Photonuclear reactions in MCS

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Introduction to photonuclear reactions

- **Important for radiation shielding, heavy water reactors and beryllium reflectors**
- **Incident photon interacting with the nucleus**
  - **Creation of neutrons, alphas, protons, gammas**
  - **Photofission**
- **Photonuclear reactions are characterized by threshold energies**
  - **Between 5 and 9 MeV for neutron-producing reactions of most nuclides**
  - **= 2.2259 MeV for (gamma,n) reaction on deuterium**
  - **= 1.6659 MeV for (gamma,n) reaction on beryllium 9**
- **XS of photonuclear reactions are always small (<5%) compared to total photoatomic XS of element**
- **Photonuclear XS are nuclide-dependent (like neutron XS) unlike photo-atomic XS (which are element-dependent)**

References

- [1, White] LA-13744-T, Morgan C. White, thesis, July 2000, “Development and implementation of photonuclear cross-section data for mutually coupled neutron-photon transport calculations in the MCNP Code”
- [2, Kalt.] Toni Kaltiaisenaho, “Photonuclear reactions in SERPENT 2 Monte Carlo code”, Proceeding M&C 2019, Portland, Oregon, Aug 25-29
- [3, Fynan] Douglas A. Fynan, “Photoneutron reaction kinematics and error of commonly used approximations”, Nuclear Instrumentation and Methods Section A, accepted for publication
- [4, Caro] Edmund Caro, “Relativistic kinematics for photoneutron production in Monte Carlo transport calculations”, Annals of Nuclear Energy, 96:170-175, 2016
- [5, Bensch] F. Bensch, F. Vesely, "Yields and spectra of some spherical photoneutron sources," Journal of Nuclear Energy, 23: 537-550, 1969

Outline

I. Photonuclear ACE data

II. Photonuclear forced collision scheme

III. Russian roulette for photoneutrons

IV. Photonuclear kinematics

V. First MCS studies of photoneutron sources

I. Photonuclear ACE data

List of photonuclear MT reactions (ENDF format)

- **MT=5 (gamma, anything)**
- **MT=16 (gamma, 2n) (sum of MT=875-891)**
- **MT=17 (gamma, 3n)**
- **MT=18 (gamma, fission)**
- **MT=22 (gamma, neutron+alpha)**
- **MT=28 (gamma, neutron+proton)**
- **MT=29 (gamma, neutron+2alpha)**
- **MT=50-91 (gamma, neutron)**
- **MT=102 (gamma, gamma)**
- **MT=103 (gamma, proton) (sum of MT=600-649)**
- **MT=104 (gamma, deuteron) (sum of MT=650-699)**
- **MT=105 (gamma, triton) (sum of MT=700-749)**
- **MT=106 (gamma, helium 3) (sum of MT=750-799)**
- **MT=107 (gamma, alpha) (sum of MT=800-849)**
- **MT=111 (gamma, 2proton)**

“endf7u” photonuclear data from MCNP package

- “endf7u” file (~380 MB), extension .70u
  - Photonuclear data based on ENDF/B-VII.0
  - Data compilation for 157 nuclides in one file (~5 million lines)
  - No temperature dependence
- 141 nuclides have only 1 reaction: MT=5 (gamma, anything)
- List of the remaining 16 nuclides
  - 1002 hydrogen-2 MT=50
  - 4009 beryllium-9 MT=16/28/29/102-106
  - 6012 carbon-12 MT=5/50/600
  - 7014 nitrogen-14 MT=5/102/103
  - 8016 oxygen-16 MT=5/50/600
  - 23051 vanadium-51 MT=16/22/28/50-65/91/102-107/111
  - 74180 tungsten-180 MT=16/17/22/28/50-57/91/102-107/111
  - 74182 tungsten-182 MT=16/17/22/28/50-71/91/102-107
  - 74183 tungsten-183 MT=16/17/22/28/50-69/91/102-107
  - 74186 tungsten-186 MT=16/17/22/28/50-71/91/102-107
  - 92235 uranium-235 MT=5/16/18
  - 92238 uranium-238 MT=5/16/17/18
  - 93237 neptunium-237 MT=5/16/17/18
  - 94239 plutonium-239 MT=5/16/17/18
  - 94240 plutonium-240 MT=5/16/17/18
  - 95241 americium-241 MT=5/16/18

"tendl17u" photonuclear data from TENDL-17 library

- **ACE file available in online repository of JEFF3.3 library**
  - https://www.oecd-nea.org/dbdata/jeff/jeff33/index.html
- **"tendl17u" file (~349 MB), extension .17u**
  - Photonuclear data based on TENDL-17 (TALYS-generated ENDF)
  - Data compilation for 283 nuclides in one file (~5 million lines)
  - No temperature dependence
- **All the nuclides have only 1 reaction: MT=5 (gamma, anything)**
- **Notable missing nuclides compared to endf7u**
  - hydrogen-2
  - neptunium-237
  - plutonium-239 and -240
  - americium-241
- **Notable nuclide present in tendl17u but not in endf7u**
  - uranium-234

