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Implementation of photonuclear attenuation in EGSnrc

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Abstract

This report supplements the publication: Ali *et al*, "Towards a more-realistic estimate of the uncertainty of photon cross sections at radiation therapy energies", YYYYYY **ZZ**, xxxx – xxxx, (201n). It describes our implementation of photonuclear attenuation in EGSnrc (without modelling secondary particles) and outlines how to implement it into a standard EGSnrc distribution (prior to its expected inclusion into the standard distribution). The final section outlines the work required for a complete implementation. A goal is that the details in this report aid colleagues in carrying this effort forward.

1 Introduction

In our recent transmission analysis studies (Ali and Rogers 2012; Ali *et al* 2012a; Ali *et al* 2012b), comparisons were made between detailed transmission measurements and their corresponding EGSnrc (Kawrakow 2000; Kawrakow *et al* 2011) calculations. The results indicate that the accuracy of photon cross sections is the ultimate limiting factor for the accuracy of the calculated transmission data, and consequently the accuracy of any extracted spectral information. Photonuclear cross sections have a resonance which spans the energy range from a few MeV to tens of MeV (depending on the isotope). The most accurate cross section data available in EGSnrc are the XCOM database from NIST (Berger *et al* 2010), but that database does not include photonuclear data. A useful first step towards improving photon cross section accuracy in EGSnrc is to take the photonuclear effect into account (without modelling secondary particles), which is done as part of the study of Ali *et al* (2012). The details of the implementation in EGSnrc are presented here.

2 Generating the photonuclear cross sections

Photonuclear cross sections are generated using the comprehensive IAEA compilation of evaluated photonuclear data (IAEA 2000) (http://www-nds.iaea.org/photonuclear/). The compilation is available in the Evaluated Nuclear Data File format (ENDF-6), but the IAEA website allows for interpreted retrieval of the ENDF data (http://www-nds.iaea.org/exfor/endf.htm). Since EGSnrc does not directly handle the ENDF format, we used the IAEA interface to extract the total photonuclear cross section data for the most-common constituent isotopes of each natural elements (Z = 1 – 100) in a two-column format: [photon energy (eV), cross section (barns/atom)].

The extracted data correspond to the following three options combined: NSUB=0: photonuclear data, MF=3: reaction cross sections, and MT=3: total cross section – note that only the *total* photonuclear cross sections are needed because the current version of the implementation in EGSnrc does not model secondary particles. In the IAEA online interface, it is misleading that MT=3 is called the "nonelastic neutron cross section" (probably a naming artifact caused by terminology migration from incident neutron data), whereas the ENDF documentation states that MT=3 is the "total absorption or total reaction cross section". For some isotopes, MT=3 is not available and the alternative is MT=5: sum of all reaction cross sections not explicitly given in another MT number.

Data for each isotope are searched for in the IAEA ENDF/B-VII.1 library since it has the most recommended evaluated data. If data are not available, the Japanese library, JENDL/PD-2004, is used. If not, the database TENDL-2011 (ftp://ftp.nrg.eu/pub/www/talys/tendl2011/tendl2011.html) is used, which is based on calculations using the TALYS nuclear-model code system. Compared with other libraries, TENDL-2011 has available data for the largest number of isotopes. However, we searched in it last because we found that, for many of the isotopes that have data from the three libraries, the JENDL/PD-2004 library gives a closer match to the ENDF/B-VII.1 library, whereas the TENDL-2011 library tends to under-estimate the cross sections. Additionally, TENDL-2011 is a newly-established library (first release in 2008). For H-1 and He-4, no evaluated data are available, therefore the IAEA EXFOR interface (http://www-nds.iaea.org/exfor/exfor.htm) is used to look for individual publications for these two isotopes. Respectively for H-1 and He-4, data from the two publications with sub-entry: M0732002 and sub-entry: M0040002 are used. Table 1 shows the most-common isotopes considered for each natural element, and the source of their data.

