Verification of inputs for the Zr and Pb benchmarks carried out in IPPE, VNIITF and TUD labs and checking the current performance of the ENDF/B-VIII.1, ENDF/B-VIII.0, JEFF-3.3 and JENDL-5 libraries *)

S. Simakov [a)], M. Kostal [b)]

[a] Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

[b] Research Center Rez, Husinec-Rez, Czech Republic

* *will appear as Report INDC(NDS)-0XXX*, IAEA, 2026

IAEA Consultant Meeting on Shielding Benchmarking of Lead and Zirconium Evaluations, 15 - 19 December 2025

Content

I. Verification and modernization of necessary input data (including transport code input decks) for:

- IPPE (Obninsk) : three Pb spheres with ^{252}Cf(s.f.) source, neutron and gamma leakage
- TUD (Dresden) : one Pb sphere with D-T source, neutron leakage and activation/fission reaction rates
- VNIITF (Snezhinsk): one Pb and Zr (hemi-)spheres with D-T source, neutron and gamma leakage

and Validation of ENDF/B-VIII.1, ENDF/B-VIII.0, JEFF-3.3 and JENDL-5

- against measured results in these three spherical benchmarks:
- search for reasons of discrepancies

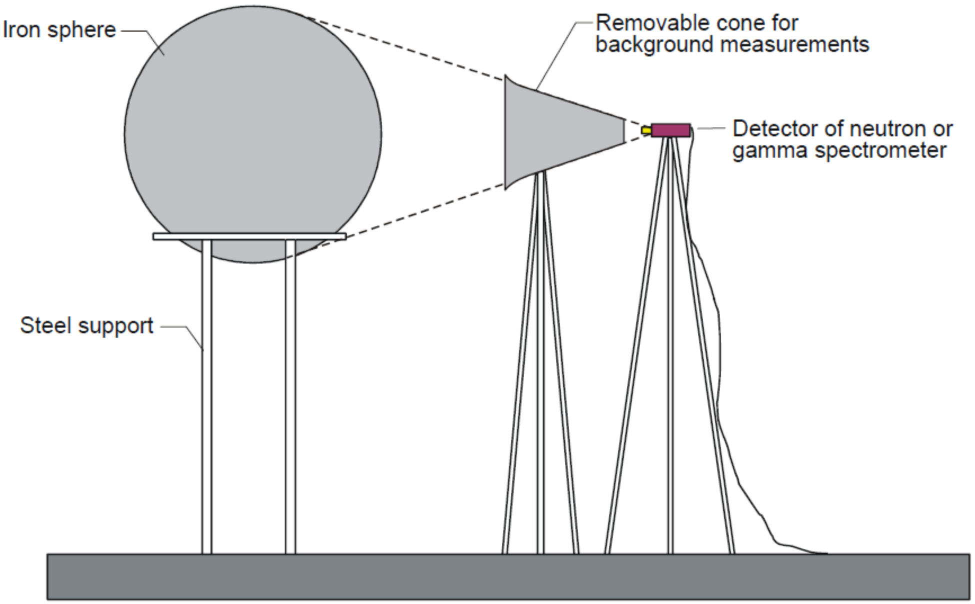
II. Performance of ENDF/B-VIII.1, ENDF/B-VIII.0, JEFF-3.3 and JENDL-5 evaluations vs. relevant cross sections for:

- (n,x)n and (n,x)γ emission cross sections on $^{nat,208}Pb$ at 14 MeV and lower energies
- (n,x)n and (n,x)γ emission cross sections on ^{nat}Zr at 14 MeV
- ENDF/B-VIII.1 vs. neutron induced discrete and continuous gamma production cross sections for ^{208}Pb at ≤ 15 MeV

III. Conclusions

I.1 IPPE three Pb sphere benchmarks with ^{252}Cf(s.f.) sources: overview

Typical set-up of IPPE sphere benchmarks with Cf source:



Benchmark most important parameters:

- Year of measurement: 1985
- Pb sphere outer diameters 20, 40 and 60 cm
- Encapsulated Cf(s.f.) in center
- Neutron detectors (at distance 3 x R):
  - Stilbene crystal viewed by PM, PSD
  - Hydrogen Recoil Spectrometer
- Gamma detector (at distance 3 x R):
  - Stilbene crystal viewed by PM, PSD
- Measuring Methods:
  - spectrometry of pulse height distribution
  - unfolding into energy spectra
  - shielding cone to detect room-return
- Measured energy range:
  - neutron spectra from 0.01 to 17.0 MeV
  - gamma spectra from 0.35 to 8.25 MeV

Availability:

detailed description of Benchmark, Measure numerical data, two MCNP sample input decks, References etc. are available in ICSBEP database in Entry:
G. Manturov, Y. Rozhikhin, L. Trykov (Evaluators), "Neutron and photon leakage spectra from Cf-252 source at centers of three lead spheres of different diameters", ICSBEP handbook, Vol. VIII, ALARM-CF-PB-SHIELD-001

I.1 IPPE three Pb sphere benchmarks with ^{252}Cf(s.f.) sources: our modifications of set-up

Cf(s.f.) source Capsules and Cavity in Pb spheres

<u>**from IPPE sample 1-D MCNP input deck to modified 3-D:**</u>

- real Geometry and Materials for Cf source:
Corundum (Al_2O_3) with 444 µg ^{252}Cf
encapsulated in SS and Cu containers

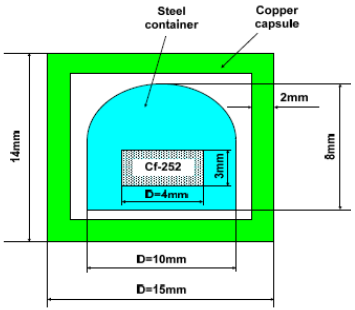
- real Geometry of Cavity in Pb sphere/plug for Cf source

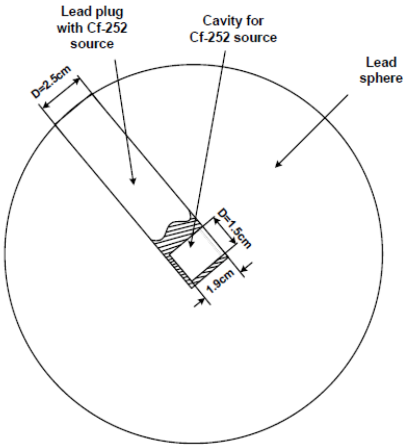
- impurities of Lead Cf(s.f.): 22 elements (instead of 9)
including heavy ones Cd, Ba …