Format of photonuclear ACE data file

- specificity of photonuclear ACE files: all secondary-particle emission is referenced through the IXS construct

- lin-lin interpolation assumed for photonuclear XS (ESZ/TOT/SIG)

NXS(1): LXS length of XSS block

NXS(2): ZA = Z*1000+A

NXS(3): NES number of energy points

NXS(4): NTR number of MT reactions

NXS(5): NTYPE number of secondary particle types

NXS(6): NPIXS number of parameter entries in IXS array per secondary particle = 2 in endf7u/tendl17u

NXS(7): NEIXS number of entries in IXS array per secondary particle = 12 in endf7u/tendl17u

JXS(1): ESZ main energy grid locator

JXS(2): TOT total XS data locator

JXS(3): NON = TOT for endf7u/tend17u

JXS(4): ELS = 0 for endf7u/tend17u

JXS(5): THN heating number locator

JXS(6): MTR MT reaction list locator

JXS(7): LQR Q-value list locator

JXS(8): LSIG locator of XS locators

JXS(9): SIG XS data locator

JXS(10): IXSA First word of IXS array

JXS(11): IXS First word of IXS block

Size of one IXS array = NEIXS = 12

1 secondary particle = 1 IXS array & 1 IXS block

Photonuclear ACE format : IXS construct [1, White]

Table 3-4. Description of the IXS Array elements in a photonuclear class 'u' ACE format.

Entry	Parameter	Fixed number descriptive
IXS(1,J)	IPT(J)	Particle IPT number
IXS(2,J)	NTRP(J)	Number of MT reactions producing this particle
Entry	**Locator**	**Offset to array of…**
IXS(3,J)	PXS(J)	Total particle production cross-section data
IXS(4,J)	PHN(J)	Particle average heating number data
IXS(5,J)	MTRP(J)	Particle production MT reaction numbers
IXS(6,J)	TYRP(J)	Reaction coordinate system data
IXS(7,J)	LSIGP(J)	Reaction yield locators (relative to SIGP)
IXS(8,J)	SIGP(J)	Primary locator for reaction yield data
IXS(9,J)	LANDP(J)	Reaction angular distribution locators (relative to ANDP)
IXS(10,J)	ANDP(J)	Primary locator for angular distribution data
IXS(11,J)	LDLWP(J)	Reaction energy distribution locators (relative to DLWP)
IXS(12,J)	DLWP(J)	Primary locator for energy distribution data

Particle Name	Symbol	IPT
neutron	n	1
photon	p	2
electron	e	3
proton	h	9
deuteron	d	31
triton	t	32
helium_3	s	33
alpha	a	34

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Examples: endf7u deuterium and beryllium

- **Hydrogen-2 1002.70u**
  - **NTR=1 : MT=50 ; NTYPE=2 ; IPT=1/9**
  - **Number of reactions producing neutrons=1 : MT=50**
    - **Tabulated angular distribution in center-of-mass system**
    - **Energy distribution: level scattering LAW=33**
- **Beryllium-4 4009.70u**
  - **NTR=8 : MT=16/28/29/102-106 ; NTYPE=4 ; IPT=1/2/9/34**
  - **Number of reactions producing neutrons=3 : MT=16/28/29**
    - **Isotropic angular distribution in center-of-mass system**
    - **Tabulated energy distribution LAW=4**
  - **Number of reactions producing photons=1 : MT=28**
    - **Isotropic angular distribution in center-of-mass system**
    - **Tabulated energy distribution LAW=4**

Example: endf7u versus tendl17u for ^{235}U

- **endf7u 92235.70u**
  - NTR=3 : MT=5/16/18 ; NTYPE=2 ; IPT=1/2
  - Number of reactions producing neutrons=3 : MT=5/16/18
    - MT=5/16: correlated energy-angle tabulated distribution in center-of-mass system LAW=44
    - MT=18: isotropic angular distribution in laboratory system
    - MT=18: simple Maxwell fission spectrum LAW=7
  - Number of reactions producing photons=2 : MT=5/16
    - Isotropic angular distribution in center-of-mass system
    - Tabulated energy distribution LAW=4
- **tendl17u 92235.17u**
  - NTR=1 : MT=5 ; NTYPE=7 ; IPT=1/2/9/31/32/33/34
  - Number of reactions producing neutrons=1 : MT=5
    - Correlated energy-angle tabulated distribution in center-of-mass system LAW=44
  - Number of reactions producing photons=1 : MT=5
    - Isotropic angular distribution in center-of-mass system
    - Tabulated energy distribution LAW=4

Lack of photoneutron data in endf7u tungsten [2, Kalt.]

