LA-UR-12-00018

Approved for public release;
distribution is unlimited.

Title:	Further Notes on MCPLIB03/04 and New MCPLIB63/84 Compton Broadening Data For All Versions of MCNP5
Author(s):	Morgan C White
Intended for:	Web Based Distribution to the MCNP Users Forum

Form 836 (7/06)

Los Alamos
NATIONAL LABORATORY
memorandum
Materials & Physical Data
Computational Physics Division
Phone (505) 667-7780

To: MCNP User Forum
From/MS: Morgan C White, XCP-5, MS F663
Email: morgan@lanl.gov
Symbol: XCP-5:MCW-12-011 (U)
Date: January 3, 2012

SUBJECT: Further Notes on MCPLIB03/04 and New MCPLIB63/84 Compton Broadening Data For All Versions of MCNP5

CAUTION Users of MCNP 5 ***SHOULD NOT*** use the photon transport libraries MCPLIB03 and MCPLIB04.

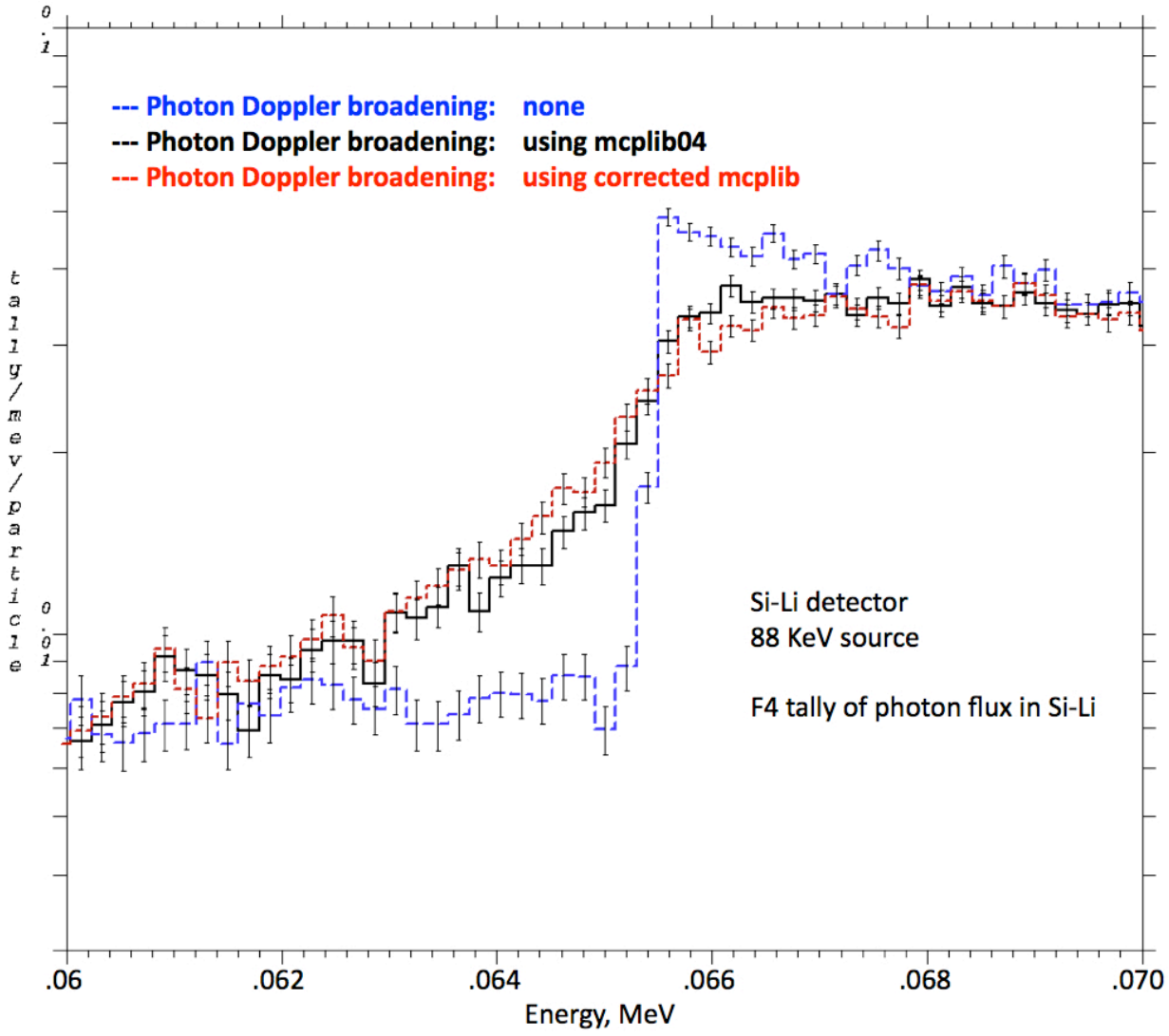
It has recently been brought to the attention of the nuclear data team that the algorithm encoded in MCNP5 incorrectly assumes that the photon Compton broadening data provided in the MCPLIB03 and MCPLIB04 libraries provides the probability of interacting with a given electron shell as a cumulative probability distribution (CDF). The data are given as a probability density function (PDF) as this was the original way in which the data where provided and this maintains higher precision for the stored data. **The expectation was that the code would convert these to a CDF distribution on-the-fly before sampling. This is *NOT* the case. MCNP5 (and MCNPX) uses the photon Compton broadening algorithm by default when the data are available and thus will give incorrect simulation results.** This problem does not affect MCNP4C3 and earlier, they did not contain coding for this algorithm, nor will it affect the final releases of MCNP6 and later (though it does affect the Beta 1 and Beta 2 releases).

