ELECTRON PHYSICS ABOVE 1 GEV IN MCNP6

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ABSTRACT

Most synchrotron light sources and x-ray free electron lasers operate at energies in the range 1-10 GeV. Simulation of electron physics above 1 GeV is thus necessary to accurately calculate the secondary radiation production and the shielding required at such facilities. The maximum electron energy in earlier versions of MCNP was 1 GeV, so the code could not be applied to shielding problems at light sources. This limitation was largely due to the implementation of a condensed-history transport approach developed for the ITS series of codes and the upper energy limit of the associated data libraries. Starting with MCNP6 a single-event electron physics option was introduced which can handle the transport of electrons up to 100 GeV. We will discuss the electron physics treatments available in MCNP6, present results of calculations of secondary radiation due to electron interactions with materials commonly found at light sources, and show that the condensed-history physics treatment gives answers which are very close to those obtained from the more resource-intensive single-event treatment.

KEYWORDS
MCNP, electron transport, bremsstrahlung

1. INTRODUCTION

Synchrotron light sources worldwide operate with electron energies in the range 1-8 GeV. Other light sources can use even higher energies. For example, the European XFEL will be able to accelerate electrons up to 20 GeV. When the electron beams strike materials, electron energy is converted to photons, which constitute a prompt radiation source. Photons are in turn converted into neutrons, which are a prompt radiation source and can also activate materials. Correct electron physics above 1 GeV is thus necessary to accurately calculate the secondary radiation sources and to estimate the shielding required to reduce doses to appropriate levels at such facilities. Being able to calculate all the electron/photon/neutron physics in a single code leads to a more consistent treatment and fewer opportunities to introduce errors.

Historically, electron physics in MCNP has been restricted to a maximum energy of 1 GeV. It was possible to exceed this limit and run condensed-history simulations up to 10 GeV, albeit with uncertain results. Recent enhancements to MCNP have added a capability to consider interactions for electrons with energies greater than 1 GeV. We will discuss the electron physics treatments available in MCNP6 and compare the existing condensed-history physics with the new single-event physics.

2. A BRIEF HISTORY OF ELECTRON PHYSICS IN MCNP

Electrons were introduced into MCNP Version 4 in 1990, and photonuclear physics was made available starting with Version 4C2 in 2001. The highest electron energy available was 1 GeV even though photons could be treated up to 100 GeV. In MCNP5, electron energies above 1 GeV lead to a fatal error with the message "`fatal error. electron emax > 1000 mev`". [Here the MCNP output is reproduced exactly as it is printed, and the notation "mev" should be interpreted as "MeV".] MCNPX gives a warning message "`warning. electron emx .gt. parameter emax_top`" for electron energies > 1 GeV, but continues to run. In both cases, MCNP5/X processes the input file, reading in the electron data file and producing a table of ranges and stopping powers for each material in the problem.

In output tables for MCNP6 Beta 2 [1] and MCNP6 1.0 [2], electron physics was still listed as limited to 1 GeV. Up to MCNP6 Beta 3, the code contained a variable `electron_maximum` for the maximum electron energy, which was set to 1 GeV "until a high-energy model for electrons is implemented". But in the initial production release, a variable `cond_hist_maximum`, the maximum energy for valid condensed-history electron transport, was defined as 1000 MeV, with another variable `single_event_maximum`, the maximum energy for single-event electron transport, set at 100 GeV.

2.1. Condensed-History Physics

Electrons take a large number of collisions to slow down to energies at which they can be captured – on the order of 10^5 interactions, as opposed to around 25 collisions for neutrons slowing down in water or only a few collisions for photons interacting in most media. As a result, it is generally not practical in terms of computational resources to model each interaction individually. Rather, most codes rely on approximations based on analytical and semi-analytical charged-particle transport theory to combine the effects of multiple collisions into probability distributions for angular deflections and energy loss. This is called the condensed-history approach. A more complete description of condensed-history physics can be found in References [3] and [4], and the references contained therein.