For each natural element, we generate the total photonuclear cross sections using the data for the most-common constituent isotopes and their corresponding isotopic abundances (also called molar fractions) in atom per cent. The most-common isotopes and their abundances are taken from the NIST database (http://www.nist.gov/pml/data/comp.cfm). The energy grid for the cross sections is 200 points, equi-spaced on a linear energy scale between the lowest threshold energy among the constituent isotopes and the highest energy that has data available. Interpolation is done separately for each isotope because each isotope has its own energy grid from the IAEA libraries. The interpolation is linear in energy and cross section to be consistent with the IAEA interpolation. As a check, some of the generated photonuclear cross section data for the natural elements are visually compared against the graphical data available for some natural elements in the Atlas of Giant Dipole Resonances (Varlamov *et al* 1999). The final file used by EGSnrc is iaea_photonuc.data which contains the total photonuclear cross section data for the 100 elements in the typical EGSnrc format of [ln(energy in MeV), ln(cross section in barns/atom)]. These photonuclear cross sections are used as the default, but the user is given the option to use their own photonuclear data as well – see below. Similar to how other cross sections are handled in EGSnrc, photonuclear cross sections for mixtures and compounds are generated internally at runtime using the standard mixing rules. Figures 1 to 4 shows examples of the photonuclear cross sections, as used during EGSnrc simulations.

Table 1: A list of the isotopes in this study for elements with atomic numbers, Z, from 1 to 100, and the source of their total photonuclear cross section data. The listed isotopes are the most-common for the natural elements, according to the NIST database. Elements with a (*) do not have stable isotopes; for those elements, the NIST database gives the longest-lived isotope, and it is used here. The pair (A, library) is the atomic mass number of the isotope and 'library' is an index representing the evaluated data library used to obtain its total photonuclear cross sections where 1≡ENDF/B-VII.1, 2≡JENDL/PD-2004, and, 3≡TENDL-2011. For H-1 and He-4, no evaluated data are available, therefore index 4≡publications with sub-entry: M0732002 and 5≡publication with sub-entry: M0040002. After any library index, the letter 'a' is for MT=3: total cross section, and the letter 'b' is for MT=5: sum of all reaction cross sections not explicitly given in another MT number. A given library/MT number index implies that data from sources with lower indices are not available – e.g., '3a' implies that data are not available for that isotope for 1a, 1b, 2a and 2b. Data for the different isotopes of a given natural element are not necessarily from the same library and/or using the same MT number (H, He, C, O, V, Ta, W, and Pb). The table continues on the following two pages.

Z	element	# iso.	(A, library) for each isotope
1	H	2	(1,4a), (2,1a)
2	He	2	(3,2a), (4,5a)
3	Li	2	(6,2a), (7,2a)
4	Be	1	(9,1a)
5	B	2	(10,2a), (11,2a)
6	C	2	(12,1a), (13,1b)
7	N	2	(14,1b), (15,1b)
8	O	3	(16,1a), (17,1b), (18,1b)
9	F	1	(19,2a)
10	Ne	3	(20,3a), (21,3a), (22,3a)
11	Na	1	(23,1b)
12	Mg	3	(24,1b), (25,1b), (26,1b)
13	Al	1	(27,1b)
14	Si	3	(28,1b), (29,1b), (30,1b)
15	P	1	(31,2a)
16	S	4	(32,1b), (33,1b), (34,1b), (36,1b)
17	Cl	2	(35,1b), (37,1b)
18	Ar	3	(36,1b), (38,1b), (40,1b)
19	K	3	(39,3a), (40,3a), (41,3a)
20	Ca	6	(40,1b), (42,1b), (43,1b), (44,1b), (46,1b), (48,1b)
21	Sc	1	(45,3a)
22	Ti	5	(46,1b), (47,1b), (48,1b), (49,1b), (50,1b)
23	V	2	(50,3a), (51,1a)
24	Cr	4	(50,1b), (52,1b), (53,1b), (54,1b)
25	Mn	1	(55,1b)

... continuation of table 1 from the previous page.

