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LLNL Proposed Modifications to the Treatment of Photofission in MCNPX

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October 24, 2008

1 MCNPX photon collision sampling

In MCNPX, all of the photonuclear reactions are grouped together, so that whenever a photon undergoes such a reaction, the number of emitted particles (and their energy and angle) are sampled from a single distribution made by averaging over all reactions. This is obviously not correct on an event-by-event basis. Furthermore, the mean number of particles produced is not done with analog sampling, but instead is either n or $n+1$ in order to give the measured average.

MCNPX determines the distance to the next photon collision based on the total photon cross-section computed from the sum of photoatomic (incoherent, coherent, photoelectric, pair production) and photonuclear (nonelastic (gamma,n), elastic, photofission (gamma,f), ...) cross-sections using the material composition and density. Then it decides whether a photonuclear or photoatomic interaction occured in the subroutine *collpn*, and then with which nucleus. The mean number of secondary particles produced for each type (e.g., neutron, photon, proton, ...) is extracted from external data (ratio of production cross-section to the total cross-section). This is sampled such that n or n+1 particles are produced to give the correct mean number. For each available particle type the secondaries are assigned to sub-processes, e.g. 3 photons from photofission and 2 photons from some other photonuclear reaction (gamma,n). Thus multiple processes are happening at the same time, which is non-physical.

Libraries are used when available, and models are used otherwise. MCNPX has a mix-and-match capability enabling mixing and matching of physics models and data tables. It is possible to specify some nuclides with models and other nuclides with data tables (isotope “mixing”). It is also possible to use data tables up to their maximum energy value and then use models above that energy, even when maximum table energy differs from nuclide to nuclide (energy “matching”). Photonuclear physics is modeled with the new CEM model [1] [2], regardless of whether CEM is used for other particles.

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2 Proposed photofission treatment

In this project, we are implementing an alternative method for photonuclear reactions. The default is still the original method as described above, but the new alternative method can be turned on by the new 'illnlphfis' switch (7^{th} entry of the photon physics card PHYS:P). It also requires the photonuclear reaction treatment to be set to analog by setting the 'ispn' switch (4^{th} entry of the photon physics card PHYS:P) to -1. With the new method, the first 2 steps are identical to the ones for the default method: The code first determines whether to follow the photoatomic or the photonuclear path and then picks a nuclide with which to interact. For that nuclide, the code computes the probability of photofission, which is the ratio of photofission cross-section to total cross-section, themselves read from data libraries. The code then determines probabilistically if a photofission occurs. If photofission is the chosen photonuclear reaction, mcnpx banks the neutrons and gammas generated by the LLNL photofission library. The numbers of neutrons and gammas, as well as their respective energies, are all coming from this single photofission library. On the other side, if we determine that a different photonuclear took place in lieu of photofission, we revert to the original treatment in the *collpn* routine. However, in this case, to avoid counting twice particles emitted by photofission (reaction which was already accounted for in the new part of the code), we also drop any particle coming from the photofission process from the "reverted-to" default method.

In other words, this new 'illnlphfis' option on the PHYS:P card allows the user to simulate the photofission process exactly, and therefore enables coincidence counting of photofission neutrons and gammas for instance. This is different from the default, where secondary particles emitted by photonuclear interactions are only correct on average over a large number of interactions, because the number of secondary particles, as well as their energies and directions are averaged over all possible photonuclear interactions.

Regardless of the option chosen in the 7^{th} entry of the PHYS:P card, delayed neutrons and gammas from photofission can be turned on and off independently via a different switch.

3 Proposed new entries to the mcnpx summary tables

The 7^{th} entry (illnlphfis) on the PHYS:P card enables the user to count exactly how many photofission interactions occured versus other photonuclear interactions. Therefore, we can now report the number of these photofission interactions in the summary tables as well as in the different 130 tables.

3.1 Changes to the summary table for neutrons

In the neutron creation column, a 'prompt photofission' entry was added that counts how many prompt neutrons are created from photofission. The 'photonuclear' entry that used to count neutrons from all photonuclear processes (including prompt neutrons from photofission) will no longer include the prompt neutrons from photofission, which are tallied separately in 'prompt photofission'.

3.2 Changes to the summary table for photons

In the photon creation column, a 'prompt photofission' entry was added that counts how many prompt photons are created from photofission. The 'photonuclear' entry that used to count photons from all photonuclear processes (including prompt photons from photofission) will no longer include the prompt photons from photofission, which are tallied separately in 'prompt photofission'.

In the photon loss column, the 'photonuclear abs' entry that used to count the photons absorbed in all photonuclear processes (including photofission), will no longer count the photons absorbed in photofission, which will be tallied separately in the 'loss to photofission' entry. The 'loss to photofission' entry in the photon loss column will be zero unless the 7^{th} entry (illnlphfis) of the PHYS:P card is set to 1 and the 4^{th} entry (ispn) is set to -1. This is because the original setting (illnlphfis=0) does not generate secondary particles adequately on a reaction per reaction basis. It only works correctly in average over a large number of reactions. When illnlphfis=0, the photons absorbed by photofission reactions are counted towards the 'photonuclear abs' entry.

3.3 Changes to table 130 for neutrons (physical events)

The 'photofission' entry was added to count the neutrons created by photofission. These used to be counted together with the other neutrons created by all other photonuclear processes in the 'photonuclear' entry.

3.4 Changes to table 130 for photons (physical events)

The 'photofission' entry was added to count the photons created by photofission. These used to be counted together with the other photons created by all other photonuclear processes in the 'photonuclear' entry.

The 'loss to photofission' entry was added to the physical events for photons. Photons lost to photofission will be counted in that entry, instead of being counted towards the 'photonuclear abs' entry. 'lost to photofission' is populated only when illnlphfis=1. If illnlphfis=0, photons lost to photofission are counted towards the 'photonuclear abs' entry.

References

[1] S.G. Mashnik and A.J. Sierk, "Recent Developments of the Cascade-Exciton Model of Nuclear Reactions," Los Alamos National Laboratory report LA-UR-01-5390, and International Conference on Nuclear Data for Science and Technology, Tsukuba, Japan, October 7-12, 2001.

[2] S.G. Mashnik, K.K. Gudima, R.E. Prael, A.J. Sierk, M.I. Baznat, and N.V. Mokhov, "CEM03.03 and LAQGSM03.03 Event Generators for the MCNP6, MCNPX, and MARS15 Transport Codes," Los Alamos National Laboratory report LA-UR-08-2931, and invited lectures at the Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, Trieste, Italy, February 4-8, 2008.