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PHOTONUCLEAR PHYSICS IN MCNP(X)

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ABSTRACT

Photonuclear physics has long been overlooked within mainstream Monte Carlo radiation transport codes for some time. Primarily, this has been due to a lack of complete, evaluated data. Recent efforts have produced such data and the MCNP and MCNPX transport codes at Los Alamos National Laboratory (LANL) are now being updated to make use of it. The code modifications are still in the developmental stages but a prototype version of MCNP is completed and has passed early verification/validation tests.

I. INTRODUCTION

A. Previous Photonuclear Data Usage

Photonuclear physics has been the neglected stepchild of photon transport. Hubbell recently published a review paper[9] in which he states that for photons above 5 MeV one "in principle" should include photonuclear interactions in transport simulation but that photonuclear data have not been included in current evaluations because the data are not amenable to systematic calculation and tabulation. This observation is easily seen when looking at the difference between a compilation of photoatomic[b] data (e.g. see Storm & Israel[14]) and a compilation of photonuclear data (e.g. see Dietrich & Berman[6]). It is this lack of complete, evaluated data that is the key to why photonuclear physics has not been handled in a comprehensive manner in radiation transport codes to date.

Photonuclear data are isotopic in nature showing irregular dependence for cross section shape and magnitude as a function of atomic number (Z) and atomic mass number (A). Thus, where photoatomic data is readily tabulated by element, photonuclear data must be tabulated for each isotope of an element. Unfortunately, the experimental data that exists is incomplete or inconsistent even for the major isotopes of interest and the theoretical models that could bridge the gaps have not been fully validated. However, the need for such data is readily apparent when reviewing existing literature.

The past attempts to model photonuclear interactions have focused mainly on neutron production. The medical physics community recognized the need to provide guidance for neutron protection measures within electron accelerators resulting in NCRP Report No. 79 on Neutron Contamination from Medical Electron Accelerators[11] being issued in 1984. More recently was the case involving the redesign of the electron beamstop for the LANL Dual-Axis Radiographic Hydrotest Facility (DARHT) after discovering that neutron dose would be a factor of 9 greater than the photon dose for a point of interest[3,5]. Another case was an ORNL sponsored study that found photoneutrons as the cause of an increased fast neutron flux within and outside of the heavy water or beryllium reflector of certain test reactors[8]. Other studies surely exist.

These studies highlight the difficulty of integrating photonuclear data into simulation models. The NCRP report gives guidance on estimating neutron yields and simple equations for estimating neutron flux in treatment rooms based on the generic equivalence of such facilities. The ORNL work made use of experimental and theoretical cross sections coupled into photon transport to produce neutrons with simple theoretical spectra. The previous LANL work used an evaluated cross section

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[b] For the purpose of this paper, photoatomic should be considered to be coherent, incoherent, photo-electric and pair-production (both atomic and nuclear) interations.

folded with a calculated photon flux as the starting point for producing neutrons from a generic spectrum. They all showed good methodology for solving specific problems but suffered from the lack of comprehensive data descriptions and from incomplete integration into the transport codes.

B. Recent Photonuclear Evaluations

The recent interest in photonuclear has brought about the formation of a Research Coordination Project (CRP) on "Compilation and Evaluation of Photonuclear Data for Applications"[13] under the auspices of the International Atomic Energy Agency (IAEA). It includes researchers from the Chinese Nuclear Data Center (CNDC), the Japanese Atomic Energy Research Institute (JAERI), the Korean Atomic Energy Research Institute (KAERI), Moscow State University (MSU), IPPE Obninsk, the University of Sao Paulo, Brookhaven National Laboratory (BNL) and LANL. The group intends to update the EXFOR library[7] at the National Nuclear Data Center (http://www.nndc.bnl.gov/) to include all relevant experimental data and release a library, through the IAEA, of ENDF evaluated data files covering the major isotopes of structural, shielding, activation analysis, fission, transmutation, astrophysics and biological importance.