Z	element	# iso.	(A,library) for each isotope
26	Fe	4	(54,1b), (56,1b), (57,1b), (58,1b)
27	Co	1	(59,1b)
28	Ni	5	(58,1b), (60,1b), (61,1b), (62,1b), (64,1b)
29	Cu	2	(63,1b), (65,1b)
30	Zn	5	(64,1b), (66,1b), (67,1b), (68,1b), (70,1b)
31	Ga	2	(69,3a), (71,3a)
32	Ge	5	(70,1b), (72,1b), (73,1b), (74,1b), (76,1b)
33	As	1	(75,3a)
34	Se	6	(74,3a), (76,3a), (77,3a), (78,3a), (80,3a), (82,3a)
35	Br	2	(79,3a), (81,3a)
36	Kr	6	(78,3a), (80,3a), (82,3a), (83,3a), (84,3a), (86,3a)
37	Rb	2	(85,3a), (87,3a)
38	Sr	4	(84,1b), (86,1b), (87,1b), (88,1b)
39	Y	1	(89,3a)
40	Zr	5	(90,1b), (91,1b), (92,1b), (94,1b), (96,1b)
41	Nb	1	(93,1b)
42	Mo	7	(92,1b), (94,1b), (95,1b), (96,1b), (97,1b), (98,1b), (100,1b)
43	Tc(*)	1	(98,3a)
44	Ru	7	(96,3a), (98,3a), (99,3a), (100,3a), (101,3a), (102,3a), (104,3a)
45	Rh	1	(103,3a)
46	Pd	6	(102,1b), (104,1b), (105,1b), (106,1b), (108,1b), (110,1b)
47	Ag	2	(107,1b), (109,1b)
48	Cd	8	(106,1b), (108,1b), (110,1b), (111,1b), (112,1b), (113,1b), (114,1b), (116,1b)
49	In	2	(113,3a), (115,3a)
50	Sn	10	(112,1b), (114,1b), (115,1b), (116,1b), (117,1b), (118,1b), (119,1b), (120,1b), (122,1b), (124,1b)
51	Sb	2	(121,1b), (123,1b)
52	Te	8	(120,1b), (122,1b), (123,1b), (124,1b), (125,1b), (126,1b), (128,1b), (130,1b)
53	I	1	(127,1b)
54	Xe	9	(124,3a), (126,3a), (128,3a), (129,3a), (130,3a), (131,3a), (132,3a), (134,3a), (136,3a)
55	Cs	1	(133,1b)
56	Ba	7	(130,3a), (132,3a), (134,3a), (135,3a), (136,3a), (137,3a), (138,3a)
57	La	2	(138,3a), (139,3a)
58	Ce	4	(136,3a), (138,3a), (140,3a), (142,3a)
59	Pr	1	(141,1b)
60	Nd	7	(142,3a), (143,3a), (144,3a), (145,3a), (146,3a), (148,3a), (150,3a)

... continuation of table 1 from the previous page.

