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Title: Some Notes on EPRDATA and MCNP

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Some Notes on EPRDATA and MCNP

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EPRDATA in MCNP comes in 2 libraries, EPRDATA12 and EPRDATA14. The acronym EPR stands for Electron Photon, and atomic Relaxation. The libraries are in an extended form[(1)] of the ACE format. This extended data includes more physics than the more common MCPLIB photo-atomic libraries, such as MCPLIB63 and MCPLIB84.

Table 1: Major MCNP Code Versions and EPRDATA

Code Version	**EPR data**	**Notes**
MCNP 5 or 6	not available	
MCNP 6.1	EPRDATA12 (only)	
MCNP 6.2 and forward	EPRDATA14	(EPRDATA12 can be used but is obsolete)

Table 2: Comparison of Electron Transport Methods in MCNP

Electron Transport	**Notes**
Condensed History[(2)]	default method, useful at higher electron energies & more efficient
	lowest electron energy = 1 keV
Single Electron[(3)]	available at lower e energies but less efficient (i.e., more physics)
	Uses EPRDATA14 or 12, lowest electron energy = 10 eV

Within the default condensed history approach, the original MCNPX version of electron transport has been changed in MCNP6 to have better physics. If the original MCNPX CH (Condensed History) treatment is still desired[(4),] set the dbcn card as follows:

DBCN 17j 0 8j 1 10j 1 1 3j 0 8j 1

To run single electron transport in MCNP 6.1 and beyond, use plib = EPRDATA12 or EPRDATA14 library (in lieu of plib = MCPLIB84) and set the 15th flag of the phys:e card to the energy below which EPR data will be used. In the past, the 18th flag on the card was also set, but this is no longer necessary since the default has been changed.

One difference between CH – Condensed history and SE – Single Electron transport can be seen on Figure 1 below. MCNP6.2.1 was used for this calculation of electrons produced by 15 keV photons impinging onto a thin gold plate. Notice the much richer physics of the epr results using the single electron method. The electron peaks correspond to various shell and sub-shell transition energies. This figure compares very favorably with Figure 3 of Reference 5.

