LA-UR-09-0467

Approved for public release;
distribution is unlimited.

Title:

Testing of Photon Doppler Broadening in MCNP5.1.50 and MCNP5.1.51

Author(s):

Avneet Sood
X-1 Transport Applications
Applied Physics (X) Division
Los Alamos National Laboratory

Intended for:

Internal documentation

Testing of Photon Doppler Broadening in MCNP5.1.50 and MCNP5.1.51

Los Alamos National Laboratory Report:

LA-UR-09-0467

Avneet Sood
Los Alamos National Laboratory,
Applied Physics (X) Division,
X-1 Transport Applications Group,
P.O. Box 1663, MS A143,
Los Alamos, NM 87545

January 26, 2009

Abstract

MCNP5-1.50 was released by RSICC in December, 2008 as part of RSICC package CCC-740. A significant error in the photon Doppler broadening routine that could lead to incorrect results was discovered. Notification to MCNP users was given along with a patch file that corects this error [1]. This research note documents some test problems that will detect problems with this feature.

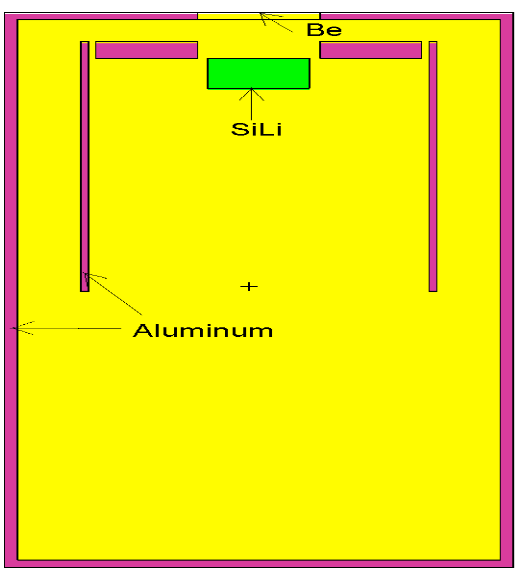
Introduction

Incoherent scattering of an incident photon can occur with a bound electron in a shell of a material and will generate a Compton electron and a scattered photon. These bound electrons carry momentum which can add or subtract to the momentum of the incoherently scattered photon. These binding effects change the anglular- and energy-distributions of the scattered photon. These effects become important when the incident photon energy is near a few hundred keV. MCNP (MCNP5 and MCNPX) has accounted for these electron binding effects on the scattered photon's energy.

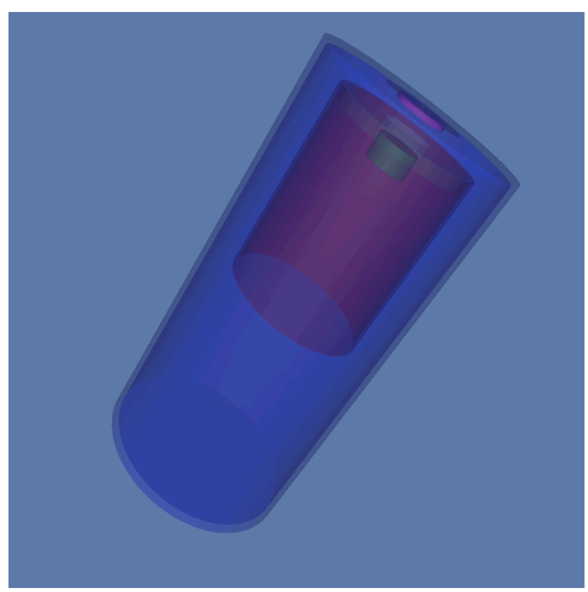
The Hartree-Fock Compton profiles are used to account for the effects of a bound electron on the energy distribution of the scattered photon. These Compton profiles are a collection of orbital and total atom data tabulated as a function of the projected precollision momentum of the electon. Values of the Compton profiles for the elements are published in tabular form and are included in the nuclear data libraries distributed with MCNP5 (mcplib03, mcplib04). The scattered energy of a Doppler broadened photon can be calculated by selecting an orbital shell, sampling the projected momentum from the Compton profile, and calculating the scattered photon energy. The details of this treatment are documented in the references [2, 3].