- **5 tungsten isotopes: W-180, -182, -183, -184 and -186**
- **Issue with two isotopes: 182 and 186**
- **Example 74182.70u (identical issue with 74186.70u)**
  - **NTR=33 : MT=16/17/22/28/50-71/91/102-107 ; NTYPE=1 ; IPT=1**
  - **Number of reactions producing neutrons=5 : MT=16/17/22/28/91**
  - **Only 5 reactions are considered to produce neutrons**
  - **All the photoneutron production by discrete-level (gamma,n) reaction (MT=50-71) is missing! 22 reactions neglected!**
- **Suggested solution**
  - **Generate anew tungsten photonuclear ACE with NJOY... if the original ENDF file indeed contains the photoneutron production data**

Isotope	W-180	W-182	W-183	W-184	W-186
Natural abundance	0.12%	26.50%	14.31%	30.64%	28.43%

II. Photonuclear forced collision scheme

Based on [2, Kalt.]

Photon mean free path

$$\Sigma_{tot} = \Sigma_{PA,tot} + \Sigma_{PN,tot}$$

- Σ_{tot} total macroscopic photon XS
- $\Sigma_{PA,tot}$ total macroscopic photo-atomic XS
- $\Sigma_{PN,tot}$ total macroscopic photonuclear XS
- Photon mean free path MFP = $1/\ \Sigma_{tot}$ instead of $1/\ \Sigma_{PA,tot}$
- In a given material composition
  - Macroscopic photo-atomic XS is summed up element-wise

$$\Sigma_{PA,tot} = \sum_{ele} N_{ele} \times \sigma_{PA,tot,ele}$$

  - Macroscopic photonuclear XS is summed up nuclide-wise

$$\Sigma_{PN,tot} = \sum_{nuc} N_{nuc} \times \sigma_{PN,tot,nuc}$$

MCS photon transport – until now

- **Sample distance to collision dtc = -log(RNG)/($\Sigma_{PA,tot}$)**
- **Compute distance to boundary dtb**
- **If (dtc < dtb) ! collision of photon with weight W and energy E**

  - **Sample collision element**
  - **Sample photo-atomic reaction for collision element**

MCS photon transport – forced photonuclear collision

- **Sample distance to collision dtc = -log(RNG)/$(\Sigma_{PA,tot} + \Sigma_{PN,tot})$**
- **Compute distance to boundary dtb**
- **If (dtc < dtb) ! collision of photon with weight W and energy E**
  - **Sample collision nuclide**
  - **Sample photonuclear reaction for collision nuclide**
  - **Bank outgoing photoneutrons for further transport**
  - **Adjust weight of incident photon**

$$W' = \left(1 - \frac{\Sigma_{PN,tot}}{\Sigma_{tot}}\right) W = \frac{\Sigma_{PA,tot}}{\Sigma_{PA,tot} + \Sigma_{PN,tot}} W$$

  - **Sample collision element**
  - **Sample photo-atomic reaction for collision element**

Sampling of collision nuclide & photonuclear reaction

- **Only the photonuclear reactions that produce photoneutrons are forced**
  - **Note: photonuclear reactions producing photoneutrons may also produce photons (e.g. photofission). Those inelastic outgoing photons are neglected in MCS for the time being.**
- **Probability of selecting the collision nuclide *nuc***
  - **Index *rea* includes only the photonuclear reactions listed in MTRP field of IPT=1 (neutron) IXS block of each nuclide**

$$P_{nuc}(E) = \frac{N_{nuc} \sum_{rea} \sigma_{nuc,rea}(E)}{\sum_{nuc} \left[N_{nuc} \sum_{rea} \sigma_{nuc,rea}(E) \right]} = \frac{N_{nuc} \sum_{rea} \sigma_{nuc,rea}(E)}{\Sigma_{PN,forced-reactions}}$$

- **Probability of selecting the photonuclear reaction *rea* for the collision nuclide *nuc***

$$P_{rea}(E) = \frac{\sigma_{nuc,rea}(E)}{\sum_{rea} \sigma_{nuc,rea}(E)}$$

Weight of outgoing photoneutrons and photons

- **Reaction *rea* of nuclide *nuc* produces photoneutrons (and maybe also photons)**
  - **Multiplicity of the outgoing particle X = $\nu_{nuc,rea,X}$**
- **Particle multiplicity is computed from SIGP data in the relevant IXS block of the nuclide**
  - **Direct multiplicity (MF=6/12/16)**
  - **Production cross section (MF=13)**
- **Set the weight W_X of the outgoing particle as a function of the weight W of the incident photon**

$$W_X = \nu_{nuc,rea,X} \frac{\Sigma_{PN,forced-reactions}}{\Sigma_{tot}} W$$

  - **[2, Kalt.] *"This weight adjustment takes into account both the forced collision and the exclusion of reactions which don't produce desired particle types."***