Z	element	# iso.	(A,library) for each isotope
61	Pm(*)	1	(145,3a)
62	Sm	7	(144,1b), (147,1b), (148,1b), (149,1b), (150,1b), (152,1b), (154,1b)
63	Eu	2	(151,3a), (153,3a)
64	Gd	7	(152,2a), (154,2a), (155,2a), (156,2a), (157,2a), (158,2a), (160,2a)
65	Tb	1	(159,1b)
66	Dy	7	(156,3a), (158,3a), (160,3a), (161,3a), (162,3a), (163,3a), (164,3a)
67	Ho	1	(165,1b)
68	Er	6	(162,3a), (164,3a), (166,3a), (167,3a), (168,3a), (170,3a)
69	Tm	1	(169,3a)
70	Yb	7	(168,3a), (170,3a), (171,3a), (172,3a), (173,3a), (174,3a), (176,3a)
71	Lu	2	(175,3a), (176,3a)
72	Hf	6	(174,3a), (176,3a), (177,3a), (178,3a), (179,3a), (180,3a)
73	Ta	2	(180,3a), (181,1b)
74	W	5	(180,1a), (182,1a), (183,1a), (184,1b), (186,1a)
75	Re	2	(185,3a), (187,3a)
76	Os	7	(184,3a), (186,3a), (187,3a), (188,3a), (189,3a), (190,3a), (192,3a)
77	Ir	2	(191,3a), (193,3a)
78	Pt	6	(190,3a), (192,3a), (194,3a), (195,3a), (196,3a), (198,3a)
79	Au	1	(197,1b)
80	Hg	7	(196,2a), (198,2a), (199,2a), (200,2a), (201,2a), (202,2a), (204,2a)
81	Tl	2	(203,3a), (205,3a)
82	Pb	4	(204,3a), (206,1b), (207,1b), (208,1b)
83	Bi	1	(209,1b)
84	Po(*)	1	(209,3a)
85	At(*)	1	(210,3a)
86	Rn(*)	1	(222,3a)
87	Fr(*)	1	(223,3a)
88	Ra(*)	1	(226,3a)
89	Ac(*)	1	(227,3a)
90	Th	1	(232,1a)
91	Pa	1	(231,3a)
92	U	3	(234,1a), (235,1a), (238,1a)
93	Np(*)	1	(237,1a)
94	Pu(*)	1	(244,3a)
95	Am(*)	1	(243,3a)
96	Cm(*)	1	(247,3a)
97	Bk(*)	1	(247,3a)
98	Cf(*)	1	(251,3a)
99	Es(*)	1	(252,3a)
100	Fm(*)	1	(257,3a)

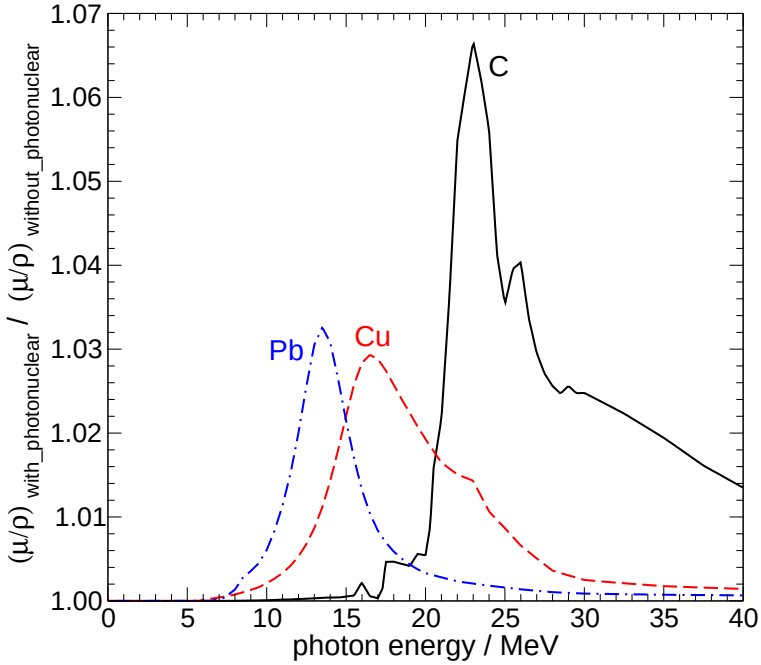

Figure 1: For the attenuators used in our recent transmission analysis work (Ali and Rogers 2012; Ali *et al* 2012a; Ali *et al* 2012), the figure shows the fractional increase in the total photon cross sections when the `IAEA` photonuclear data are added to the `XCOM` cross sections. Data are generated within `EGSnrc` for the default 2000-point energy grid.