The Test Problem

A simple test problem has been created to demonstrate the effects of photon Doppler broadening. The test problem consists of a simplified model of a SiLi detector with a Cd-109 (88 keV) photon point source 3 cm away from the surface. Figure 1(a) and 1(b) is an MCNP plot of the geometry. The SiLi crystal is surrounded by an aluminum sleeve and contained in an aluminum cannister. A thin beryllium window is located above the SiLi detector crystal. The input file describing the geometry, materials, source, and tallies is given in Appendix A.



(a)



(b)

Figure 1: MCNP plot of SiLi detector

Results

Figure 2 shows the results of the pulse-height distribution in the SiLi detector crystal using the RSICC release of MCNP5.1.40. The black line represents a calculation using the default physics (i.e. photon Doppler broadeing ON) and the blue dotted-line represents the same result with the photon Doppler broadening turned OFF (disabled with *phys:p 4j 1*). The 180^o Compton scatter peak, located near 0.02 MeV, shows the expected broadening effects of photon Doppler broadening.

.

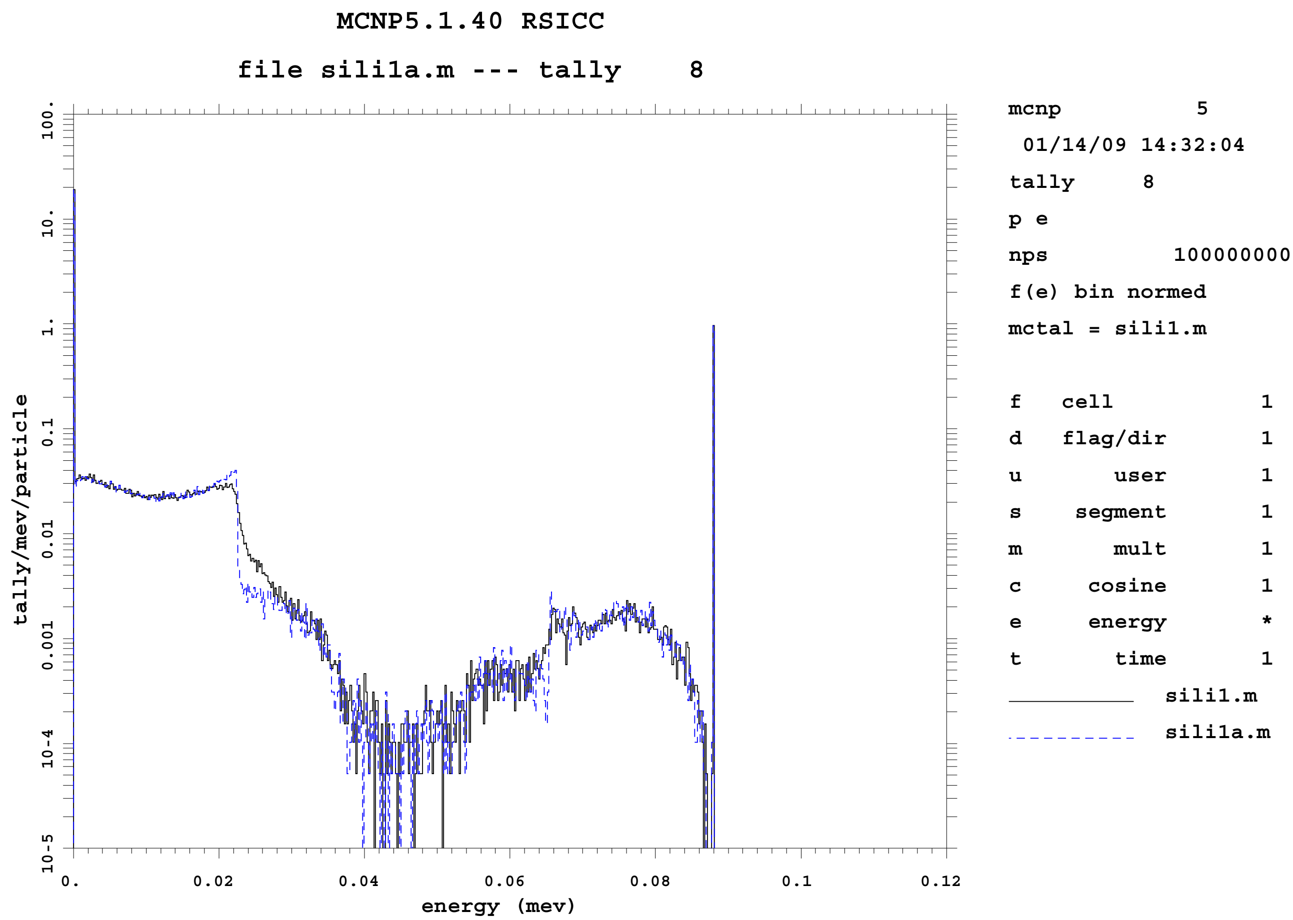


Figure 2: MCNP5.1.40 comparison of pulse-height spectra with (black line) and without (blue dotted line) photon Doppler broadening

Figure 3 shows the same results using the December 2008 RSICC release of MCNP5.1.50. As before, the black line represents a calculation using the default physics (i.e. photon Doppler broadeing ON) and the blue dotted-line represents the same result with the photon Doppler broadening turned OFF. There is a substantial difference in the result.