Photonuclear data, by definition being nuclear and thus isotopic in nature, are being compiled separately from traditional elemental photoatomic data. The library is due to be released early in 2000 and will be available as ENDF-6[12] formatted files containing complete interaction descriptions, i.e. double differential cross sections, suitable for use in transport calculations. In coordination with the CRP, the LANL Nuclear Theory and Applications group (T-2) is producing a series of photonuclear evaluations for the Accelerator Production of Tritium (APT) project's LA150 nuclear data library[4]. Preliminary data from T-2 has been made available for the purpose of integration into the MCNP code family.

II. EXTENDING MCNP

Photonuclear physics is dominated by a giant resonance phenomena occurring in the energy range of a few MeV to a few tens of MeV. This range is particularly well suited to tabulated data driven Monte Carlo radiation transport simulations and MCNP[2] is probably the most widely used such code and is particularly well suited for the addition of photonuclear physics. It provides generalized geometry and tally routines for input and simulation of electron, photon and neutron transport at low energy (neutrons less than 150 MeV and electrons and photons less than one GeV). The MCNPX code[10] extends the transport capability of MCNP to include 34 particles over a more complete energy range (less than one TeV).

A. Material Definition

The first step necessary to use the new photonuclear data is to be able to specify which data sets are associated with a material definition. An MCNP input deck contains materials defined by isotope (ZA) and atomic (or mass) fraction. Cross section data is then associated with each material component using a library ID; e.g., ENDF/VI neutron data for $^{74}W_{184}$ would be referenced by ZAID equal to 74184.60c. Unfortunately, photoatomic data ignores the atomic mass number (in the example, A equal 184) portion of the ZAID and thus $^{74}W_{184}$ data would load ZAID equal 74000.02p. It was therefore necessary to establish a new container for photonuclear data separate from the photoatomic data and then to associate two sets of photon data to each component.

MCNP therefore recognizes photonuclear data as a new class of data and uses the identifier 'u' with its associated data. Thus, the tungsten example above could load 74000.02p photoatomic data, 74184.60c neutron data and 74184.01u photonuclear data. An interesting new option is also added due to the lack of data for all isotopes. On a separate card, isotopic substitution can be made, e.g. each component of elemental tungsten can be specified on the material card such that all available neutron data is used but then each isotope can be made to refer only to W_{184} photonuclear data or to refer to no table at all. In this manner, photonuclear data can be specified where available without affecting the other data associations.

Photonuclear data have not been generally available before and some trial and error will be necessary before it becomes a routine part of the code base. As such, the current default is not to load photonuclear data. This has been generally acceptable in the past and still presents a good option for most problems due to the relatively small influence of photonuclear data to many applications and the unavailability of all necessary data. As experience is gained, this could change such that it would default on and simply make use of whatever data were available.

B. Photon Collision Sampling

Photonuclear physics was implemented in the traditional Monte Carlo style as a purely statistical based process. This means that photons undergoing a photonuclear interaction produce an average number of emission particles each having a sampled energy/angle though not necessarily from the same reaction. This method was chosen as it produces good results for generalized problems and lends itself to an uncomplicated biasing scheme. Further, the availability of traditional ENDF neutron sampling laws, suitably adapted, simplifies coding for determining the photonuclear emission parameters.

The photonuclear data are used as an extension of the photon collision routines. The total photon cross section, photoatomic and photonuclear, is used to determine the distance to the next photon collision. The type of collision is then sampled as photonuclear or photoatomic. If the collision is photoatomic, the traditional photon collision routine is used. For photonuclear events, the routine chooses the collision isotope from the separately maintained photonuclear list. Then for each available secondary particle type, an integer number of emission particles are sampled based on the ratio of the production cross section to the total cross-section. The emission parameters for each particle are then sampled independently from the reaction laws provided in the data. Tallies and summary information are appropriately updated, applicable variance reduction games are performed and the emitted particle is banked for further transport.

Biasing of the photonuclear collision can be thought of as forcing a photonuclear interaction. At the collision site, the particle is split into two parts; one forced to undergo photoatomic interaction and the other photonuclear. The weight (a measure of particle importance) of each new particle is adjusted by the ratio of their actual collision probability. The reaction can be further biased to increase the number of secondary particles to be sampled, again adjusting their weights to account for the multiplicity. Like all biasing techniques, this can give rise to particles with extreme weight variations. Thus it is very important to examine the summary information and for cases with poor statistics use weight windows or non-biased sampling.