In condensed histories, the effects of many individual interactions are sampled over "steps" and "sub-steps". The step size is chosen to be small enough that the electron's energy is roughly constant over a step in order to satisfy approximations in the theory that require the electron energy to be constant. The sub-steps must be chosen small enough to keep angular deflections small over a sub-step, which improves the calculation of the electron's trajectory. The default step size in MCNP6 is $2^{-1/8} = 0.917$, but can be set by the user to be anything between 0.8 and 0.99. The number of sub-steps per step depends on the material (larger for higher Z) and can also be set by the user. Angular deflections and the production of secondary particles (e.g., bremsstrahlung photons) take place at sub-step boundaries. Ranges and stopping powers are calculated in MCNP based on data contained in the electron interaction data files (e.g. el or el03). The energy loss is dominated by collisions at low energy and by radiative processes at high energy.

2.2. Single-Event Physics

With MCNP6, many enhancements [5,6] were made to electron and photon physics to enable more accurate transport at low energies, and to extend the low-energy limit below 1 keV. In single-event physics, the microscopic distribution data in ENDF/B-VI.8 (valid for 10 eV $\leq$ E $\leq$ 100 GeV) and contained in the mcplib12 data file are sampled directly instead of using the multiple-scattering theories and probability distributions from condensed histories. ENDF data include both cross sections for the various processes (electron elastic scattering, atomic excitation, electro-ionization, and bremsstrahlung production) and distribution functions for secondary particle production and energy loss. While intended for use below 1 keV, they can also be used to extend electron transport above the traditional 1 GeV limit recommended for condensed histories. MCNP6 has not yet been tested extensively for electron energies above 1 GeV, and much work needs to be done before such usage can be considered to be reliable.

3. MCNP6 CALCULATIONS

MCNP6 was used to calculate photon and neutron emission due to 10 GeV electrons striking one of the circular faces of a 30.48 cm long x 10.16 cm diameter iron target. Particle fluxes and doses were tallied over a spherical surface located 10 m from the center of the cylinder. The sphere was segmented to give angular distributions with respect to the incident beam direction. The cylinder dimensions and electron energy correspond to the conditions of dose measurements [7] made at SLAC in the 1960s, which provide a useful experimental benchmark. The authors of Ref. [7] fit the measurements with the equation

$$H(\theta) = 52.55 E_0 \left(e^{-0.959\sqrt{\theta}}\right) + 12.97\left(e^{-\theta/72.2}\right) \qquad \mu\text{Sv/J} \qquad (1)$$

(where the units of Joules refers to the energy content of the electrons). The results of the MCNP6 calculations using both condensed-history and single-event physics are shown in Figures 1 and 2. In these figures, the fractional standard deviation on the MCNP6 results are a few percent or lower, except for angles less than 0.2°, where they can be as high as 10%. The results using single-event physics are generally closer to the measured data (as represented by the equation of Nelson & Jenkins) than the condensed-history results, for angles larger than about 10°. Below about 3° the results using single-event physics diverge upward. The condensed-history results show a forward peak starting at angles just above 0.1 degrees. This may be due to differences in the MCNP6 treatment of electron scattering (and/or bremsstrahlung production) for angles above and below 1.4 milliradians (0.08°).

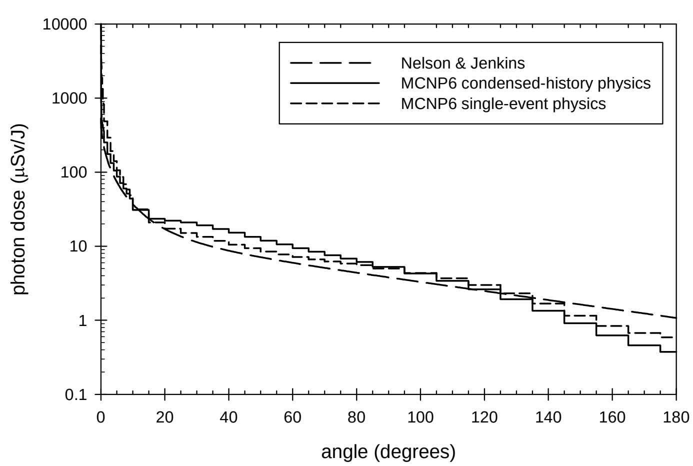

Figure 1. Photon dose for 10 GeV electrons incident on a 30.48 cm x 10.16 cm Fe target.