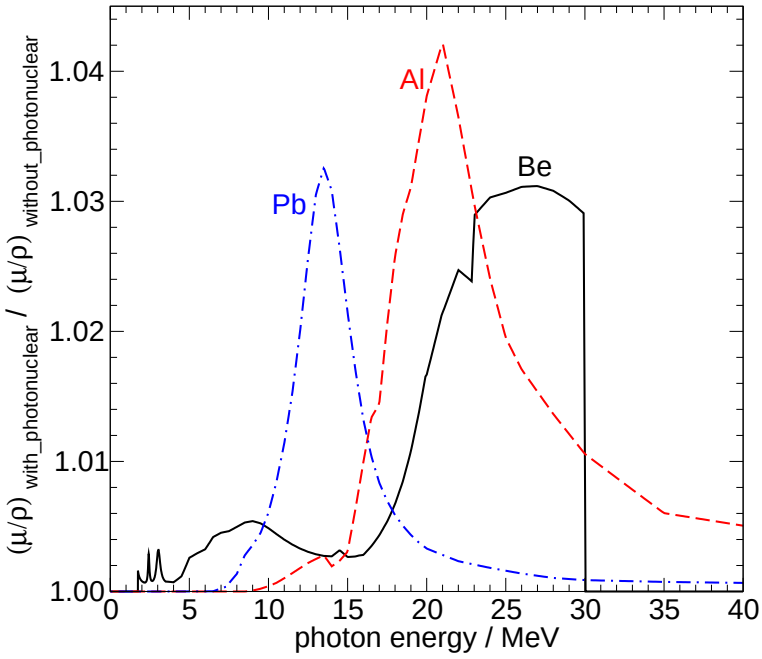

Figure 2: Same as figure 1 but for the target materials used with the electron beam from the NRC Vickers research linac.

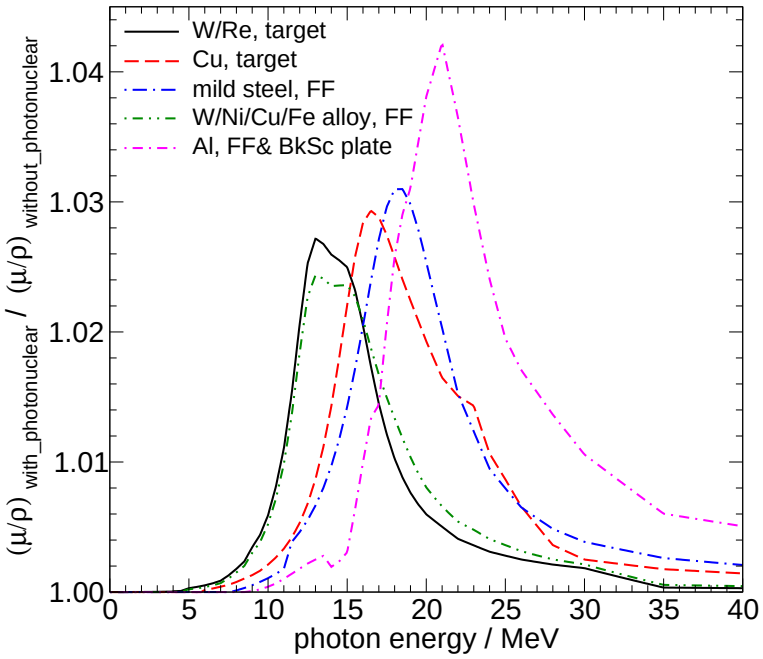

Figure 3: Same as figure 1 but for the major materials in the path of the photon beams in the NRC Elekta *Precise* linac – i.e., target, flattening filter (FF) and backscatter (BkSc) plate.