(Intermediate NB remark: above listed modifications
have impact ≤ 2% on n- and g-leakage spectra)

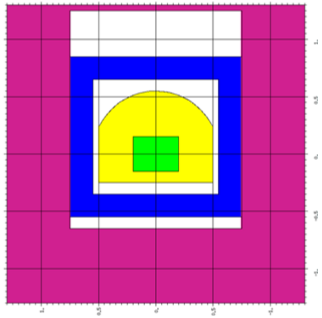
- contemporary knowledge about multiplicities and
energy distributions for neutrons and gammas after ^{252}Cf(s.f.)
(see next 2 slides)

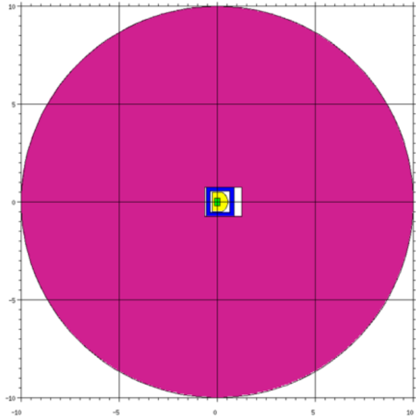
<u>given in ICSBEP/IPPE Pb benchmark:</u>





<u>Implemented now in 3-D input deck:</u>





I.1 IPPE Pb spheres: upgrade of ^{252}Cf(s.f.) source for sampling by MCNP - (i) general and for emission of neutrons

Present status: two IPPE original 1-D MCNP input decks with ^{252}Cf(s.f.) for

- 1st deck with Cf as a source of neutrons => for neutron-gamma transport
- 2nd deck with Cf as a source of gammas => for gamma transport
- 2 MCNP outputs should be then summed and compared with measured n- and g-leakages

Our upgrade of original input deck:

^{252}Cf(s.f.) is now source of Prompt & Delayed Neutrons & Gammas (we use MCNP capability to sample several source particles in one run, i.e. we sample Cf n- and g-emission fully analogous to s.f. of ^{252}Cf)

Our 3-D input MCNP deck sample Cf source either:

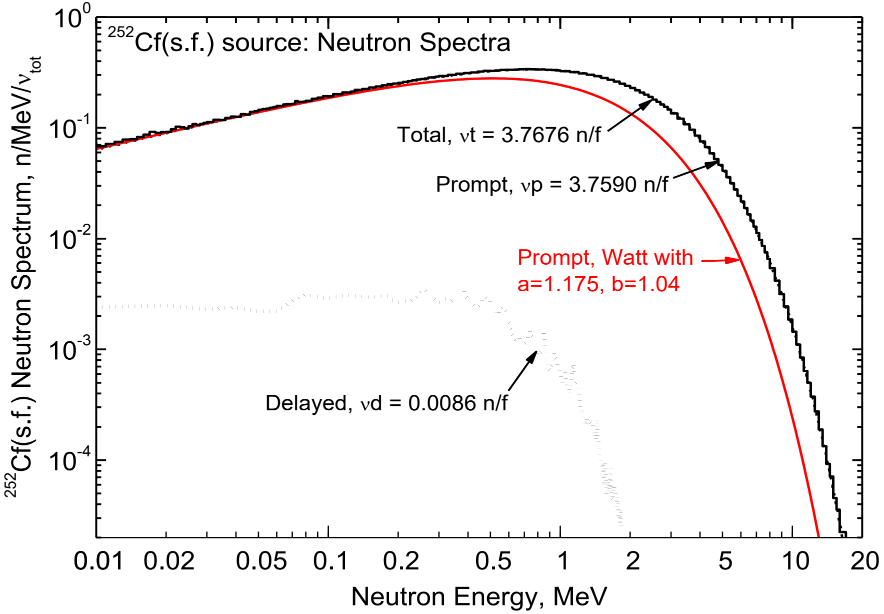
(i) simultaneously 4 particles (n_p , n_d , γ_p , γ_d)
- with proper Multiplicities (ν_p , ν_d , M_p , M_d)
- and proper Energy Spectra (which are read-in from external files):
  1. Prompt Fission Neutron Spectrum (PFNS) = Standards
  2. Delayed Fission Neutron Spectrum (DFNS) = ENDF/BV-VIII.1
  3. Prompt Fission Gamma Spectrum (PFGS) = GMA Fit to PFGS
  4. Delayed Fission Gamma Spectrum (DFGS) = Stoddard'65

(ii) or alternatively (combining Prompt and Delayed gammas in Total)
- simultaneously 3 particles (n_p , n_d , γ_t)
- with proper Multiplicities (ν_p , ν_d , M_t)
- and proper Energy Spectra (which are read-in from external files):
  1. Prompt Fission Neutron Spectrum (PFNS) = Standards
  2. Delayed Fission Neutron Spectrum (DFNS) = ENDF/BV-VIII.1
  3. Total Fission Gamma Spectrum (TFGS) = GMA fit to TFGS

Specific Modification of input for ^{252}Cf(s.f.) as source of Neutrons

1. one Watt neutron distribution (in IPPE 1st deck) was replaced by two energy spectra:
   - PFNS from Neutron Standards and
   - DFNS from ENDF/B-VIII.1

2. Neutron Multiplicities are taken from Standards or ENDF/B-VIII.1



I.1 IPPE Pb spheres: upgrade of ^{252}Cf(s.f.) source for sampling by MCNP - (ii) for emission of gammas

Modification of MCNP input for ^{252}Cf(s.f.) as a source Gamma

2nd original MCNP input deck serves for transport of ^{252}Cf(s.f.)gamma.
It has Total FGS from library ABBN-93 (*we did not find detailed information*).

