

rleigh.txt

rleigh is an MCNPX simulation that demonstrates an error in how MCNPX handles Rayleigh scattering.

This scattering depends on the parameter ν , defined as

$$\nu = \alpha \kappa (1 - \mu)^{0.5}$$

with $\alpha = E/mc^2$, $\kappa = 29.1445/\text{\AA}$, and $\mu = \cos \theta$. Here, E is the incident photon energy, m is the mass of the target particle, and θ is the scattering angle. We take $mc^2 = 0.511$ MeV, the rest mass of the electron. Note that $\mu = 1 - [(v/\kappa)^2] / \alpha^2 = 1 - (v/\kappa)^2 * (mc^2 / E)^2$.

MCNPX only has data for the range $0 < \nu < 6/\text{\AA}$, which corresponds to $1 > \mu > 0.996166$, or $0 < \theta < 5.01882$ degrees. For larger scattering angles, MCNPX ignores Rayleigh scattering entirely!

This simulation demonstrates the errors that can come about by this omission. 1.699 MeV gamma rays are incident on a 10 μm -thick natural uranium target. The tallies are taken over a range of scattering angles to show the sharp drop in scattering effects beyond $\nu = 6/\text{\AA}$. The tallies are:

Bin 1: $0^\circ < \theta < 0.0256235^\circ$
Bin 2: $0.0256235^\circ < \theta < 2.56256^\circ$
Bin 3: $2.56256^\circ < \theta < 3.13861^\circ$
Bin 4: $3.13861^\circ < \theta < 4.43922^\circ$
Bin 5: $4.43922^\circ < \theta < 5.01882^\circ$
Bin 6: $5.01882^\circ < \theta < 5.43760^\circ$
Bin 7: $5.43760^\circ < \theta < 6.27958^\circ$
Bin 8: $6.27958^\circ < \theta < 7.25225^\circ$
Bin 9: $7.25225^\circ < \theta < 8.10961^\circ$
Bin 10: $8.10961^\circ < \theta < 60^\circ$
Bin 11: $60^\circ < \theta < 90^\circ$

The attached plot shows the differential uranium cross-section within each angular bin. The graphs are normalized by the solid angle subtended by each bin, i.e.

Bin 1: $\Omega = 0.000000628319$ steradians
Bin 2: $\Omega = 0.00628256$ steradians
Bin 3: $\Omega = 0.00314159$ steradians
Bin 4: $\Omega = 0.00942478$ steradians
Bin 5: $\Omega = 0.00524018$ steradians
Bin 6: $\Omega = 0.00418460$ steradians
Bin 7: $\Omega = 0.00942478$ steradians
Bin 8: $\Omega = 0.01256637$ steradians
Bin 9: $\Omega = 0.01256637$ steradians
Bin 10: $\Omega = 3.07876$ steradians
Bin 11: $\Omega = 3.14159$ steradians

(These numbers are obtained using $\Omega = 2\pi |\cos \theta_1 - \cos \theta_2|$.)
MCNPX F1 tallies give total counts per source particle across a surface. Using the density of natural uranium as 19.1 g/cc with a molar mass of 238.02891 g/mol, we get a number density of $4.832 * 10^{22}$ atoms/cc. The target itself is 10 μm thick, which gives $N = 4.832 * 10^{17}$ atoms/cm² for interaction with the photons. Also, the sphere over which the tallies were taken has a radius of 10 cm. Thus, the interaction cross-section within the target is

$$\sigma = [\text{fluence}] * \Omega * r^2 / N$$

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which gives σ in units of cm^2 . For example, a fluence of 0.0005 counts/ cm^2 /source particle across bin 2 would yield $\sigma = 0.0005 * 0.00628256 * 10^2 / 4.832 * 10^{17} = 6.5001 * 10^{-22} \text{cm}^2 = 65001 \text{ barns}$.

Two tests were run, to isolate the effects due to incoherent scattering. One run had all scattering physics turned on, while the other used the NOCOH physics card. Subtracting the results of the NOCOH run gives the effects due only to coherent (Rayleigh) scattering.