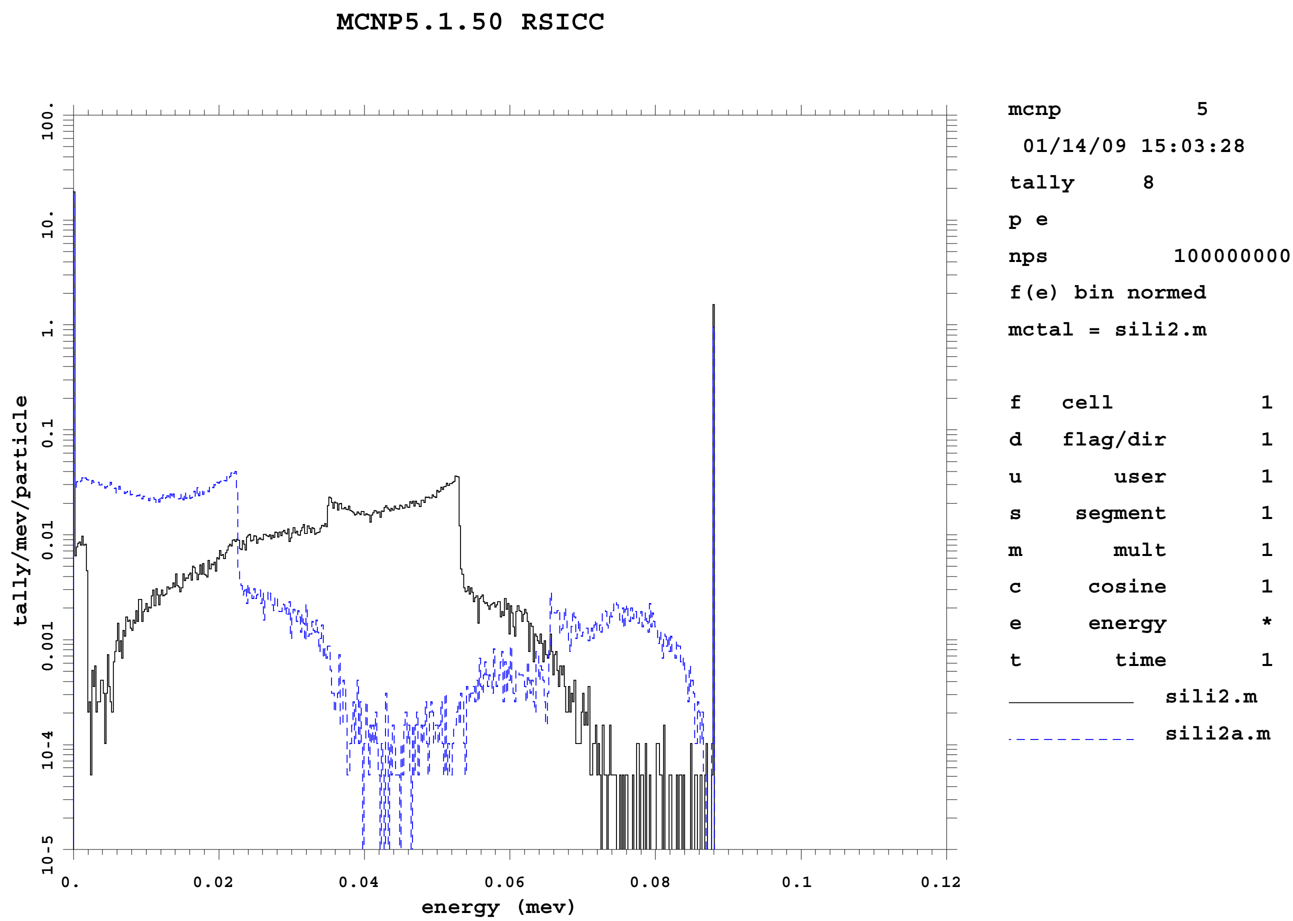


Figure 3: MCNP5.1.50 comparison of pulse-height spectra with (black line) and without (blue dotted line) photon Doppler broadening

A significant error was discovered in subroutine dopplerp that could lead to incorrect results and was reported to MCNP5.1.50 users [1]. A patch to the RSICC release of MCNP5.1.50 was issued that fixed this mistake. Figure 4 shows the result of the patch for the same problem. As before, the black line represents a calculation using the default physics (i.e. photon Doppler broadeing ON) and the blue dotted-line represents the same result with the photon Doppler broadening turned OFF. These results are statistically identical to the numerical values presented in figure 2.

Regression Test Suite Problems

Two regression test problems were developed to include in the installation test suite for MCNP5.1.51 (inp98, inp99). The two regression test problems are designed to test the photon Doppler broadening routine using a simplified geometry and materials while completing within a few seconds. The geometry is a small cylinder of silicon and hydrogen with a Cd-109 point source in the center. The tallies (pulse-height and volumetric flux) are binned into three energy groups that encompass the low-energy scatter (eg. several Compton scatters followed by escape) continuum, single Compton scatter region, and few Compton scatters.