Comparisons were also made for the case of 7 GeV electrons incident on a 14 cm x 10 cm copper cylinder, which approximates the dimensions of the transition piece at the entrance to an insertion device at the Advanced Photon Source. These results are shown in Figure 3, along with the equation of Nelson & Jenkins. Fractional standard deviations for the MCNP6 results are under 1%. The equation has been modified using factors described in [7] to account for the difference in electron energy and in target size and composition, but these are only rough corrections based on photon attenuation. Because different adjustment factors apply to angles below and above 90 degrees, the equation exhibits a small inflection at that point. For this case, the MCNP6 data lie below the equation for angles larger than a few degrees, and are only a bit higher for smaller angles. Photon energy spectra are shown in Figures 4 and 5. In these data, fractional standard deviations are less than a few percent except for the single-event results at 90°, where the standard deviations are more than 10% for energies > 10 MeV due to the lower yield and longer computational time (so that fewer histories could be run). The spectra appear to have roughly the same shape, although better statistics are needed at high energies to make a conclusive statement.

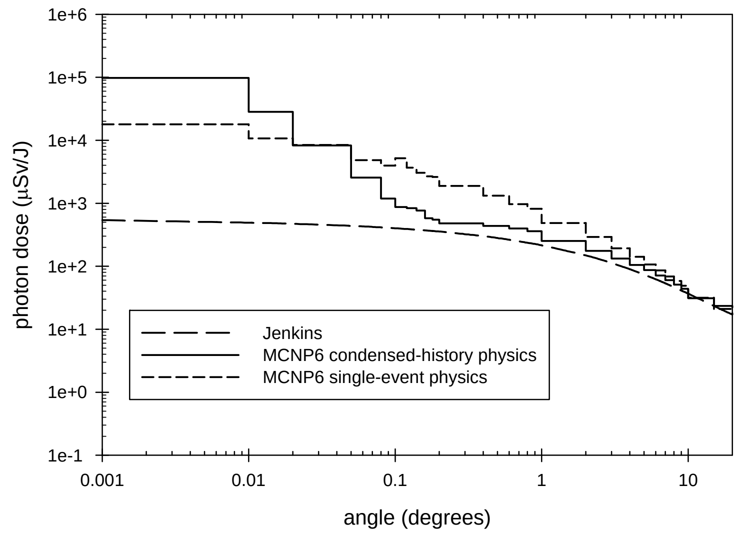

Figure 2. Photon dose for 10 GeV electrons incident on a 30.48 cm x 10.16 cm Fe target.

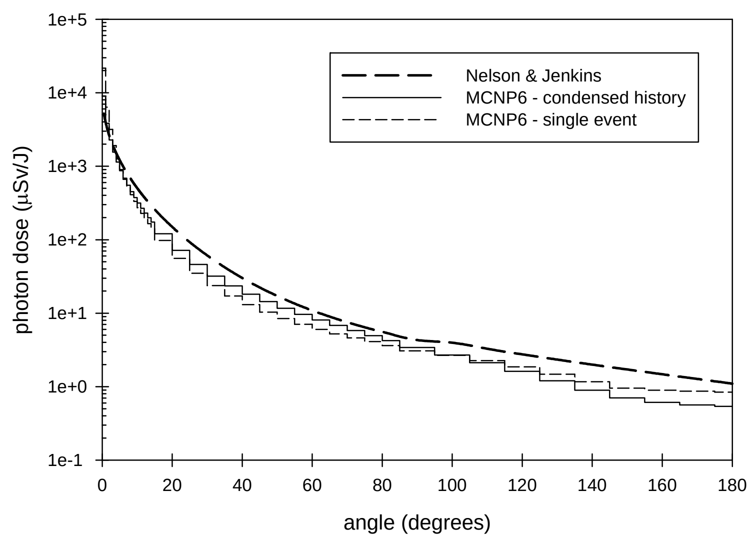

Figure 3. Photon dose for 7 GeV electrons incident on a 14 cm x 10 cm cylindrical Cu target.