III. Russian roulette for photoneutrons

Parameters of Russian roulette for photoneutrons

- **The Russian roulette is applied <u>after a neutron collision</u>**
  - **Default Russian roulette: B(1) = 0.25 and B(2) = 2*B(1) = 0.5**
  - **If w < B(1) {if RNG*B(2) < w then w = B(2) else neutron is killed}**
- **Weight of photoneutrons** $W_X = \nu_{nuc,rea,X} \frac{\Sigma_{PN,forced-reactions}}{\Sigma_{tot}} W \leq \sim 5\%$
- **Russian roulette applied for photoneutrons = RR_factor*B**
- **Description of test case**
  - **Heavy water sphere with leakage boundary condition**
  - **Point isotropic photon source at the center of the sphere**
  - **Uniform energy distribution of source photons between 2 MeV and 10 MeV**
  - **(Threshold of (gamma,n) reaction on deuterium = ~2.2 MeV)**
  - **Neutron flux tallied in the sphere in units [cm per photon source]**
  - **10 statistical tests on to measure the figure of merit**
  - **1,000,000 source photons with 100-cm-radius sphere tested**
  - **Volume of sphere = 4.19E6 cm^3**

Test case: statistics on initial weights of photoneutrons

- **1000 source photons → 1142 photoneutrons are generated**
  - **Median weight = 0.47%**
  - **Average weight = 0.42%**
  - **Minimum weight = 0.04%**
  - **Maximum weight = 0.52%**
- **Impact of different RR parameters on photoneutron survival**
  - **If w < B(1) {if RNG*B(2) < w then w = B(2) else neutron is killed}**
  - **Russian roulette applied for photoneutrons = RR_factor*B**

RR_factor	B(1)	B(2)	% photoneutrons surviving RR = median weight/B(2)
1.0	25%	50%	~1%
0.5	12.5%	25%	~2%
0.2	5%	10%	~5%
0.1	2.5%	5%	~10%
0.05	1.25%	2.5%	~20%
0.01	0.25%	0.5%	>50%

Results: 1E6 source photons / 100 cm radius

- **B(1) = 25%: photoneutrons with weights 0.5% and 50% co-exist → bigger relative error**
- **Simulation time explodes with decreasing B(1): more and more photoneutron tracks with smaller weights are simulated**
- **All the photoneutron tracks contribute to the tally, so FOM increases when B(1) decreases**

P	RR_factor	B(1)	Neutron flux	Relative error	Figure of Merit	Time (min)
Photonuclear turned off		N/A	N/A	N/A	N/A	0.265
~1%	1.0	25%	6.24886E+00	1.28891E-02	1.5596022E+04	0.386
~2%	0.5	12.5%	6.20942E+00	8.97452E-03	2.6758815E+04	0.464
~5%	0.2	5%	6.24708E+00	5.62096E-03	4.3202376E+04	0.733
~10%	0.1	2.5%	6.24454E+00	3.89518E-03	5.7218630E+04	1.15
~20%	0.05	1.25%	6.25778E+00	2.74266E-03	6.8299026E+04	1.95
>50%	0.01	0.25%	6.26654E+00	9.56405E-04	1.1732326E+05	9.32

Russian roulette of photoneutrons AT BIRTH

- **The Russian roulette is applied at photoneutron birth and at neutron collision**
  - **Default Russian roulette: B(1) = 0.25 and B(2) = 2*B(1) = 0.5**
  - **If w < B(1) {if RNG*B(2) < w then w = B(2) else neutron is killed}**
- **Russian roulette applied for photoneutrons = RR_factor*B**
- **Results for 1E6 source photons / 100 cm radius**

P	RR_factor	B(1)	Neutron flux	Relative error	Figure of Merit	Time (min)
Photonuclear turned off		N/A	N/A	N/A	N/A	0.259
~1%	1.0	25%	6.22465E+00	1.27056E-02	1.6490619E+04	0.376
~2%	0.5	12.5%	6.23580E+00	9.00510E-03	2.7455915E+04	0.449
~5%	0.2	5%	6.24468E+00	5.72662E-03	4.4053288E+04	0.692
~10%	0.1	2.5%	6.25715E+00	3.98856E-03	5.5463032E+04	1.13
~20%	0.05	1.25%	6.26278E+00	2.75182E-03	6.6623324E+04	1.98
>50%	0.01	0.25%	6.26973E+00	9.52019E-04	1.1545637E+05	9.56

of scoring photon histories for photoneutron RR at birth

- **The Russian roulette is applied <u>at photoneutron birth and at neutron collision</u>**
  - **Default Russian roulette: B(1) = 0.25 and B(2) = 2*B(1) = 0.5**
  - **If w < B(1) {if RNG*B(2) < w then w = B(2) else neutron is killed}**
- **Russian roulette applied for photoneutrons = RR_factor*B**
- **Results for 1E6 source photons / 100 cm radius**