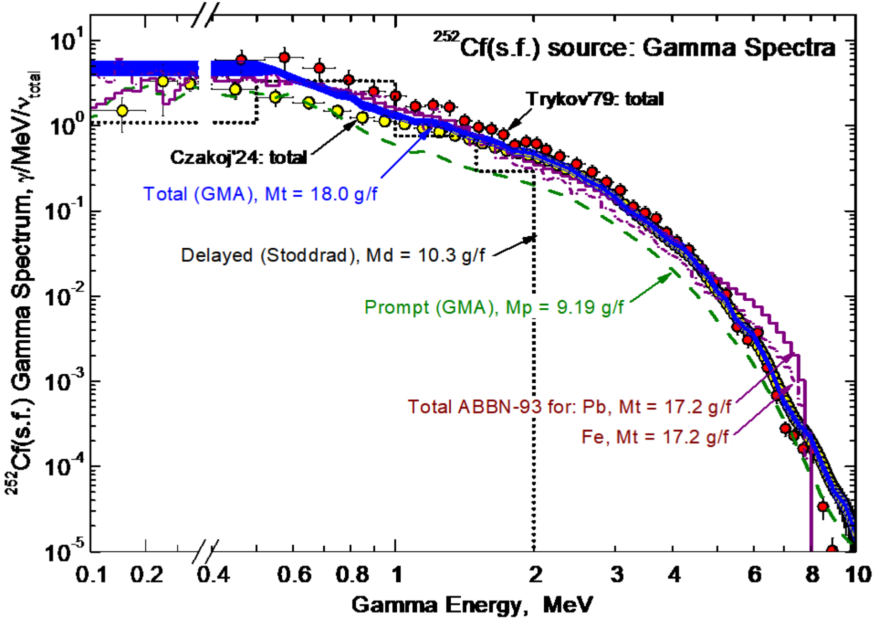
Instead of ABBN-93 we use either 2 gamma spectra:
- **PFGS from GMA fit to 18 measurements of ^{252}Cf(s.f.)PFGS [1] plus**
- **DFGS from Stoddrard'65 evaluation [2]**

or 1 gamma spectra:
- **TFGS from GMA fit to scarcely measured ^{252}Cf(s.f.)TFGS [3]**

Neutron Multiplicities were taken from extrapolated GMA Fits or Stoddard

[1] S.Simakov, "Evaluation of the prompt gamma-ray spectrum from spontaneous fission of ^{252}Cf", Report INDC(NDS)-0887, 2024
[2] D.H.Stoddard, "Radiation Properties of Californium-252", Report DP-986, Savannah River Laboratory, 1965
[3] S.Simakov, M.Kostal, present work, to be appeared as Report INDC(NDS)-XXX, IAEA, 2026

^{252}Cf(s.f.) Gamma Spectra

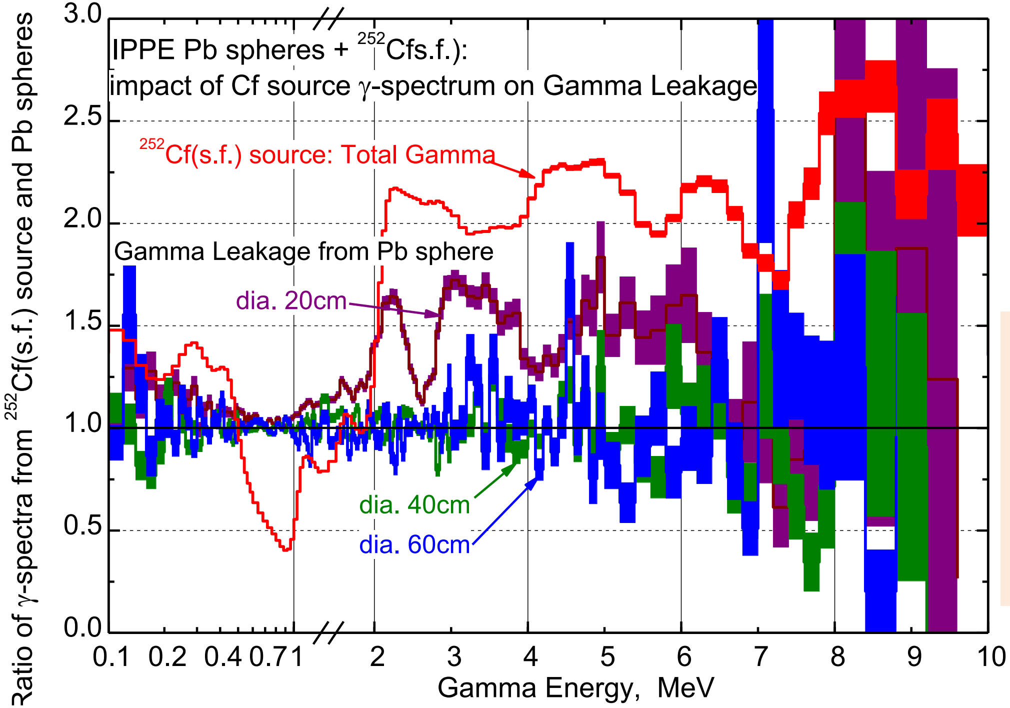


Measured ^{252}Cf(s.f.)TFGS: known 5 measurements, but only two provide enough details and g-spectrum in wide energy range ***(see overview in Report INDC(NDS)-0887, 2024):***

[2] L.A. Trykov et al., "Experimental Researches of outflow spectra of neutron and gamma radiations for spheres from Iron", IPPE-943, Obninsk, 1979
[3] T. Czakoj et al., "Measurement of total fission gamma spectrum of ^{252}Cf(s.f.)", Eur. Phys. Journ. A60 (2024) 228 .