Figure 6 shows neutron doses for the 14 cm x 10 cm Cu target. Standard deviations are again under a few percent, except for the first and last angular bins. The condensed-history and single-event results are in general agreement with each other, and both lie well below the equation of Ref. [7] for all angles. The neutron energy spectra shown in Figure 7 show good agreement between the two MCNP6 results, for which standard deviations are under a few percent except for the single-event results at $E_n > 10$ MeV.

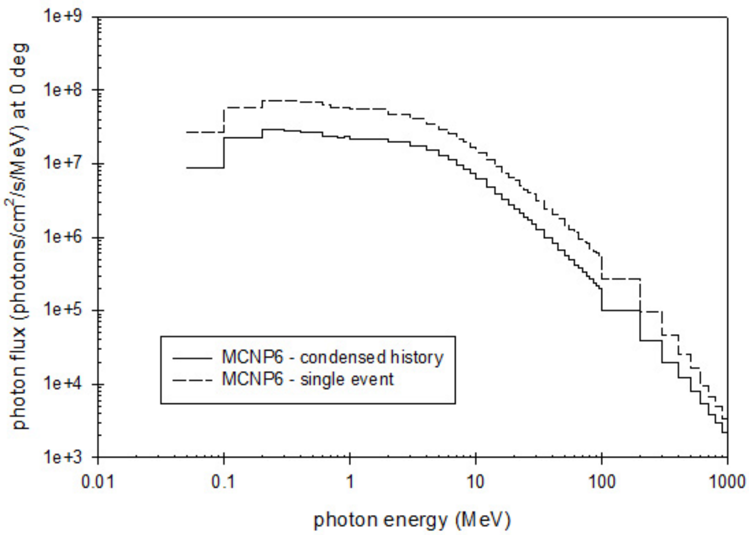

Figure 4. Photon energy spectra over the angular range 0-1 degree for 7 GeV electrons incident on a 14 cm diameter x 10 cm long Cu cylinder.

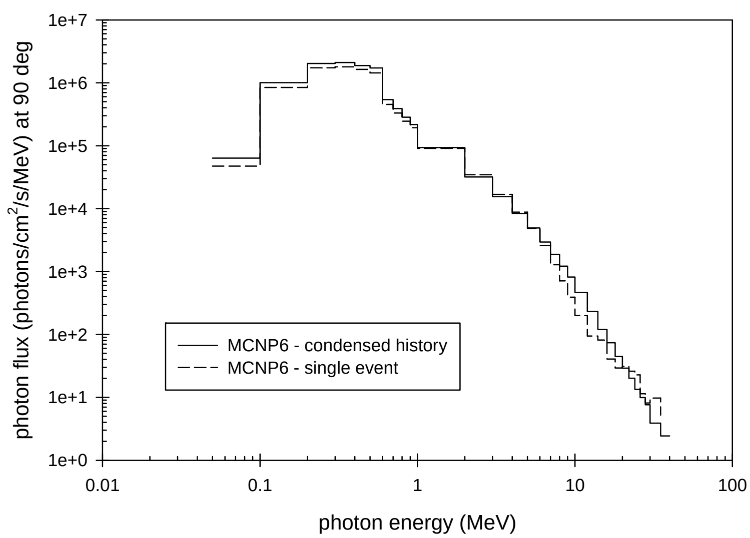

Figure 5. Photon energy spectra over the angular range 85-95 degrees for 7 GeV electrons incident on a 14 cm diameter x 10 cm long Cu cylinder.

4. CONCLUSIONS

Preliminary results using single-event physics above 1 GeV in MCNP6 agree well with measurements on an iron cylinder and show promise for the application of single-event physics above 1 GeV. They also indicate that the condensed-history approach also gives reasonable results for the limited set of problems considered and may be a good approximation for some problems in this energy range.