P	RR_factor	B(1)	#
No RR at birth		N/A	885,282
~1%	1.0	25%	9,509
~2%	0.5	12.5%	18,988
~5%	0.2	5%	47,476
~10%	0.1	2.5%	94,412
~20%	0.05	1.25%	184,812
>50%	0.01	0.25%	839,997

IV. Photonuclear kinematics

Kinematics data in photonuclear ACE files

- "tendl17u" : only MT=5 (γ, anything) is used
  - Neutron production uses LAW=44 (correlated energy-angle distribution) in center-of-mass system
  - Photon production uses LAW=4 (tabulated energy distribution) and isotropic angular distribution in center-of-mass system
- "endf7u": many different cases
  - MT=50-90 discrete (γ,n) uses LAW=33 (level scattering) and tabulated angular distributions in center-of-mass system
  - MT=18 (γ,f) uses LAW=7 (Maxwell) or LAW=4 (tabulated energy distribution) with isotropic distribution in laboratory system
  - MT=16/17/22/28/29/91 (γ, X) with X=2n/3n/n+α/n+p/n+2α/(n in continuum) are all sampled in center-of-mass system
    - Either LAW=44 (correlated energy-angle distribution)
    - Or LAW=4 with isotropic angular distribution

Issues to solve

- **Implementation of LAW=33 (level scattering) for discrete (γ,n) reactions**
  - **Wrong implementation in MCNP**
  - **Relativistic implementation shown in next slides**
- **Conversion from center-of-mass system to laboratory system**
  - **With one exception, sampling in center-of-mass is used for all the reactions in endf7u and tendl17u**
  - **One exception: endf7u MT=18 (γ,f) sampled in laboratory frame**
  - **Relativistic solution presented in next slides for MT=50-91 (γ,n) reactions**
  - **What about neutron production for the reactions MT= 5 / 16 / 17 / 22 / 28 / 29 (γ, X) with X= anything / 2n / 3n / n+α / n+p / n+2α?**
    - **Approximation: those reactions are assumed as (γ, n) for relativistic conversion from center-of-mass to laboratory**

LAW=33 Level scattering

- **[1, White] “*Law 33 indicates any combination of particles incident and emitted. Its use is allowed for photonuclear interactions though the parameters must be chosen for photonuclear kinetics instead of neutron kinetics*”**
- **LAW=33 is not implemented correctly in MCNP**
  - **Calling LAW=33 is the same as calling LAW=3 in MCNP**
  - **But LAW=3 is only for neutron kinematics (incident neutron, outgoing neutron)**
  - **[3, Fynan]: modelling the photoneutron energy in center-of-mass system (CMS) according to LAW=3 gives very wrong results (negative energies!)**

$$E_{photoneutron-law3} = \frac{A}{A+1}[E_{in} + Q]$$

- **Fully relativistic implementation of LAW=33 for discrete (γ,n) reactions detailed in [3, Fynan][4, Caro] and next slides**

Photoneutron energy from (γ,n) reaction in center-of-mass

- Notations
  - CMS center-of mass system ; LAB laboratory system
  - E_G energy of incident gamma
  - m_N neutron mass; m_T mass of target nucleus; m_R mass of residual nucleus
  - $E'_N = T'_N + m_N c^2$ total energy of photoneutron in CMS
  - $E_N = T_N + m_N c^2$ total energy of photoneutron in LAB
- Four-momentum Lorentz invariant s (unit = mass.energy)

$$sc^2 = \left(m_T c^2\right)^2 + 2 m_T c^2 E_G$$

- Total energy of photoneutron in CMS from Eq. (29) [3, Fynan]

$$E'_N = \frac{sc^2 + \left(m_N c^2\right)^2 - \left(m_R c^2\right)^2}{2\sqrt{sc^2}}$$

- Neutron kinetic energy in CMS

$$T'_N = E'_N - m_N c^2 = \frac{sc^2 + \left(m_N c^2\right)^2 - \left(m_R c^2\right)^2}{2\sqrt{sc^2}} - m_N c^2$$