A simple solution presents itself to fix this issue without the need for distributing a code update and recompiling, verifying and validating the code for other purposes. New versions of the MCPLIB03 and MCPLIB04 data libraries have been produced where the probability of interacting with a given shell is stored using as a cumulative distribution function. These alternate versions of the libraries are being released as MCPLIB63 and MCPLIB84 using the library IDs '63p' and '84p', respectively. The choice of IDs is intended to keep these updates out of the general sequence of releases and indicate their special nature. It is highly recommended that users of MCNP5 ***download*** these updated libraries and ***replace*** their existing XSDIR file with a version that includes the MCPLIB63 and MCPLIB84 entries and does not include any reference to the MCPLIB03 and MCPLIB04 versions. These libraries and instructions on this process will be available through the MCNP web site.

http://mcnp-green.lanl.gov/

This memorandum constitutes the official release documentation for the MCPLIB63 and MCPLIB84 photon transport libraries. These libraries are identical to the MCPLIB03 and MCPLIB04 data with the exception of the XSS[LPIPS] array given using a cumulative distribution function rather than a probability distribution function.

It should be noted that this issue does not have a significant impact for most simulations. This algorithm was implemented for performing specialized calculations of detector efficiency curves for photon measurements. It makes small corrections to the Compton edge in simulations of scattering. The figure below shows three curves: no photon Doppler broadening (blue), broadening using incorrectly sampled shells (black), and correctly sampled shells (red). While this is a small affect on this example problem, there may yet be cases where a more significant impact is found. As always, the end user is reminded that validation for a given application is ultimately the responsibility of the user. As much care is taken as possible to ensure the code and data are as accurate and bug free as possible but mistakes can and do slip in. See, for example, that the original validation of these data for use in computing detector efficiency curves did not catch this issue.



At the time these data were adopted as part of MCPLIB03 and MCPLIB04, they were only spot checked to determine that they reproduced the values given in the original publication. Having

now had to deal with issues in this algorithm on multiple occasions, it was felt a bit more time should be spent looking over the data. It is now felt that the data, like the original algorithm, are a bit deficient. There are inconsistencies with the number of electron shells between the latest ENDF/B atomic relaxation data and the data referenced herein. In addition, the binding energies have been updated over the years since these data were created and, due to formatting and translation issues, some of the binding energies stored on the data libraries are given as zero. This all points to the obvious conclusion that users with a serious need for these data should sponsor an updated evaluation and that these evaluated data should be folded into the ENDF/B database so such that their production, verification and use can be better controlled and validated.

As part of the post-mortem looking over this issue, changes are being made to "Appendix F" which is the official definition of the ACE data formats. This updated document will be released as a separate document. It is felt that a separate document of the data format is a good idea for multiple reasons: it is intended for unrestricted distribution, there are other users of the ACE data, and it can be updated independent of other release schedules. The updated format will now allow for either PDF or CDF data to be stored for the probability of interacting with a given shell. The recommended value will be the PDF. The code using the data will be required to check if the last value is unity and, if so, recognize it as CDF data, otherwise, it is PDF data. This unfortunate condition will allow all of the MCPLIB data distributed to be used with codes like MCNP6.

References:

A. Sood, Doppler Energy Broadening for Incoherent Scattering in MCNP, Part I, Los Alamos National Laboratory internal memorandum X5:AS-02-16 (LA-UR-04-0487), July 31, 2002.

A. Sood and M.C. White, Doppler Energy Broadening for Incoherent Scattering in MCNP, Part II, Los Alamos National Laboratory internal memorandum X5:AS-02-17 (LA-UR-04-0488), July 31, 2002.

Morgan C White, Photoatomic Data Library MCPLIB03: An Update to MCPLIB02 Containing Compton Profiles for Doppler Broadening of Incoherent Scattering, Los Alamos National Laboratory internal memorandum X-5:MCW-02-110 (LA-UR-03-0787), December 19, 2002.

Morgan C White, Photoatomic Data Library MCPLIB04: A New Photoatomic Library Based On Data from ENDF/B-VI Release 8, Los Alamos National Laboratory internal memorandum X-5:MCW-02-111 (LA-UR-03-1019), Revised February 7, 2003.

Distribution:

MCNP User Forum
MCNP Team, XCP-3, LANL
Nuclear Data Team, XCP-5, LANL
Robert C. Little, XCP-DO, LANL