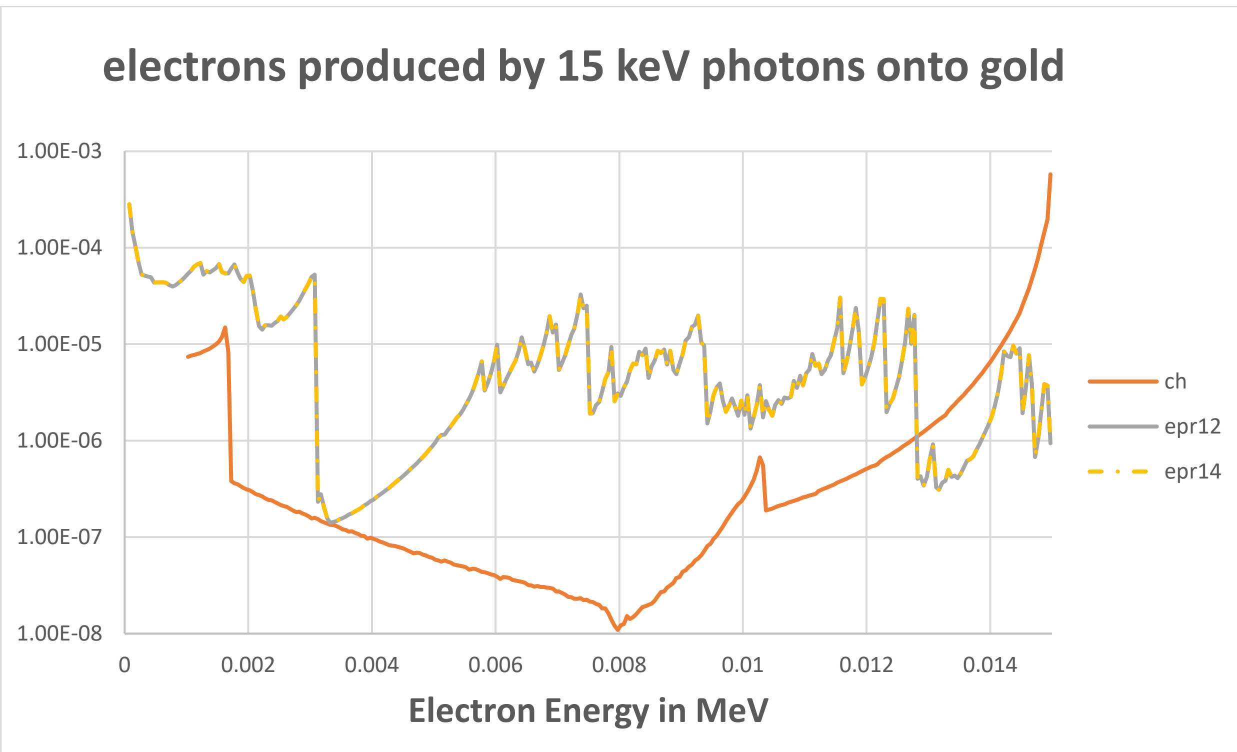

Figure 1: Relative Number of Electrons produced by 15 keV gammas onto gold

Between MCNP 6.1 and 6.2, the EPR electron transport was also upgraded, and the results now look more like other related codes. In Figure 2 below, the electron dose (use the *F8 tally) from a 1 keV beam of electrons onto water (for biological applications) is shown for the Single Electron method using MCNP6.1 and 6.2. This figure compares very favorably with Figure 2b of Reference 6. Condensed history results are not shown since 1 keV is the lower limit the CH method.

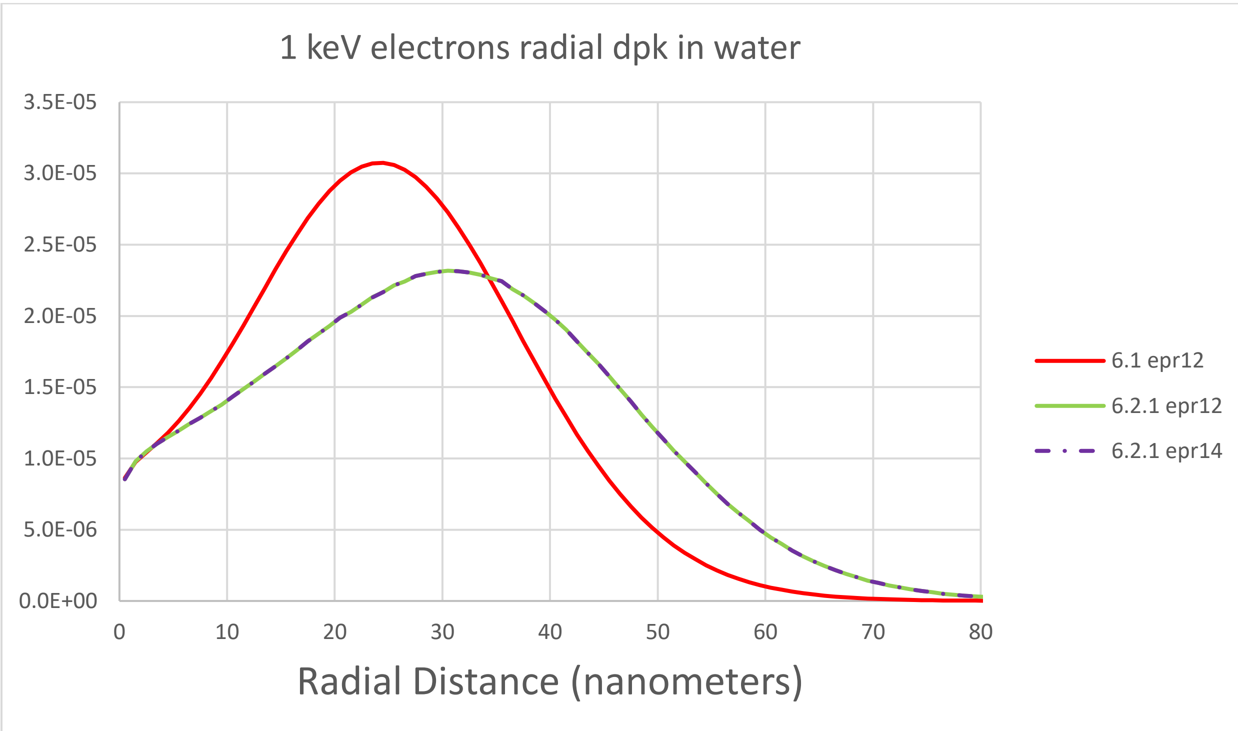

Figure 2: Relative Electron Dose Rates in Water from a 1 keV Electron Beam

The differences between EPRDATA12 and EPRDATA14 are corrections and the addition of more physics[7]. To date, no significant changes have been noticed in integral results. However, the EPRDATA14 library does NOT track the EPRDATA12 library. Also note that MCNP 6.1 will not run the EPRDATA14 library. In the future, it is anticipated that an EPRDATA17 library will be generated from EPICS-2017 data[8].