C. Summary Information

MCNP includes a robust tally package that is fully integrated in the new sampling routines. Since photonuclear interactions are simply generating traditional particles for further transport, it was only necessary to set the appropriate parameters for each created particle. Point detectors and dxtran spheres have been implemented though they required modification of some routines to differentiate between particles created from photons as opposed to particles from neutrons.

Appropriate summary information has also been added to the output file to reflect photonuclear contributions. Traditional summary tables give broad outlines for each particle as to how particles were created or lost. These tables now include photonuclear absorption and emission. Additionally, more detailed information has also been included such that photonuclear contributions can be viewed by cell and by nuclide.

D. Verification and Validation

Verification of all implemented options has been performed. This includes testing of input options to ensure that all valid material specifications result in expected data associations. The data loading routines were tested to ensure that photonuclear data was stored appropriately in memory. The calculation of the total photon cross-section was checked to ensure that the photon sampling density reflected the addition of the photonuclear contribution. The unbiased and biased collision algorithms were checked to ensure that they produced equivalent tally results. Collisional biasing in its various permutations was checked. Appropriate sampling of photonuclear emission parameters by the sampling routines was verified. With the completion of these tests, validation of the data can be performed with confidence in the repeatability and precision of the results.

Only one set of validation results is available for reporting at this time. Barber and George[1] reported neutron yields per incident electron as a function of incident electron energy for various materials and material thickness. Note that calculations for comparison implicitly depend on bremstrahlung generation for photon production being correct. Comparisons have been performed against the complete set of data available though only tantalum and copper results are presented here. These two results show the best and worse case for the calculations performed.

The comparative agreement between the calculation and experimental data for tantalum (see

Table 1) is exceptionally good. Comparison is made in the table by presenting the ratio of the calculated value of neutron yield per incident electron divided by the experimental value. The only large discrepancy seen is near the threshold energy. Several hypothesis could reasonably explain this – by extrapolating to different values for the energy threshold; by changing the initial shapes of the neutron production cross-section; or by achiving better energy resolution in the experimental measurements. Further study is needed to determine which of these, if any, is correct.

Energy (MeV)	Exp. Yield (10^{-4} n / e)	Ratio Calc. / Exp.
10	0.88	0.055
19	5.3	1.042
28	13.7	1.005
34	18	0.942

Table 1. Experimental neutron yield compared to calculation for various electron energies incident on 6.21 g/cm^2 (0.374 cm) thickness tantalum.

The comparative agreement between the calculation and experimental data for copper (see Table 2) is not so good. This calculation (and most of those not shown) consistently under-predicts the experimental data. All the data examined also show the same difficulty in predicting yields near the threshold energy. However, one general conclusion drawn was that the general shape of the various calculated yield versus energy curves match well to the shape of the original experimental data (this is not shown here).

Energy (MeV)	Exp. Yield (10^{-4} n / e)	Ratio Calc. / Exp.
19	6.1	0.464
28	21.5	0.728
34	33.5	0.768

Table 2. Experimental neutron yield compared to calculation for various electron energies incident on 53.13 g/cm^2 (5.93 cm) thickness copper.

The definitive conclusion drawn at this time is that evaluated photonuclear data is still in its infantile stages. The one comparison to experimental data shown here is not the complete answer. It is not clear whether the discrepancy is in the experimental measurements, the evaluated data, or the calculation. There is much left to do before proper error estimation can be made for this new data. It will be an ongoing process for some time to come to actually refine the accuracy of this type of calculation.

III. SUMMARY

Evaluated photonuclear data for a large range of isotopes is necessary before generalized problems can be solved. Such data is now being produced by several international organizations. The MCNP family of codes is being updated to incorporate use of the evaluated tabular data and to do so in a fully coupled manner. This capability will improve the ability to simulate a variety of problems including accelerator shielding, dosimetry calculations and photon induced transmutation. This capability currently exists in a developmental version of MCNP and will soon be integrated into the release versions of MCNP and MCNPX.

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