I.1 Results of Upgrade: Impact of ^{252}Cf(s.f.)γ source on IPPE benchmark gamma leakage spectra

Ratio of gamma leakage spectra for bare Cf source and Pb spheres Ø20, 40 and 60 cm
with either (i) TFGS (= GMA fit to 5 measurements) and (ii) PFGS(GMA fit to 18 measurements) + DFGS (Stoddard)
(however gamma multiplicities were not changed)



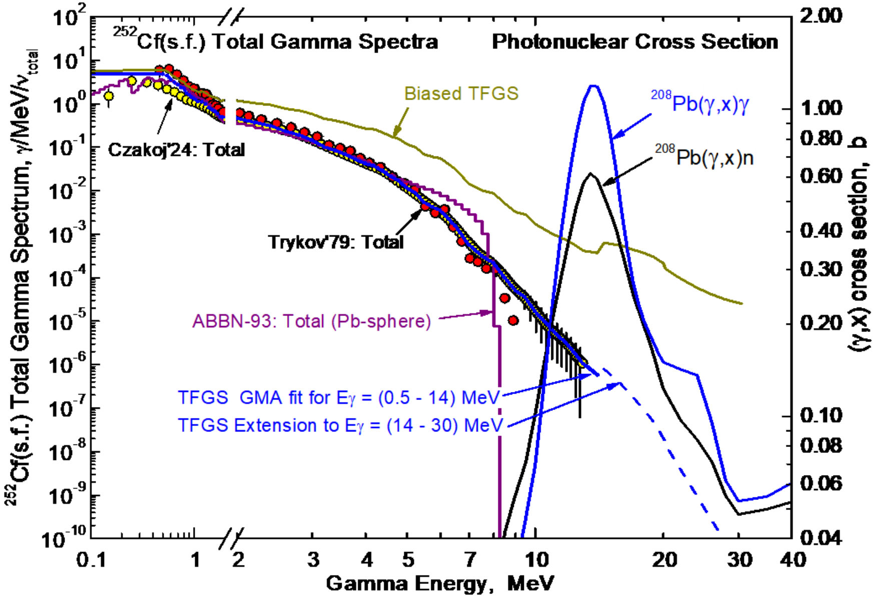
Observations - how variation of ^{252}Cf(s.f.)TFGS shape impact on:

(i) bare Cf source - total gamma spectrum is
- **systematically increased by factor of 2 above Eγ ≈ 2 MeV**
- **variations around unity below this energy**

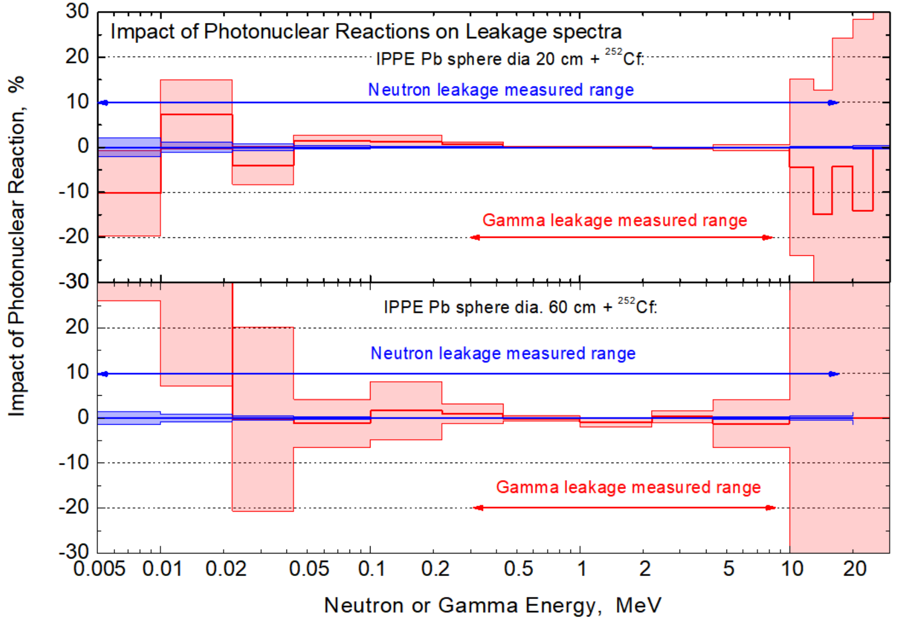
(ii) Pb spheres – gamma leakage spectrum is
- **for Ø20cm - increased by factor ≈ 1.5 for interval Eγ = 2 - 7 MeV**
- **for Ø40 and 60cm - impact becomes statistically not significant**

I.1 Results of analysis: ^{252}Cf(s.f.) γ-spectra and Photo-Nuclear (PN) reaction Impact on leakage spectra

^{252}Cf(s.f.)TFGS and photo-nuclear (PN) reaction cross sections:



Impact of PN reactions on Neutron and Gamma leakage spectra from Pb spheres of Ø20 and Ø60 cm:



<u>What is seen</u>:

^{252}Cf(s.f.)TFGS overlaps with Pb(γ,x) cross sections above 10 MeV,
=> hence attenuation of g-flux in Pb sphere and production of PN neutrons and gammas are possible
(but not in case of ABBB-93 TFGS)

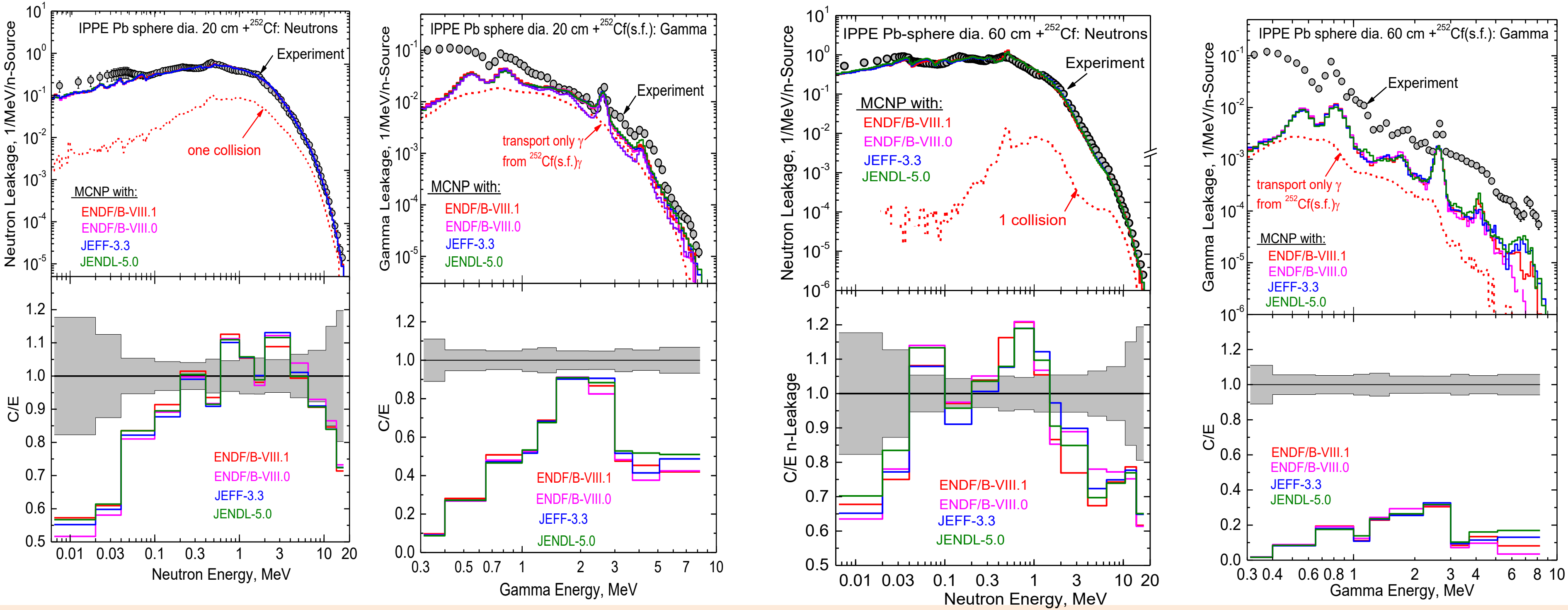
<u>The changes found in leakage spectra from Pb spheres for</u>:

- **neutrons: ≤ 0.1% in measured range En = 0.005 - 17 MeV**
- **gammas : ≈ -10% in energy domain Eγ = 10 - 20 MeV (only Ø20cm Pb)**
  ≤ 1% in measured range Eγ = 0.03 – 8.25 MeV

NB: PN impact is << Experimental Uncertainties, hence could be neglected

I.1 Evaluated data validation Results: Neutron and Gama leakage from IPPE Pb spheres with ^{252}Cf(s.f.)

Pb sphere Ø20 cm: *(Pb sphere Ø40 cm is not displayed)* **Pb sphere Ø60 cm:**

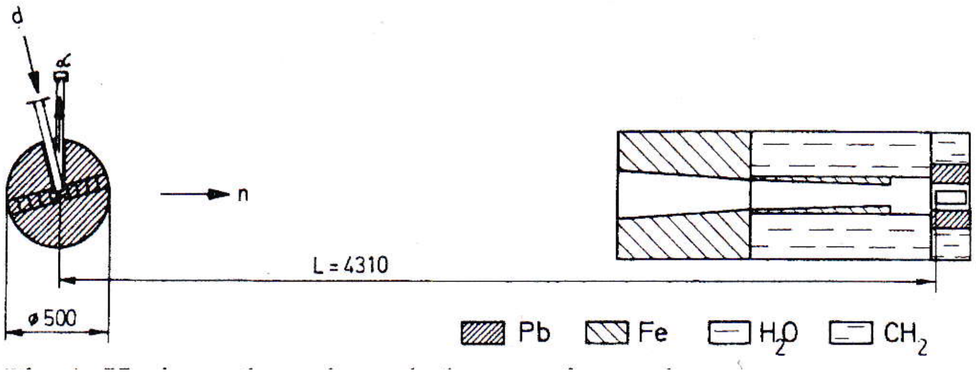


What was found:

- all libraries (ENDF/B-VIII.1, ENDF/B-VIII.0, JEFF-3.3, JENDL-5) demonstrate similar performance for n- & g-leakage spectra and for all 3 Pb spheres
- C/E for leaking neutrons: agreement within 1 - 2 experimental uncertainties only in middle of energy spectra, i.e. from ≈ 0.1 MeV to ≈ 4 MeV, but large underestimation 30 - 50% at lower (<0.1 MeV) or higher energies (for En > 3 - 10 MeV, it increases as Pb sphere becomes thicker).
- C/E for leaking gammas: is < 1.0 for all spheres (local maximum around 1 - 3 MeV or near most intensive discrete line 2.615 MeV from ^{208}Pb(n,n')γ), moreover underprediction factor increases from 2 to 5 as diameter of lead sphere increases from 20 to 60 cm.
- Fraction of first collided neutrons and primary ^{252}Cf(s.f.) gammas decreases as Pb sphere diameter increases

I.2 TUD (Dresden) Ø50 cm Pb sphere benchmark with D-T source: overview

Set-up of TUD Pb sphere benchmark with 14 MeV source:



Benchmark most important specifications:

- Years of measurements: 1984 - 1987
- Pb sphere of outer diameters 50 cm
- Neutron Source: thick TiT target + 130 keV d-beam with counting of associated α-particles
- Neutron detectors (at distance 431 cm, Θ = 106°):
  - Stilbene and NE-213 viewed by PMs, PSD, En > 1 MeV
  - Proton Recoil Spectrometer (PRS), En < 1 MeV
- Reaction rate (on Pb sphere outer surface):
  - 8 Activation foils
  - 5 Fission chambers (covered by Cd)
- Measuring Methods:
  - TOF spectrometry of
  - differentiation of PRS pulse height distribution
  - room-return background was calculated by MCNP
- Measured energy range:
  - neutron spectra from 0.01 to 17.0 MeV
  - reaction rate (SACS) for 12 reactions with kinematic threshold from 0 or 10 MeV

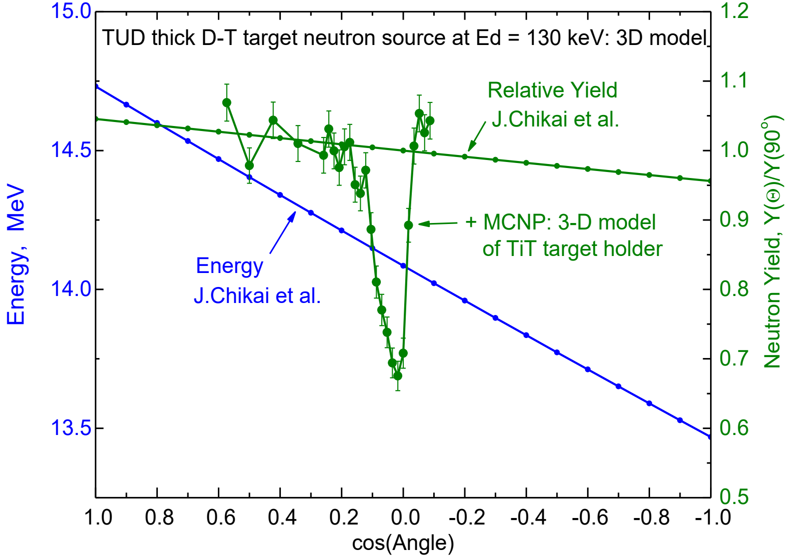
Availability of Information:

- Benchmark specifications (Pb sphere, …), Measured numerical data (D-T source & Leakage n-spectra, Reaction Rates), Refs. (but no input deck) are now available from dedicated IAEA/FENDL database in Entry FENDL-2 BENCHMARKS SUBLIBRARY [.DRESDEN.PB]
- Authors and main publications: T. Elfruth, D.Seeliger, K.Seidel et al., "The neutron multiplication of Lead at 14 MeV neutron incidence energy", Atomkernenergie Kerntechnik 49(1987)121

I.2 TUD (Dresden) Ø50 cm Pb sphere benchmark with D-T source: our modifications and verifications

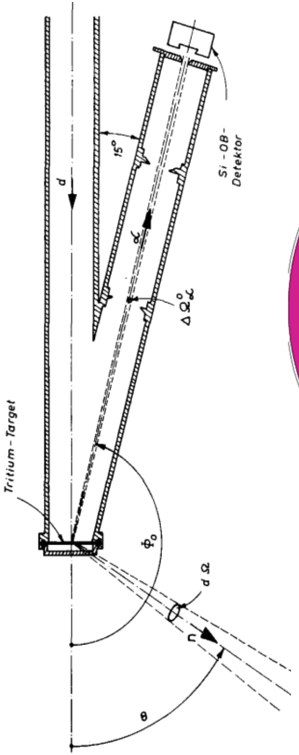
Elaboration of 3-D MCNP input deck for TUD Pb benchmark
(with guessing of several parameters not given by experimenters):

- **real Geometry and Materials for D-T source ("Holder"): thick TiT target, water cooling, SS tubes for d-beam and a-particles**
- **real Geometry of Cavity in sphere for accommodation of target Holder**
- **Angular dependence of "14MeV" Energy and Yield from thick TiT target:**

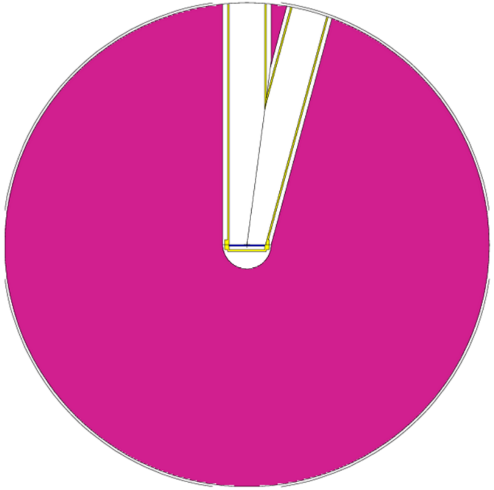


J.Csikai et al. Report IAEA-TECDOC-410, 1987, p.296

given in TUD docs:



Implemented now in 3-D input deck:



I.2 TUD (Dresden) Ø50 cm Pb sphere benchmark with D-T source: TOF correction and verifications

Verification of the energy distribution from bare D-T source

- **reasonable agreement between MC simulation with our 3-D model and TUD measured spectrum is achieved**

Analysis TOF correction for TUD Pb benchmark

(time-of-flight method (TOF) used to measure neutron leakage energy spectra from bulk spherical assemblies could result to necessity of applying of correction)

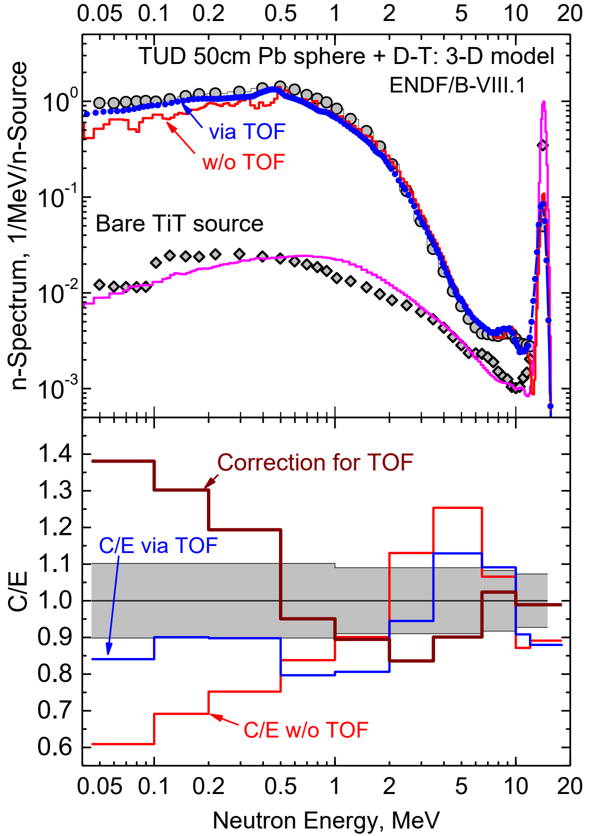
We calculated two spectra by MCNP employing 3-D model and ENDF/B-VIII.1:
- **labelled as "w/o TOF" is MCNP energy tally,**
- **labelled as "via TOF" is MCNP time tally, then transformed into energy one**

Then Ratio "via TOF"/"w/o TOF" is a correction which should be applied to experimental energy spectrum before comparison with energy distribution calculated without real travel time consideration

We found that TOF correction for TUD Ø50 cm Pb benchmark is:
- **significant as neutron energy decreases below 0.5 MeV but**
- **comparable with experimental uncertainty above 0.5 MeV.**