Materials Available in EPRDATA12 (~2009) and EPRDATA14 (~2015)

The elemental materials found in the EPRDATA libraries are listed in Table 3 below:

Table 3: Library Contents for EPR data

Number	Element	EPRDATA12	EPRDATA14
1	H	1000.12p	1000.14p
2	He	2000.12p	2000.14p
3	Li	3000.12p	3000.14p
4	Be	4000.12p	4000.14p
5	B	5000.12p	5000.14p
6	C	6000.12p	6000.14p
7	N	7000.12p	7000.14p
8	O	8000.12p	8000.14p
9	F	9000.12p	9000.14p
10	Ne	10000.12p	10000.14p
11	Na	11000.12p	11000.14p
12	Mg	12000.12p	12000.14p
13	AL	13000.12p	13000.14p
14	Si	14000.12p	14000.14p
15	P	15000.12p	15000.14p
16	Si	16000.12p	16000.14p
17	Cl	17000.12p	17000.14p
18	Ar	18000.12p	18000.14p
19	K	19000.12p	19000.14p
20	Ca	20000.12p	20000.14p
21	Sc	21000.12p	21000.14p
22	Ti	22000.12p	22000.14p
23	V	23000.12p	23000.14p
24	Cr	24000.12p	24000.14p
25	Mn	25000.12p	25000.14p
26	Fe	26000.12p	26000.14p
27	Co	27000.12p	27000.14p
28	Ni	28000.12p	28000.14p
29	Cu	29000.12p	29000.14p
30	Zn	30000.12p	30000.14p
31	Ga	31000.12p	31000.14p
32	Ge	32000.12p	32000.14p
33	As	33000.12p	33000.14p
34	Se	34000.12p	34000.14p
35	Br	35000.12p	35000.14p
36	Kr	36000.12p	36000.14p
37	Rb	37000.12p	37000.14p
38	Sr	38000.12p	38000.14p

39	Y	39000.12p	39000.14p
40	Zr	40000.12p	40000.14p
41	Nb	41000.12p	41000.14p
42	Mo	42000.12p	42000.14p
43	Tc	43000.12p	43000.14p
44	Ru	44000.12p	44000.14p
45	Rh	45000.12p	45000.14p
46	Pd	46000.12p	46000.14p
47	Ag	47000.12p	47000.14p
48	Cd	48000.12p	48000.14p
49	In	49000.12p	49000.14p
50	Sn	50000.12p	50000.14p
51	Sb	51000.12p	51000.14p
52	Te	52000.12p	52000.14p
53	In	53000.12p	53000.14p
54	Xe	54000.12p	54000.14p
55	Cs	55000.12p	55000.14p
56	Ba	56000.12p	56000.14p
57	La	57000.12p	57000.14p
58	Ce	58000.12p	58000.14p
59	Pr	59000.12p	59000.14p
60	Nd	60000.12p	60000.14p
61	Pm	61000.12p	61000.14p
62	Sm	62000.12p	62000.14p
63	Eu	63000.12p	63000.14p
64	Gd	64000.12p	64000.14p
65	Tb	65000.12p	65000.14p
66	Dy	66000.12p	66000.14p
67	Ho	67000.12p	67000.14p
68	Er	68000.12p	68000.14p
69	Tm	69000.12p	69000.14p
70	Yb	70000.12p	70000.14p
71	Lu	71000.12p	71000.14p
72	Hf	72000.12p	72000.14p
73	Ta	73000.12p	73000.14p
74	W	74000.12p	74000.14p
75	Re	75000.12p	75000.14p
76	Os	76000.12p	76000.14p
77	Ir	77000.12p	77000.14p
78	Pt	78000.12p	78000.14p
79	Au	79000.12p	79000.14p
80	Hg	80000.12p	80000.14p
81	Tl	81000.12p	81000.14p

82	Pb	82000.12p	82000.14p
83	Bi	83000.12p	83000.14p
84	Po	84000.12p	84000.14p
85	At	85000.12p	85000.14p
86	Rn	86000.12p	86000.14p
87	Fr	87000.12p	87000.14p
88	Ra	88000.12p	88000.14p
89	Ac	89000.12p	89000.14p
90	Th	90000.12p	90000.14p
91	Pa	91000.12p	91000.14p
92	U	92000.12p	92000.14p
93	Np	93000.12p	93000.14p
94	Pu	94000.12p	94000.14p
95	Am	95000.12p	95000.14p
96	Cm	96000.12p	96000.14p
97	Bk	97000.12p	97000.14p
98	Cf	98000.12p	98000.14p
99	Es	99000.12p	99000.14p
100	Fm	100000.12p	100000.14p

The Lockwood Validation Suite for EPR Data

Based on some work at Sandia(9), 167 experiments involving electron beams were carried out. In the MCNP validation suite, there are test calculations (one with CH – and one with SE) for each of the configurations. Results are available(10) in json-formatted files for EPRDATA14 and MCNP versions 6.2.0 and 6.2.1.

References

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4. Michael R. James, “MCNPX to MCNP6 Migration Notes”, LA-UR-13-22964, Los Alamos National Laboratory, 2013.
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8. See https://www-nds.iaea.org/epics/, accessed July 2022.
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