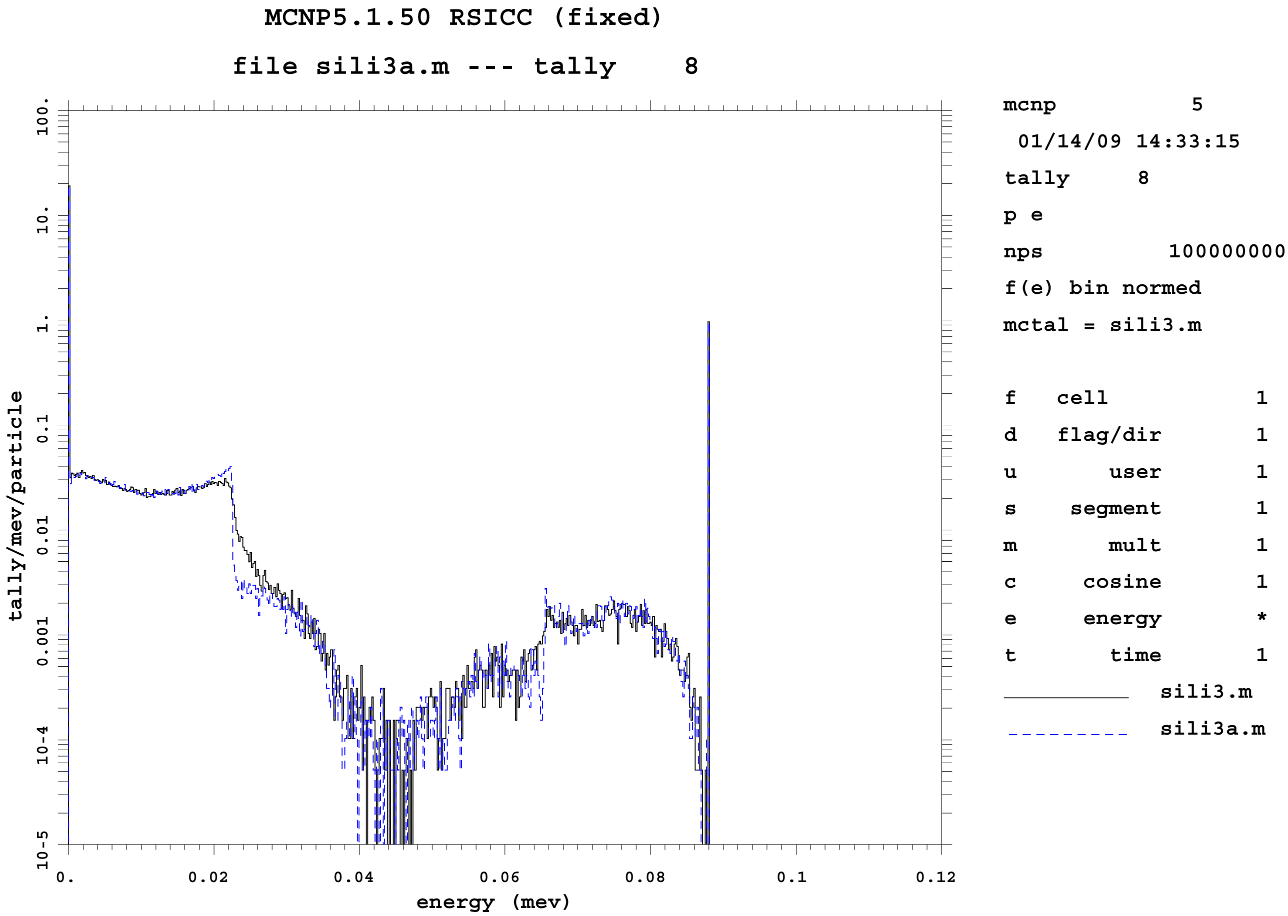


Figure 4: MCNP5.1.51 comparison of pulse-height spectra with (black line) and without (blue dotted line) photon Doppler broadening

These large energy bins capture the Doppler broadening effects and will detect any future changes in this routine. (Furthermore, if more energy bins are used, similar results to figures 4 are produced.) Numerical regression test set results with photon Doppler broadening on and off are given for MCNP5.1.40 in tables 1-2. Similarly, numerical regression test set results are given for MCNP5.1.51 in tables 3-4.

Energy (MeV)	Volume flux ($1/cm^2$)	Relative Error
0.0625	8.05244E-03	0.0103
0.0675	2.10212E-02	0.0065
0.100	7.17338E-01	0.0002
total	7.46412E-01	0.0003

Energy (MeV)	Pulse-height	Relative Error
1.0E-10	7.80555E-01	0.0005
0.020	1.29960E-01	0.0026
0.025	2.22710E-02	0.0066
0.100	6.72140E-02	0.0037
total	1.00000E+00	0.0000

TABLE 1: Regression test results for MCNP5.1.40 with photon Doppler broadening