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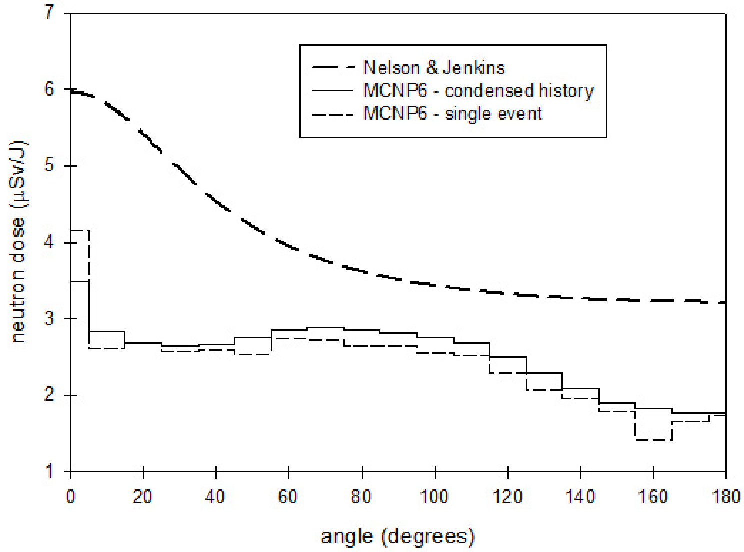

Figure 6. Neutron dose for 7 GeV electrons incident on a 14 cm x 10 cm cylindrical Cu target.

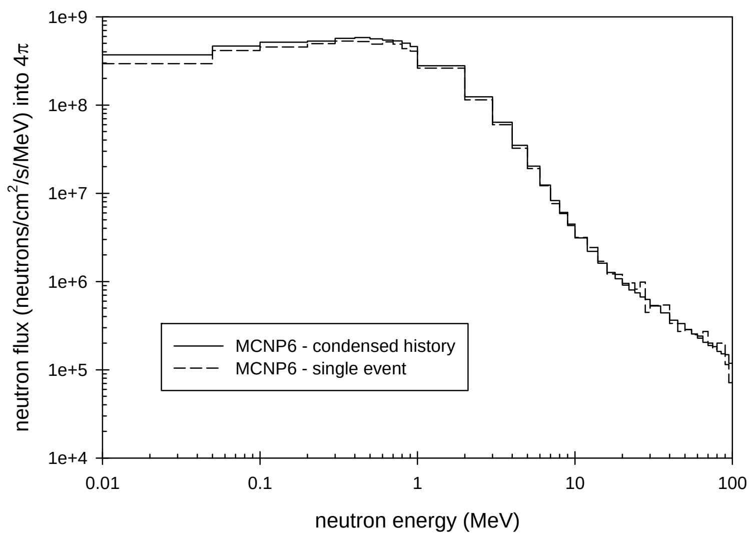

Figure 7. Neutron energy spectra over all angles for the 14 cm diameter x 10 cm long Cu cylinder.

REFERENCES

1. T. Goorley et al., "Initial MCNP6 Release Overview," *Nucl. Tech.* **180** (3), pp. 298-315 (2012).
2. T. Goorley et al., "Initial MCNP6 Release Overview – MCNP6 Version 1.0," LA-UR-13-22934 (April 2013).
3. X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory," LA-UR-03-1987 (April 2003, revised Feb. 2008).
4. K. Adams, "Electron Upgrade for MCNP4B," LA-UR-00-3581 (May 2000).
5. H. G. Hughes, "Quick-Start Guide to Low-energy Photon/Electron Transport in MCNP6," LA-UR-12-21068 Rev. 3 (April 2013).
6. H. G. Hughes, "Enhanced Electron-Photon Transport in MCNP6," LA-UR-13-27632 (Oct. 2013).
7. W. R. Nelson and T. M. Jenkins, "The SHIELD11 Computer Code," SLAC-R-737 (Feb. 2005).