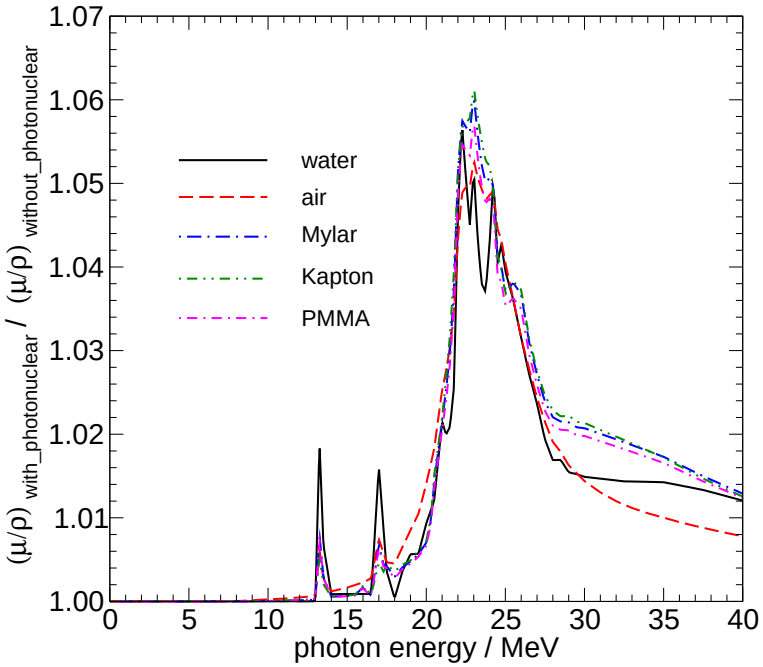

Figure 4: Same as figure 1 but for other materials commonly found in the path of photon beams (through monitor chambers, ambient air, phantoms, etc).

3 Implementation in EGSnrc

The outline of the implementation is as follows. The photonuclear effect can be turned ON or OFF on a region-by-region basis. When ON in a region, the gamma mean free path (GMFP) in the medium of that region is shortened accordingly. After transporting the photon to the interaction site, an interaction type is sampled according to the relative cross section of each interaction. In the current version of the implementation, when the interaction is photonuclear, the photon is discarded without energy deposition and without generating secondary particles. The implementation requires making additions/changes to the following five EGSnrc files: egsnrc.macros, egsnrc.mortran, get_inputs.mortran, egs_utilities.mortran, and transportp.macros. The changes can be spotted by searching for the exact string Ali:photonuc (case sensitive) in those files. Without exception, any new variable/macro/subroutine/etc has the string photonuc for ease of search. The details of the implementation are parallel to the existing implementation of Rayleigh scattering in EGSnrc.

The user's inputs for the photonuclear option are handled in a way similar to the inputs for typical EGSnrc transport parameters. The following are the phrases (VALUES_SOUGHT) needed in the input file anywhere between the two delimiters :start MC transport parameter: and :stop MC transport parameter: (order of the photon nuclear parameters with respect to each other or to other transport parameters is irrelevant)

```
Photonuclear attenuation=     OFF (default), ON, OFF in regions, or ON in regions
Photonuclear start region=    ir1, ir3, ...
Photonuclear stop region=     ir2, ir4, ...
Photonuclear cross sections=  photonuc_xsections
```

Note that the word attenuation in the VALUES_SOUGHT is meant as a reminder that the current implementation only eliminates the photon **but does not model the secondary particles**. If Photonuclear attenuation= OFF, an internal EGSnrc region switch, IPHOTONUCR($MXREG) (defined in the COMMON block MISC), is set to 0 for all regions. If ON, the switch is 1 for all regions. If OFF in regions, the switch is ON everywhere except for regions with indices between ir1 to ir2 (inclusive), ir3 to ir4, etc. If ON in regions, the switch is OFF everywhere except for regions with the indices just mentioned. An array, IPHOTONUCM($MXMED) (defined in the COMMON block MEDIA), is filled with a 0 or 1 switch for each medium based on mapping the media of the regions whose IPHOTONUCR is 1.

EGSnrc has a recent feature for user-supplied Compton cross sections in which the user provides a prefix for the custom data file name, then the full file name should be prefix_compton.data and should be located at $HEN_HOUSE/data. An identical approach is adopted for user-supplied photonuclear data where the input photonuc_xsections is a user-supplied prefix, and the custom data file should be photonuc_xsections_photonuc.data and should be located at $HEN_HOUSE/data. If photonuclear is requested but the entry for Photonuclear cross sections is missing or photonuc_xsections is set to default or is left blank, then $HEN_HOUSE/data/iaea_photonuc.data (described in the previous section) is used.