Energy (MeV)	Volume flux ($1/cm^2$)	Relative Error
0.0625	7.12226E-03	0.0107
0.0675	2.23241E-02	0.0064
0.100	7.17052E-01	0.0002
total	7.46498E-01	0.0003

Energy (MeV)	Pulse-height	Relative Error
1.0E-10	7.80555E-01	0.0005
0.020	1.29899E-01	0.0026
0.025	2.34630E-02	0.0065
0.100	6.60830E-02	0.0038
total	1.00000E+00	0.0000

TABLE 2: Regression test results for MCNP5.1.40 without photon Doppler broadening

Energy (MeV)	Volume flux ($1/cm^2$)	Relative Error
0.0625	8.22032E-03	0.0102
0.0675	2.08728E-02	0.0065
0.100	7.17346E-01	0.0002
total	7.46439E-01	0.0003

Energy (MeV)	Pulse-height	Relative Error
1.0E-10	7.80555E-01	0.0005
0.020	1.30042E-01	0.0026
0.025	2.20370E-02	0.0067
0.100	6.73660E-02	0.0037
total	1.00000E+00	0.0000

TABLE 3: Regression test results for MCNP5.1.51 with photon Doppler broadening

Energy (MeV)	Volume flux ($1/cm^2$)	Relative Error
0.0625	7.12226E-03	0.0107
0.0675	2.23241E-02	0.0064
0.100	7.17052E-01	0.0002
total	7.46498E-01	0.0003