Retrieving the mass m_R of the residual nuclide

- **Total energy of photoneutron in CMCS from Eq. (29) [3, Fynan]**

$$E'_N = \frac{sc^2 + (m_N c^2)^2 - (m_R c^2)^2}{2\sqrt{sc^2}}$$

- **Q-value of the reaction (γ,n) for a residual nucleus in ground state (MT=50), in a discrete excited state (MT=51-90) or in continuum (MT=91) available in LQR block of photonuclear ACE**

$$Q_{MT} = (m_T - m_N - m_R)c^2$$
$$m_R c^2 = (m_T - m_N)c^2 - Q_{MT}$$

- **Excited nuclides are heavier than ground state nuclides**
  - $Q_{MT=50+n} < Q_{MT=50}$ **for n=1-41 (first to 40th excited state & continuum)**
  - **Excited nuclide in nth excited state heavier than ground state nuclide by a mass of** $(Q_{MT=50} - Q_{MT=50+n})c^2$

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Relativistic conversion from CMS to LAB for (γ,n): ENERGY

- **Notations**
  - **CMS center-of mass system ; LAB laboratory system**
  - E_G **energy of incident gamma;** m_N **neutron mass;** m_T **mass of target nucleus;**
  - μ' **cosine between incident photon and photoneutron in CMS**
  - $E'_N = T'_N + m_N c^2$ **total energy of photoneutron in CMS**
  - $E_N = T_N + m_N c^2$ **total energy of photoneutron in LAB**
- **β = ratio of center-of-mass velocity to speed of light in CMS**

$$\beta = \frac{E_G}{E_G + m_T c^2}$$

- p' **= momentum of photoneutron in CMS**

$$p'c = \sqrt{\left(E'_N\right)^2 - (m_N c^2)^2}$$

- T_N **kinetic energy of the photoneutron in LAB**

$$T_N = \frac{1}{\sqrt{1-\beta^2}}\left(E'_N + \beta p' c \mu'\right) - m_N c^2$$

Relativistic conversion from CMS to LAB for (γ,n): ANGLE

- **Notations**
  - **CMS center-of mass system ; LAB laboratory system**
  - E_G **energy of incident gamma;** m_N **neutron mass;** m_T **mass of target nucleus;**
  - μ' **cosine between incident photon and photoneutron in CMS**
  - p' **momentum of photoneutron in CMS**
  - $E'_N = T'_N + m_N c^2$ **total energy of photoneutron in CMS**
  - $E_N = T_N + m_N c^2$ **total energy of photoneutron in LAB**
- **Components of photoneutron momentum parallel and perpendicular to the incident photon direction in CMS**

$$p_{\parallel} c = \frac{1}{\sqrt{1-\beta^2}} \left(p' c \mu' + \beta E'_N \right)$$

$$p_{\perp} c = p' c \sqrt{1-\mu'^2}$$

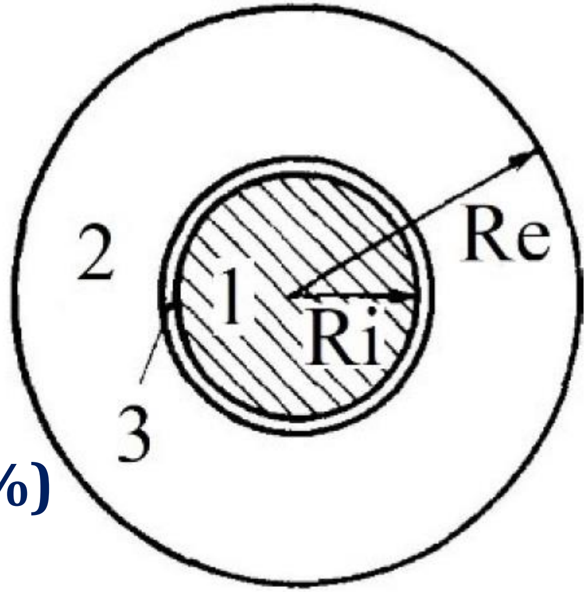
- μ **cosine between incident photon and photoneutron in LAB**

$$\mu = \frac{p_{\parallel} c}{\sqrt{\left(p_{\parallel} c\right)^2 + \left(p_{\perp} c\right)^2}}$$

V. MCS studies of photoneutron sources

Experimental data described in [5, Bensch]