A difference from the Rayleigh implementation is that an extra internal flag, IPHOTONUC, is set to 1 if *any* value of the array IPHOTONUCM($MXMED) is 1. Then in HATCH, photonuclear cross sections are read only if IPHOTONUC is 1. This is because Rayleigh data are read whether the user turns Rayleigh scattering ON or OFF. For photonuclear data, we thought that it's better to have the code deal with them only if needed. In HATCH, if IPHOTONUC is 1 the subroutine EGSI_GET_DATA is called with a new FLAG value of 3. Photonuclear data are not read under one of the existing FLAG values (0 for photoelectric, Rayleigh or Compton, 1 for pair and 2 for triplet) because of some common-sense differences. The subroutine EGSI_GET_DATA is re-coded to accommodate the new FLAG value. As discussed in the previous section, the interpolation is linear/linear. However, once the data are read, the interpolation during simulations is similar to all other cross sections (i.e., ln / ln).

Similar to the Rayleigh implementation, there is no new explicit branching ratio (i.e., no GBR3). Rather, the fraction of the total cross section without photonuclear to that with photonuclear is calculated (PHOTONUCFAC, which parallels COHEFAC). Then in PHOTON the macro $PHOTONUC-CORRECTION shortens the GMFP by the scaling factor PHOTONUCFAC. Once the photon is transported, the macro $PHOTONUCLEAR performs interaction sampling. The maximum number of AUSGAB calls ($MXAUS) is increased from 28 to 30 to allow for AUSGAB calls to be made (if requested) before and after a photonuclear event. The default for IAUSFL(29) and IAUSFL(30) is set to 0. When a photonuclear interaction is sampled, an AUSGAB call with IARG=29 is made if requested. This is followed by a call to a new subroutine (PHOTONUC) to handle the photonuclear interaction details (similar to the subroutines COMPT, PHOTO, PAIR, etc). In the current implementation of subroutine PHOTONUC, it sets the photon energy (E(NP)) and weight (WT(NP)) to zero (which causes the photon to be discarded during GOTO :PNEWENERGY:), and no energy is deposited in the medium (EDEP = PZERO). Finally an AUSGAB call with IARG=30 is made if requested. In the current implementation, the zero-energy zero-weight photon on top of the stack

is discarded before an AUSGAB call with IARG=30 ever happens. However, the IARG=30 feature is meant to provide some infra-structure for future developers who will implement secondary particle generation and transport.

If the user requests cross section output in a .xsections file, a new column is printed with the GMFP shortened due to both Rayleigh (COHE) and photonuclear (PHOTONUC) effects. Unlike the existing output column for GMFP*COHE, the column GMFP*COHE*PHOTONUC is printed *only* for the media in which photonuclear is requested to avoid confusing the user.

The current implementation does not work for user codes that use the egs++ geometry package (Kawrakow *et al* 2009) - e.g., cavity and egs_chamber user codes. This is because of the presence of files that interface EGSnrc with the egs++ geometry package (.macro and .mortran files located at $HEN_HOUSE/interface). Among other things, those interface files re-define most of the EGSnrc replacement macros and COMMON blocks. However, it should be noted that in the current implementation, if a non-egs++ user code (e.g., BEAMnrc) is used as a source for an egs++ user code (e.g., cavity), photonuclear modelling works fine for the non-egs++ part. The data presented in the validation section below are generated that way.

4 Validation

To validate the proper use of photonuclear data in EGSnrc during photon transport, the transmission measurement setup from Ali *et al* (2012a) is modelled for the case of a 30 MV beam from the NRC Vickers research linac with an aluminum bremsstrahlung target. The attenuators are graphite and lead and the detector is an Exradin A19 Farmer chamber with a tungsten-alloy cap. The transmission setup is modelled using BEAMnrc (Rogers *et al* 1995; Rogers *et al* 2011) and used as a source for cavity (Kawrakow *et al* 2009), which, in turn, models the ion chamber. Simulations are performed with photonuclear attenuation once turned ON and once turned OFF in the geometric region of the attenuator. EGSnrc results are compared to analytical calculations for the same setup using equation 1 in Ali and Rogers (2012). In this integral equation, the known detector energy response per unit energy fluence and the photon spectrum at the attenuator surface (both pre-calculated using EGSnrc) are used to calculate the transmission signals analytically using an integral equation. The cross sections employed are the same 2000-point data used in EGSnrc, once with and once without the photonuclear effect. Figure 5 shows perfect agreement between the two calculation methods, which validates the mechanics of the implementation of photonuclear attenuation in EGSnrc. Note that unlike the EGSnrc simulations, the analytical calculations do not include non-ideal attenuation effects