Energy (MeV)	Pulse-height	Relative Error
1.0E-10	7.80555E-01	0.0005
0.020	1.29899E-01	0.0026
0.025	2.34630E-02	0.0065
0.100	6.60830E-02	0.0038
total	1.00000E+00	0.0000

TABLE 4: Regression test results for MCNP5.1.51 without photon Doppler broadening

Comparing the numerical regression test set results from MCNP5.1.40 and MCNP5.1.51 for both volumetric flux and pulse-heights show the values to be within one to two standard deviations of each other (i.e. they are statistically identical). These values are considered acceptable due to the changes made to subroutine dopplerp in MCNP5.1.51.

Summary

A significant error in the photon Doppler broadening routine that could lead to incorrect results was discovered in MCNP5.1.50 released to RSICC in December 2008.. Notification to MCNP users was given along with a patch file that corrects this error [1]. This research note documents a simple but realistic test problem and gives plotted results that will detect problems with this feature. Furthermore, two new regression test problems have been described and numerical results are given. These numerical results show that MCNP5.1.51 gives statistically identical results to MCNP5.1.40 for problems using photon Doppler broadening.

References

[1] F.B. Brown, J.S. Bull, J.T. Goorley, A. Sood, and J.E. Sweezy, "MCNP5-1.51 Release Notes," Los Alamos National Laboratory report LA-UR-09-0384 (January 2009).

[2] Avneet Sood, "Doppler Energy Broadening for Incoherent Scattering in MCNP5, Part I," Los Alamos National Laboratory report LA-UR-04-0487.

[3] Avneet Sood, White,M.C. "Doppler Energy Broadening for Incoherent Scattering in MCNP5, Part II," Los Alamos National Laboratory report LA-UR-04-0488.

Appendix A

Input file for simple model of SiLi detector shown in Figure 1(a)

```
Standard example of SiLi detector
c CD 109  88 keV source
c      cell cards
 1  1  -2.70  (-1 2 -3) (4:-5:6) #2 #3    $Al  cannister
 2  2  -1.85  (-1  8 -7)                  $Be window
 3  3  -0.00129  -8  4  -9                $Unobstructed hole
 4  1  -2.70  -10  11  9  -12             $Al sleeve top
 5  1  -2.70  -10  13 -14  15             $Al sleeve
 6  4  -2.33  -11  17 -16                 $SiLi detector
998  3  -0.00129 (-4 5 -6) #4 #5 #6
999  0  (1:-2:3) -9999
1000 0 9999

c      surface cards
1   pz   0.0     $Top of outer can
2   pz -10.0     $Bottom of outer can
3   cz   2.5     $Outer Al can
4   pz  -0.13    $Top of inner can
5   pz  -9.87    $Bottom of inner can
6   cz   2.37    $Inner Al can
7   cz   0.95    $Be Window
8   pz  -0.0025  $Be Window bottom
9   cz   0.6     $Unobstructed window
10  pz  -0.53    $Top of Al
11  pz  -0.83    $Bottom of Al
12  cz   1.6     $Al cylinder
13  pz  -5.03    $Al sleeve length
14  cz   1.75    $Al sleeve outer cylinder
15  cz   1.674   $Al sleeve inner cylinder
16  cz   0.5     $SiLi Detector cylinder
17  pz  -1.375   $Bottom plane of Sili Detector
9999 so  15

c      data cards
mode p e
imp:p 1 1 1 1 1 1 1 1 0
imp:e 0 0 0 0 0 1 0 0 0
sdef   erg=0.088 pos = 0.0 0.0 3.0
c  Al
m1 13027.04p 1.0
c  Be
m2  4009.04p 1.0
c  Air
```

```
m3 7014.04p -0.767  8016.04p -0.233
c  Sili Detector
m4  14000.04p -0.99999  3006.04p -0.00001
f8:p,e   6
e8     0.0  512i 0.1
f4:p     6
e4     0.0  512i 0.1
f14:e    6
e14    0.0  512i 0.1
nps 1.0e8
prdmp 2j 1
```