Implementation of Doppler broadening in MCNP5

Introduction: One effect of bound electrons on incoherent scattering is a broadened distribution of scattered photon energies for a given incident energy and scattering angle (i.e., Doppler broadening (DB)). Many Monte Carlo (MC) codes have implemented routines to account for this effect. This work focuses on the DB model in the MCNP5 code.

Methods: Simulations were run to test the DB feature in three versions of MCNP5: v1.51, v1.60, and an in-house modified edition of v1.60 (called v1.60m). All simulations were performed using the MCPLIB04 photon data library, in which the electron subshell data for incoherent scattering is represented in probability distribution form. In v1.60m, the code was altered to sample the electron subshell from a cumulative distribution data set. This modification was made because MCNP5 samples the subshell using a binary search which must be performed on a sorted data set to work accurately. The DB model of each code was investigated for scattering angles, \( \theta \), of 15°, 30°, and 45°. Multiple incident photon energies (between 200 and 800 keV) were tested at each angle.

Results: Figures 1, 2, and 3 show three simulated spectra for each code and \( \theta \) tested.

MCNP5 v1.51: The spectra determined using v1.51 indicate that for each \( \theta \) there is an incident photon energy above which DB is not modeled. This threshold changes with scattering angle (about 760 keV, 385 keV, and 260 keV for 15°, 30°, and 45°, respectively).

MCNP5 v1.60: The spectra simulated using v1.60 indicate that energy broadening is partially modeled for all incident photon energies and \( \theta \) tested. Analysis of the MCPLIB04 data library shows that only three of the five electron subshells in silicon are sampled when used with v1.60.

MCNP5 v1.60m: When sampled from a cumulative data set all subshells are appropriately sampled. Thus, DB is more correctly modeled in v1.60m than in the other versions (see Figure 4). These results indicate that appropriate sampling of subshell data has a substantial effect on the scattered energy distribution. It is recommended that MCNP5 v1.60 be used with a data library that presents the electron subshell data in cumulative distribution form.

Impact: Accurate characterization of incoherently-scattered photons is important for kilovoltage and megavoltage spectroscopic applications. As MC methods have become popular for verifying and correcting spectroscopic measurements, many codes have implemented DB routines. This work will be valuable for accurate detector modeling in the MCNP5 code.