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Title:	New ACE Format Proton Table for Be-9
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memorandum

X-Computational Physics (XCP-DO)

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Subject: New ACE Format Proton Table for Be-9

You experienced fatal errors using MCNP® 6.2 in a MODE h n p (proton-neutron-photon) problem, seemingly dependent on the proton source energy. The error from MCNP was largely non-informative (ACECAS reported "Wrong number of discrete lines for law 4/44," but no information about the ZAID, incident particle type, incident particle energy, secondary particle type, or reaction type).

Using a combination of ptrac and debug output, you determined that the problem (in one instance at least) occurred for an incident proton in a specific material in your problem. That material, unfortunately, included about a dozen isotopes. For those isotopes for which proton ACE data tables were available, MCNP was calling tables from the ENDF70PROT library (ZAIDs ending in .70h, Reference – "The Processing of ENDF70 and ENDF70PROT: New ACE-Formatted Neutron and Proton Libraries Based on ENDF/B-VII.0," Trellue, Little, and Lee, LA-UR-08-1999).

I reviewed ENDF6-formatted files on the BNL web site https://www.nndc.bnl.gov/exfor/endf00.jsp. In particular, I was searching for any proton evaluation that included discrete-energy secondary particles. Among the isotopes included in your material, only one had such discrete-energy secondary particles: Be-9.

The p + Be-9 evaluation specifies one discrete secondary gamma (E_γ = 3.5629 MeV) in MF = 6, MT = 5 as part of all "Law 1" tabulated secondary photon energy distributions for incident proton energies from threshold (E_p = 1.8679 MeV) through E_p = 40 MeV. For such distributions from E_p = 45 MeV through the maximum energy of the evaluation (E_p = 113 MeV) the number of specified discrete secondary gammas was zero. This specification does not violate ENDF6 format rules.

The p + Be-9 evaluation also specifies "discrete 2-body scattering" for secondary neutrons from MTs 50 through 55. This type of "discrete" scattering is handled differently in MCNP than that described in the last paragraph for discrete secondary gammas, and is of no concern for this work.

Some readers might note that the evaluations easily available on the BNL web site above include ENDF/B-VII.1 but not ENDF/B-VII.0. Since ENDF70PROT was based on ENDF/B-VII.0, I checked Morgan White's very useful compilation of ENDF evaluations on the ADX LAN at /opt/local/codes/data/nuclear/endf/… to confirm that the p + Be-9 evaluation was the same in VII.0 and VII.1.

The ACE table 4009.70h faithfully reproduced the proton-induced photon energy distributions as provided in the ENDF evaluation (note that the version of NJOY used for this processing was NJOY99 Version 248). This would seem to be a good thing! However, MCNP requires that the number of discrete-energy secondary particles in any MCNP Law = 4 or LAW = 44 tabulation be identical at all incident energies comprising that tabulation. Otherwise, the code cannot interpolate between adjacent incident energy distributions. Ultimately, the discontinuity between one discrete line at E_p = 40 MeV and zero discrete lines at E_p = 45 MeV caused ACECAS to call EXPIRX with the "wrong number of discrete lines for law 4/44" message.

I verified that this was a problem by creating a very simple MCNP test problem. When I used ZAID 4009.70h in a MODE h n p problem, I quickly received the same error message as you had previously. When I changed to MODE h n only, MCNP did not fail. Using materials other than Be-9 from ENDF70PROT in MODE h n p also caused no issue. (Note – I ran MCNP on local machine varan by loading and using /opt/local/codes/mcnp/modules/mcnp6/6.2.)

Note that NJOY (even in 2008) would catch and repair instances of non-constant number of discrete lines in secondary distributions for neutron-incident evaluations. Why did NJOY not catch and repair this instance? Why did our Nuclear Data Team (NDT) checking codes not flag this as a problem (as they would for neutron-incident evaluations)? It turns out that the NDT checking code checknd (or at least today's version of that code (thanks to Kent Parson for pointing me at /usr/projects/data/nuclear/mc/endf7/acs for the NDT checking codes) *does* catch the problem. But, it simply notes it rather than flagging the problem as an *ERROR* that needs to be corrected. I recommend that the NDT consider expanding the write statement at line 145 of checknd.f to make it clear that an error has been found.

To provide a fix for this problem, I first wrote a little code to add a zero-probability discrete gamma line to the ENDF evaluation at incident proton energies of 45 MeV and above. I am confident that the resulting modified ENDF file, when processed through NJOY, would have flowed through MCNP without error.

Before completing this path, I decided to try what might have been a more obvious fix – namely running today's NJOY with the original evaluation to see if a fix to this problem had crept into NJOY over the past decade.

Thanks to Wim Haeck and Jeremy Conlin for pointing me to the current NJOY 2016 executable on Snow (/usr/projects/data/nuclear/bin/NJOY2016/bin/njoy). The NJOY version I used was 2016.43 and I executed the MODER, RECONR, BROADR, GASPR, and ACER modules. (Unfortunately, it appears that the NDT has lost the archival NJOY input / output files used in the original creation of ENDF70PROT, so my NJOY input may be different than was used in the original processing.)

It turns out that indeed the desired fix had crept into NJOY over the past decade! The resulting ACE file does specify one discrete proton-induced photon (E=3.5629 MeV) for all incident proton energies. The probability for this discrete line is zero at incident proton energies of 45

MeV and above. I used this table in my simple MCNP test problem and it flows through correctly.

I have given the resulting ACE table a ZAID of 4009.99h. The table is stored on open hpss as /hpss/rcl/proton/p+be9 (I will store in the same location on secure hpss once I figure out how to do that). I have not updated xsdir files maintained by the NDT or MCNP team. So, until and unless someone does that, the user needs to incorporate an XS card in the MCNP deck as follows (obviously assuming that the file "p+be9" is in local file space):

xs1 4009.99h 8.934761 p+be9 0 1 1 79932 0 0 2.530E-08

Other files associated with this project are also archived on the open under the same hpss directory.

In summary, the Be-9 proton table found on the ENDF70PROT library contains a flaw that will cause certain MCNP runs having both protons and photons to fail. The current version of NJOY 2016 creates an ACE table without this flaw. The resulting ACE table with a ZAID of 4009.99h has been made available for user applications. Please let the author know of any difficulties encountered with or questions about this table.

The author would like to thank the memo recipient for generously providing a few days funding for this work.

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XCP-DO files