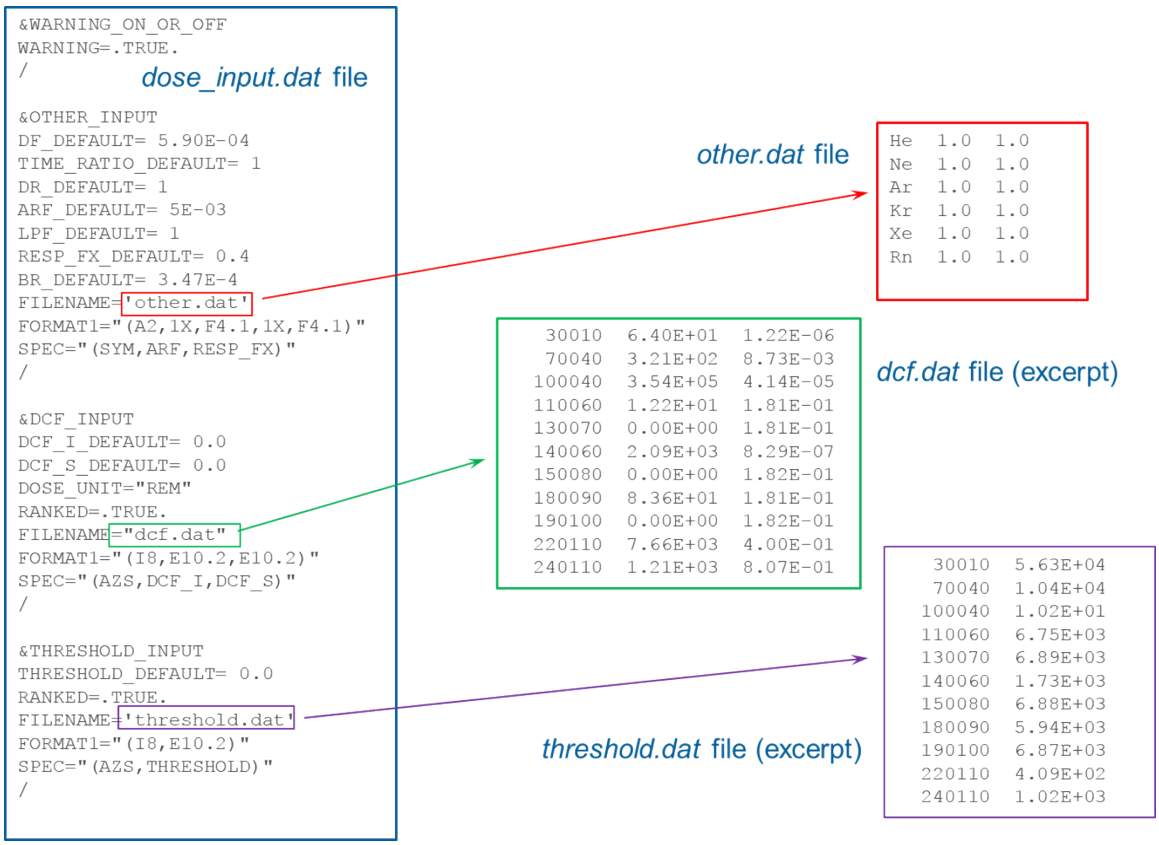

Figure 7. dose_input.dat file in CINDER example problem #3.

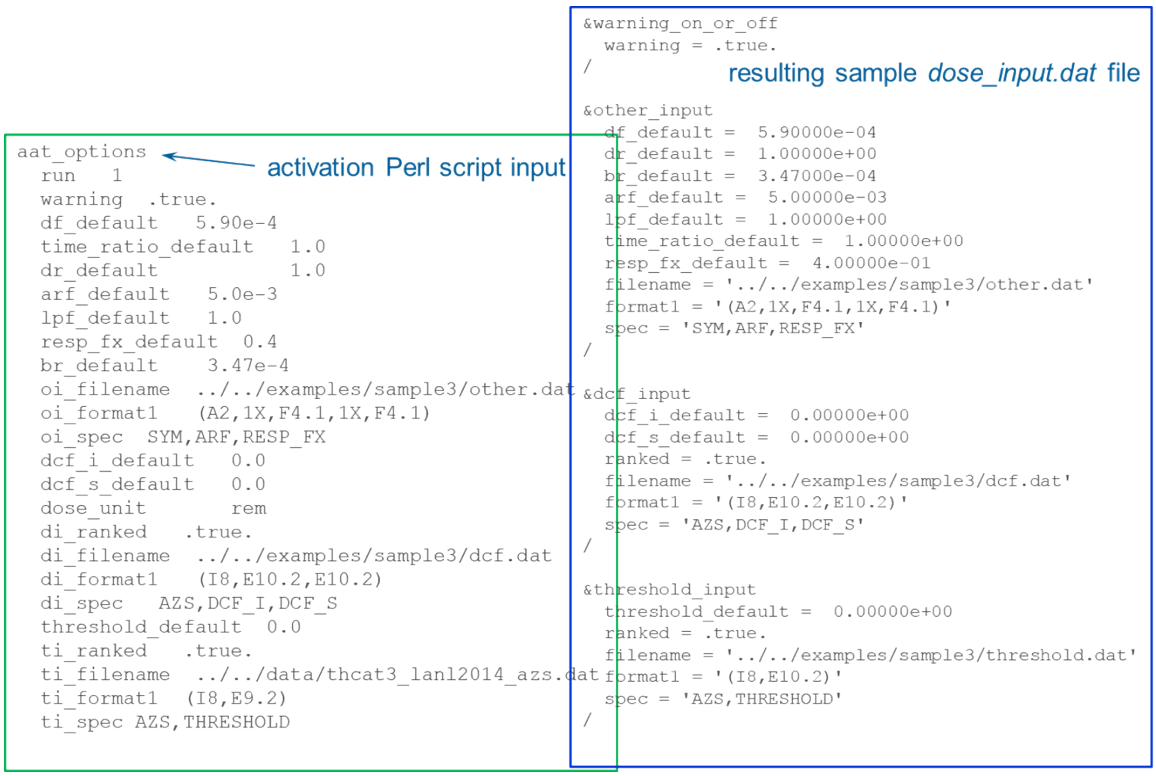

Figure 8. dose_input.dat file in CINDER example problem #3.

2.5. MCNP6 Compatability

The *activation* script processes model-based radionuclide production from either the *histp* file written by the standard version of MCNPX, or from a special version of MCNPX that writes the nuclide production and destruction rates directly into the MCNPX text output file. The original version of MCNP6 did not have the capability of writing the *histp* file. A patch to MCNP6 enabled writing the *histp* file, but only in a single-processor mode. The upcoming release of MCNP v6.2 will have this same capability. A patch that enables writing the nuclide production/destruction rates in the MCNP text output file for multi-processor problems has been developed for MCNP v6.1 and is undergoing testing.

3. SUMMARY

The CINDER2008 code package contains a completely revised version of CINDER and the auxiliary code POST. The CINDER data libraries have been updated, and revised USDOE HC-3 values are available for use with POST. Updated versions of scripting tools written in Perl provide access to several of CINDER2008's new features. Several examples of these new capabilities were presented, and more are illustrated in example problems distributed with the code package.

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