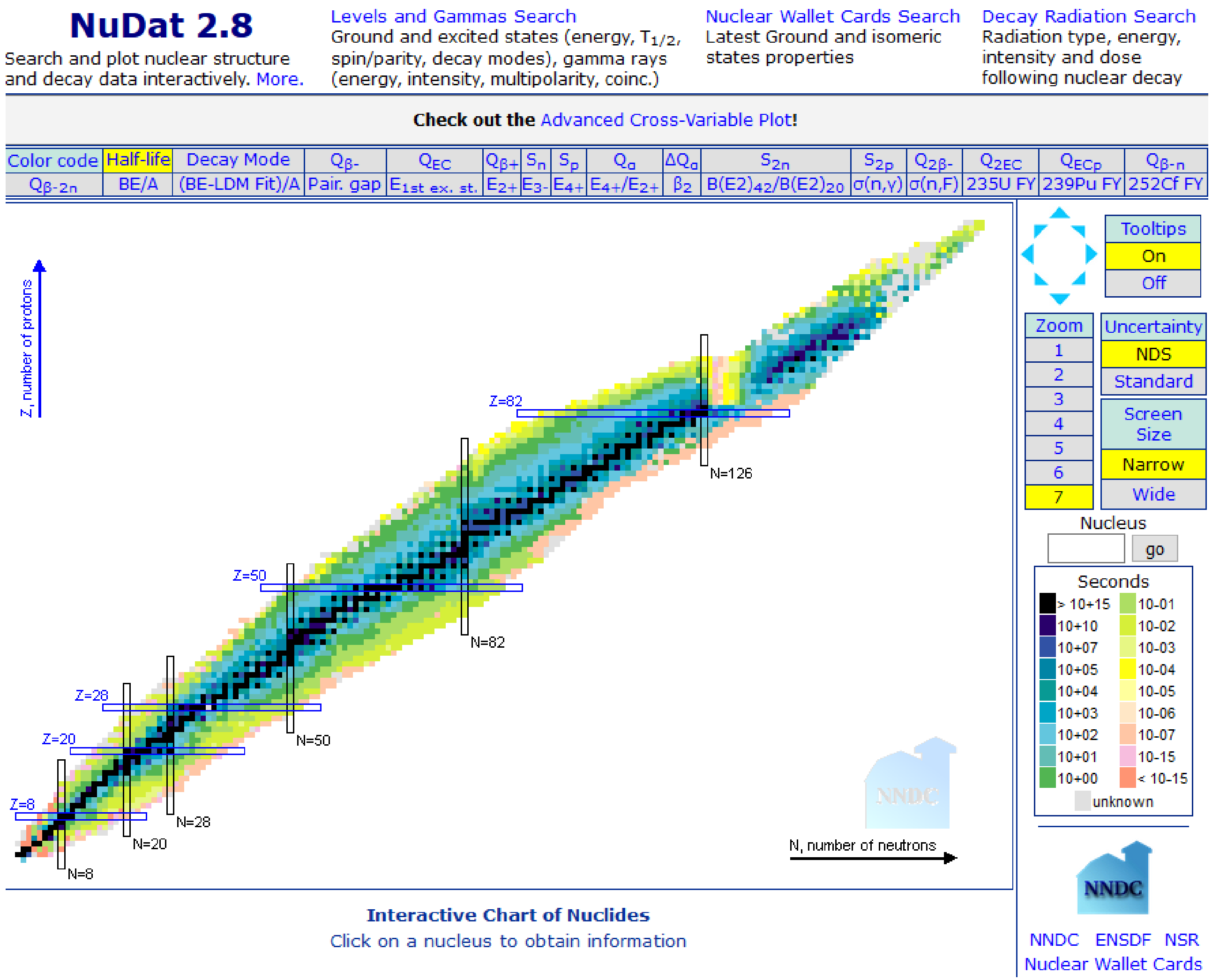
Example of a photoneutron source [5, Bensch]



- **1: radioactive core of radius Ri = 0.5 cm**
  - **Gamma-emitter nuclides**
  - **Core material: either Sb, In, Ga, La_2O_3 or NaF**
- **2: target material of external radius Re**
  - **Beryllium (ρ = 1.73 g/cm^3, purity > 99.7%)**
  - **Heavy water (ρ = 1.107 g/cm^3, purity > 99.8%)**
- **3: tin plate container**
- **Core is irradiated in reactor: gamma-emitter nuclides are produced through neutron capture**
- **Core is taken away from reactor and wrapped with target material**
- **Gamma emitted by the core interact with ^{9}Be or ^{2}H target and produce photoneutrons through (gamma,n) reactions**

Properties of gamma rays from radioactive nuclides

- **Source: Nudat2.8 database from Brookhaven National Lab.**
- **https://www.nndc.bnl.gov/nudat2/**



Properties of gamma rays emitted by the central core

- **Nudat2.8 database https://www.nndc.bnl.gov/nudat2/**
- **^{9}Be (γ,n) threshold = 1.6659 MeV**
- **^{2}H (γ,n) threshold = 2.2259 MeV**

γ-emitter nuclide	Energy of decay photons (MeV)	Yield (number of photons per decay)	Half-life
^{124}Sb	1.690971 2.090930	0.4757 0.0549	60.9 days
^{116m}In	1.75250 2.11229	0.0236 0.1509	54.1 minutes
^{140}La	2.34788 2.52140 2.54734	0.0085 0.0346 0.00101	40.2 hours
^{24}Na	2.754007	0.99855	15.0 hours
^{72}Ga	2.491026 2.507718 2.515857 2.621279 2.844160	0.0773 0.1333 0.00258 0.00141 0.00446	14.1 hours