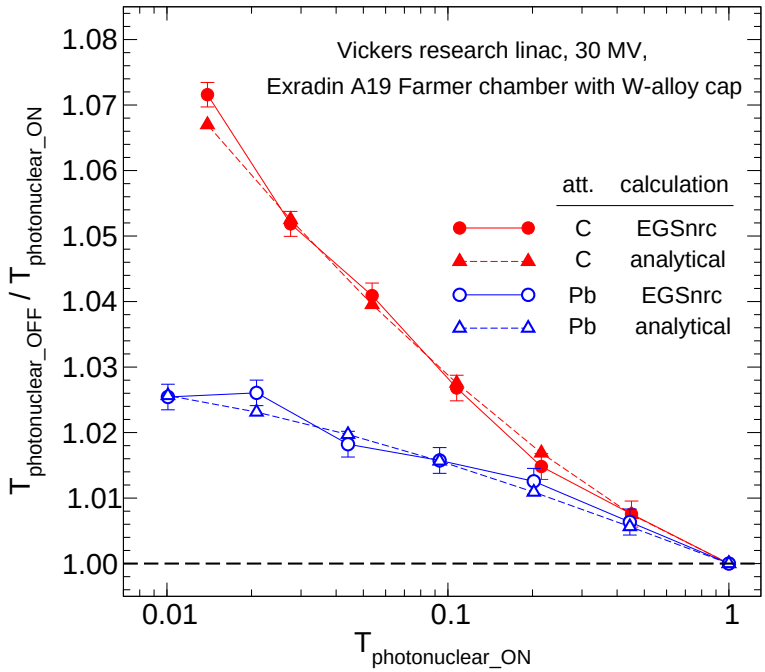

Figure 5: EGSnrc results versus analytical calculations of the effect of the photonuclear component on transmission data, T, to validate the implementation of photonuclear attenuation in EGSnrc.

such as forward scatter (Ali and Rogers 2012). However, for the ratio of the transmission data with and without photonuclear attenuation, these non-ideal effects cancel out almost identically in the EGSnrc results, which makes the comparison in figure 5 valid.

The ∼7% effect of photonuclear attenuation on the simulated transmission data (figure 5) justifies the efforts to implement it in EGSnrc. The effect of including photonuclear attenuation on the level of agreement between EGSnrc calculations and experimental transmission data is shown in Ali *et al* (2012). The indirect effect on the accuracy of the unfolded linac photon spectra is shown in Ali *et al* (2012b).

5 To-do list

The following items would improve/extend the current implementation:

- Modelling the resulting particles (n, p, α, γ, etc). The following are four implementation scenarios with increasing level of sophistication.
  (a) Breaking down the total photonuclear cross section into only a neutron component and a charged-particle component, then discarding the neutrons and depositing the energy of the charged particles on the spot.
  (b) Same as 1 but emitting the charged particles isotropically, and depositing their energy according to a range relationship.
  (c) Developing energy deposition kernels for neutrons and charged particles and using them.
  (d) Explicit full modelling of secondary particles, as done in other codes – `MCNP` (Briesmeister 1999), `GEANT4` (Agostinelli *et al.* 2003), etc.
- Extending this work to the `egs++` user codes by re-applying the changes described in this report to the `EGSnrc`-to-`egs++` interface files described in the implementation section.
- Comparing photonuclear cross sections from different sources, and possibly making each source a separate option for `EGSnrc`. In that context, it may be useful to make `EGSnrc` able to directly read the `ENDF` format so that the periodic new releases of full libraries (e.g., `TENDL`) are easily imported.
- Modifying the utility user code `examin` to output photonuclear cross section data if requested.

6 References

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