



memorandum

XCP -- Computational Physics

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SUBJECT: The NJOY Temperature Bug in PURR and a List of Affected Materials

Introduction:

A bug in the calculation of the probability tables in NJOY was reported recently by a user. The bug was resolved in 2012 by Skip Kahler but cross sections processed prior to that still contain incorrect data. This memo discusses the bug, its fix, and lists the affected materials in the MCNP ACE cross section libraries.

The Bug:

All versions of the PURR module (until NJOY version 99.387, dated Nov. 2012) for the production of probability tables for unresolved resonances have incorrect coding for non-room temperature continuous energy cross sections. This bug affects:

- continuous energy ACE files produced using ACER and PURR
 - does NOT affect multi-group cross sections produced by GROUPT
- cross sections in the unresolved resonance energy range
- unresolved resonance energy cross sections at all material temperatures
 - **except room temperature**

This is the actual NJOY update message: (from Skip Kahler)

```
*ident up387
*/ purr -- 19nov2012
*/ - the calculation of ctx in subroutine unrest includes a temperature
*/ ratio, tref/temp(_). we really should be taking the square root
*/ of this ratio, per the definition of cth in unresx. this impacts
*/ all probability tables that have not been calculated at 300K.
*/ (ornl, wiarda).
```

ACE library materials with probability tables are designated with a PTABLE entry in the xsdir directory file and with a non-zero entry in the JXS(23) array element in the first few lines of an ACE table. Not all ACE files have probability tables.

The List:

The biggest set of ACE tables affected by this bug are in the ENDF70x (where x= b,c,d,e,f,g,h,i,j,k) files and have the suffixes .71c (for 600 K), .72c (for 900 K), .73c (for 1200 K), and .74c (for 2500 K). The room temperature ACE tables with the .70c suffix are fine as are all of the .71c to .74c tables without PTABLE. Basically, most all of the ACE tables from Germanium (Z=33) thru Californium (Z=98) are incorrect in .71c through .74c. Note that the big 3 of U-235, U-238, and Pu-239 are all included in the bad list.

Fortunately, the latest and greatest ACE tables for MCNP6 based on ENDF/B VII.1 (with suffixes .80c thru .86c, or, alternatively, suffixes .710nc thru .716nc) were processed after the PURR bug fix and are therefore all ok.

Other miscellaneous old data tables are affected as well. ACE tables with PTABLE and ZAID suffixes of .61c from ACTI, .64c from endf66d, or .67c from t16_2003 are also incorrect. Fortunately, most of the ACE tables for ACTI, endf66d, and t16_2003 are at room temperature and have ZAID suffixes of .62c, .66c, and .69c, respectively.

Convenient Condensed List:

ACE table materials with the following ZAID suffixes are incorrect if they include PTABLE. The name of data file which contains the incorrect data and the assumed material temperature are also given.

.61c	actib	ACTI .61c tables are at 77 K
.64c	endf66d	all .64c tables are at 77 K
.67c	t16_2003	all .67c tables are at 77 K
.71c	endf70b thru endf70k	all .71c tables are at 600 K
.72c	endf70b thru endf70k	all .72c tables are at 900 K
.73c	endf70b thru endf70k	all .73c tables are at 1200 K
.74c	endf70b thru endf70k	all .74c tables are at 2500 K

Note: the endf70 tables with the .70c are actually at 293.6 K – but that is considered close enough to 300 K to ignore any effects from the PURR bug.

DKP:dkp