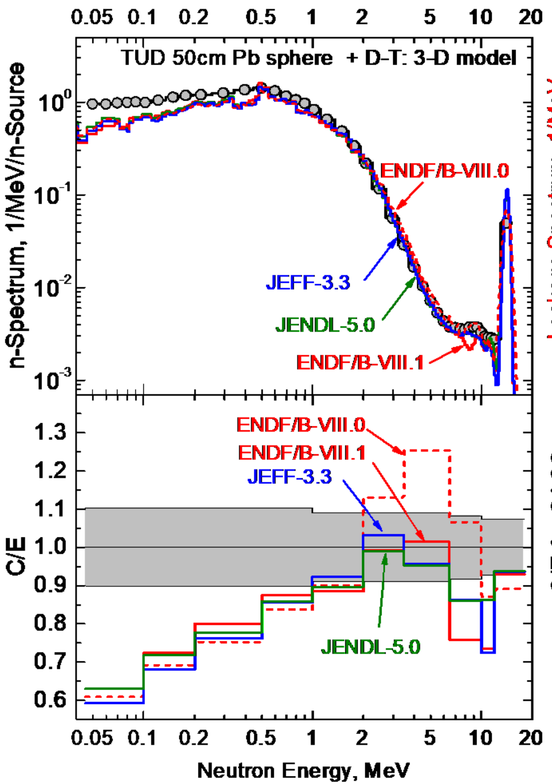
Regarding this and since neutron leakage spectrum was measured by TOF only above ≈ 0.90 MeV (at lower energies - by time-independent proton recoil spectrometry), we neglected Impact of TOF technique and corresponding TOF correction.

Bare D-T neutron source spectrum and Ø50cm Pb leakage spectra w and w/o TOF correction

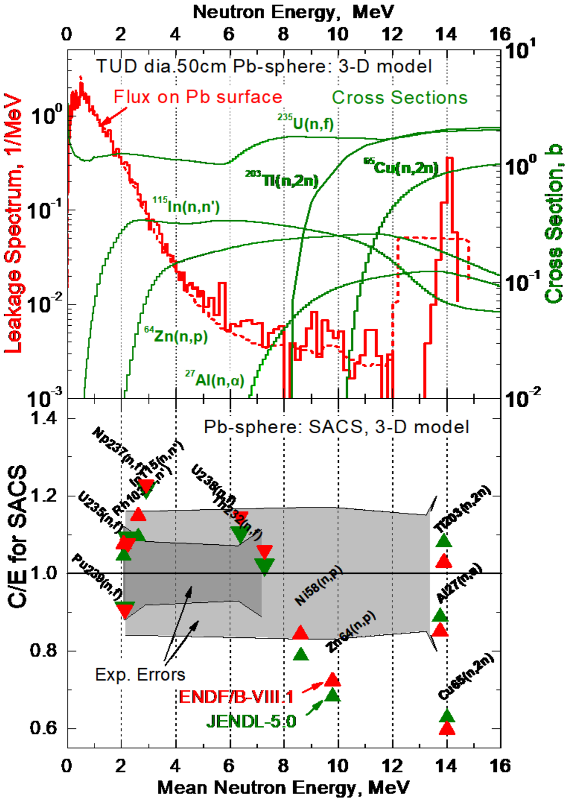


I.2 Evaluated data validation Results: Neutron leakage from TUD Ø50cm Pb sphere with D-T source

Neutron Leakage Spectrum at 431 cm from Pb sphere center:



Activation and Fission SACS on the outer surface of Pb sphere:



What was found:

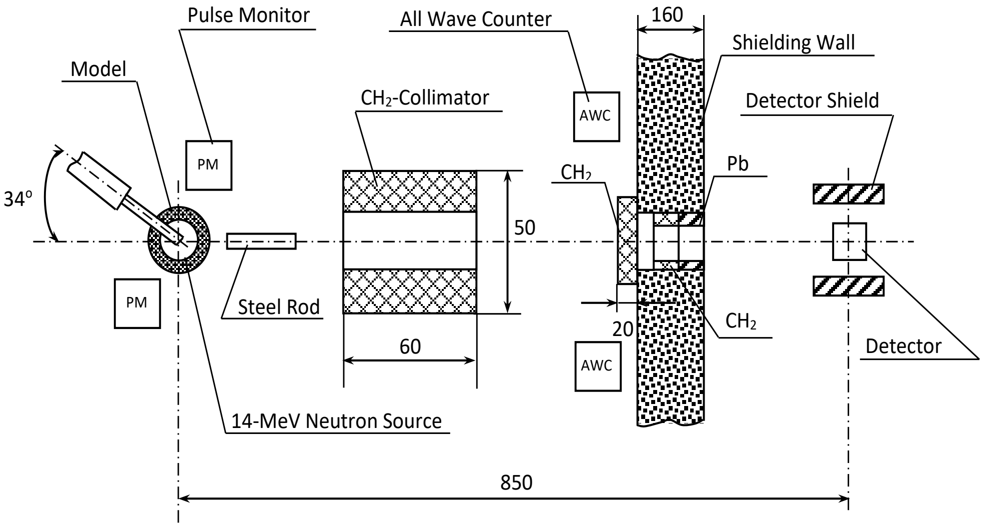
1. C/E for Neutron leakage spectrum:
   - 40 - 10% underestimation below 1 MeV and
   - agreement (one/two exp. Uncertainty) at higher energies.

   Libraries ENDF/B-VIII.1, JEFF-3.3, JENDL-5 demonstrate similar performance, except ENDF/B-VIII.0: too large yield in 4 – 6 MeV.

2. SACS for Activation/Fission reactions (XS from IRDFF-II):
   - C/E with <E>=2–14MeV confirm trend for leakage spectum
   - SACS outlier:
     1. ^{237}Np(n,f): C/E ≈ 1 + 25%, <E> = 2.9 MeV.
        Since C/E contradicts with other SACS (having similar <E>) and C/E for leakage spectrum (in bin 1.0 - 3.5 MeV), we suppose that ^{237}Np(n,f) measurement has systematic bias or uncertainty larger than declared 8.2%.
     2. ^{65}Cu(n,2n): C/E ≈ 1 - 40%, <E> = 14.0 MeV.
        We also suppose that TUD' measurement had some deficiency.
   - ^{203}Tl(n,2n) is from ENDF/B-VIII.1 (not included in IRDFF-II). However, we have satisfactory C/E = 1.0 - 1.1 (or within 20% exp. uncertainty) for all neutron transport libraries.