Photoneutron source strength calculated by MCS/MCNP

- 30 million photon histories, mode N P with photonuclear reactions on
- Isotropic / homogeneous radioactivity of spherical core
- Neutron current tallied through the sphere of radius Re
- Results expressed in [neutrons.cm^2/(g.s.curie)]

Re [cm] nuclide & target	$\mu_{EXP}^{eff} \pm 1\sigma$	$\mu_{MCS}^{eff} \pm 1\sigma$	$\mu_{MCNP}^{eff} \pm 1\sigma$	$\left(\frac{MCS}{EXP}-1\right) \pm 1\sigma$	$\left(\frac{MCNP}{MCS}-1\right) \pm 1\sigma$
1.0 cm ^{124}Sb & Be	1.026E+5 ±2.4%	1.172E+5 ±0.5%	1.181E+5 ±1.5%	+14.2% ±2.4%	+0.8% ±1.6%
1.6 cm ^{124}Sb & Be	1.046E+5 ±2.4%	1.159E+5 ±0.3%	1.178E+5 ±1.0%	+10.8% ±2.4%	+1.7% ±1.1%
2.0 cm ^{124}Sb & Be	1.047E+5 ±2.4%	1.144E+5 ±0.3%	1.157E+5 ±0.9%	+9.2% ±2.4%	+1.2% ±0.9%
2.5 cm ^{124}Sb & Be	1.032E+5 ±2.4%	1.124E+5 ±0.3%	1.140E+5 ±0.8%	+8.9% ±2.4%	+1.4% ±0.8%
2.5 cm ^{116m}In & Be	8.250E+3 ±3.5%	1.420E+4 ±0.4%	1.442E+4 ±1.3%	+72.1% ±3.5%	+1.5% ±1.3%
2.5 cm ^{140}La & Be	1.810E+3 ±4.6%	4.561E+3 ±0.4%	4.639E+3 ±1.1%	+152.0% ±4.6%	+1.7% ±1.2%
2.5 cm ^{24}Na & Be	1.013E+5 ±2.4%	8.390E+4 ±0.4%	8.547E+4 ±1.3%	-17.2% ±2.4%	+1.9% ±1.3%
2.5 cm ^{24}Na & D_2O	2.209E+5 ±2.4%	1.913E+5 ±0.3%	2.210E+5 ±1.0%	-13.4% ±2.4%	+15.5% ±1.0%
2.5 cm ^{72}Ga & D_2O	3.065E+4 ±2.4%	3.050E+4 ±0.4%	3.545E+4 ±1.1%	-0.5% ±2.4%	+16.2% ±1.2%

VI. Conclusion and perspectives

Conclusion and perspectives

- **First implementation of photonuclear reactions in MCS**
  - **Turned off by default in MCS; toggle <photonuclear>on</photonuclear>**
  - **Forced-collision scheme that produces one photoneutron particle per photon collision**
  - **Specific Russian roulette for photoneutrons at birth and after photoneutron collision**
  - **Full relativistic photoneutron kinematics for (γ,n) reactions**
- **Further validation of MCS (references next slide)**
  - **[A, Barber] contains experimental data for several target materials**
    - **Exploited in the references [B, White] [C, Heinrich] [D, Frankl]**
  - **[B, White] also contains MCNP input examples and solutions for analytical problems (semi-infinite slab etc.)**
  - **All the benchmarks involve electron sources and electron transport, which is currently unavailable in MCS**
  - **Workaround: use a third-party code to compute a bremsstrahlung photon source from electrons and use that source in neutron-photon mode in MCS**

References for further validation of MCS

- [A, Barber] W. C. Barber, W. D. George, “Neutron yields from targets bombarded by electrons,” Physical Review, 116: 1551–1559, 1959
- [B, White] LA-13744-T, Morgan C. White, thesis, July 2000, “Development and implementation of photonuclear cross-section data for mutually coupled neutron-photon transport calculations in the MCNP Code”
- [C, Heinrich] D.P. Heinrichs, E. M. Lent, “Photonuclear benchmarks with a comparison of COG and MCNPX Results,” Lawrence Livermore National Laboratory (LLNL), Livermore, California, 2003
- [D, Frankl] M. Frankl, R. Macian-Juan, “Photonuclear benchmarks of C, Al, Cu, Ta, Pb, and U from the ENDF/B-VII cross-section library ENDF7u using MCNPX,” Nuclear Science and Engineering, 183(1): 135–142, 2016

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