I.3 VNIITF (Snezhinsk) Ø20 cm Zr & Pb (back hemi-) sphere benchmark with D-T source: overview

Set-up of VNIITF (hemi-)sphere benchmark with 14 MeV source:



Benchmark most important specifications:

- Years of measurements: ≈ 1991 - 2002
- Pb & Zr (back hemi-) spheres of inner/outer diameter 10/20 cm
- Neutron Source: thick ZrT target and ≈190 keV d-beam
- Radiation Detectors (at distance 850 cm and Θ = 34°):
  n: Stilbene Ø7 × 7 cm + PM, PSD, Ethr_n = 0.25 MeV
  g: Stilbene Ø6 × 6 cm + PM, PSD, Ethr_g > 0.35 MeV
- Measuring/Processing Methods:
  - TOF spectrometry for neutrons
  - Unfolding of pulse distributions for gammas
  - Efficiencies of Detectors were measured & MC simulated
  - Steel rod Ø3 × 40 cm between D-T source and detectors
  - room-return background was calculated by MCNP
- Measured energy range of leaking radiations:
  - neutron spectra from 0.40 to 18.0 MeV
  - gamma spectra from 0.37 to 7.39/8.16 MeV for Zr hemi/sphere
    from 0.37 to 7.39/7.96 MeV for Pb hemi/sphere

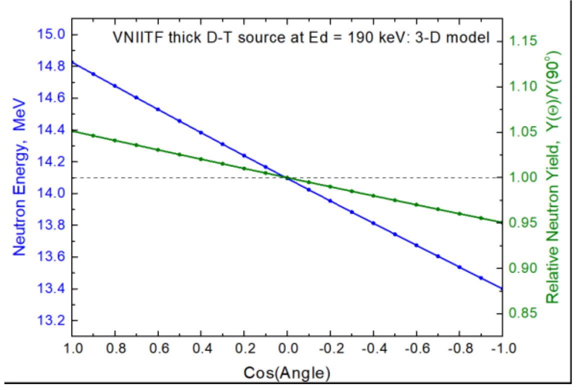
Availability of Information:

- Benchmark set-up, Pb and Zr sample specifications, Measured numerical data (only g Leakage spectra, no Neutron spectra), Ref., 1-D model only for Fe sphere (can not be used since do not contains 40 cm long SS rod and other details) are available now in SINBAD NEA-1517/74: "Measurement of photon leakage spectra from spherical and hemispherical samples of Al, Ti, Fe, Cu, Zr, Pb, 238U with a central 14-MeV neutron source", NEA Data Bank, 1992.
- Authors & main publications: A.I.Saukov et al., "Measurements of neutron and photon leakage from spherical and hemispherical samples with a central 14-MeV neutron source as a possible type of benchmarks", Int. Conf. Rad. Safety ICRS10 – RPS-2004, May 2004, Madeira.
  A.I.Saukov et al., "Photon leakage from spherical and hemispherical samples with a central 14-MeV Neutron Source", NSE 142 (2002) 158.

I.3 VNIITF (Snezhinsk) Ø20 cm Zr & Pb (back hemi-) sphere benchmark with D-T source: elaborated 3-D model

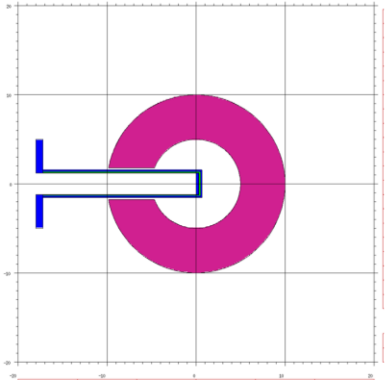
VNIITF MCNP 3-D model (but not available) accounted for:	Elaborated 3-D model
• Ang. dependence of neutron Yield (±6%) & Energy (±0.6MeV) for D-T	Yes
• size of neutron-emitting area of radius 1 cm	Yes
• deuteron tube geometry	Yes
• Cu-flange on d-tube and tube-holder pedestal behind sample (are significant for four lighter materials used in experiment)	No
• Shielding Steel Rod	Yes
• Fe-container (0.5mm thick) for samples of fragmented materials	No

Angular depence of neutron Yield and Energy for thick D-T target

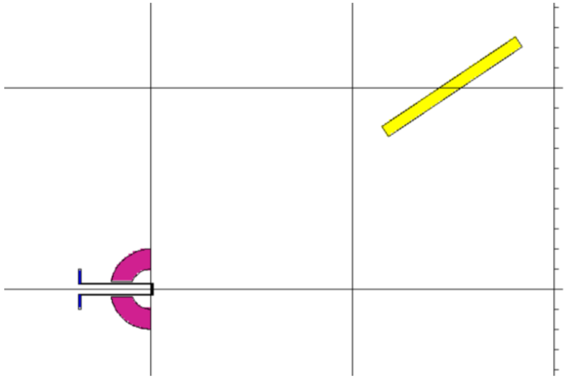


J.Csikai et al. Report IAEA-TECDOC-410, 1987, p.296

D-T holder and Cavity in Pb or Zr spheres (our 3-D)



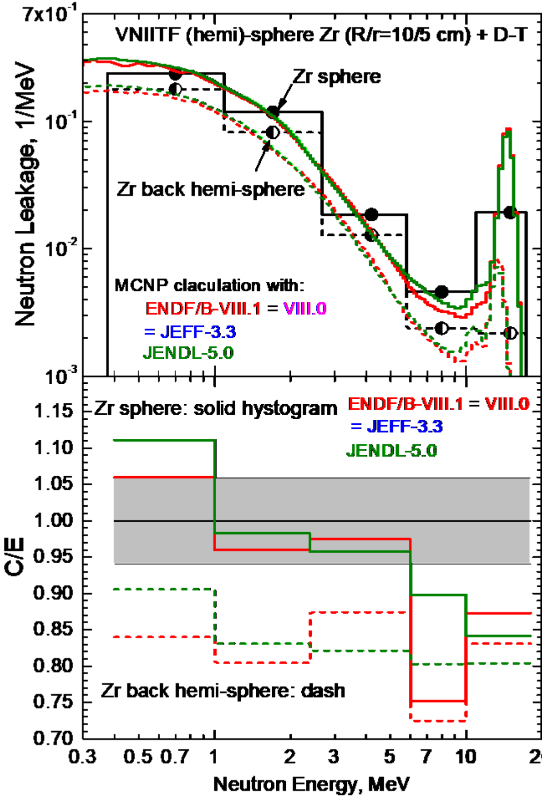
D-T holder, Cavity in Pb or Zr back hemi-spheres, SS rode (our 3-D)



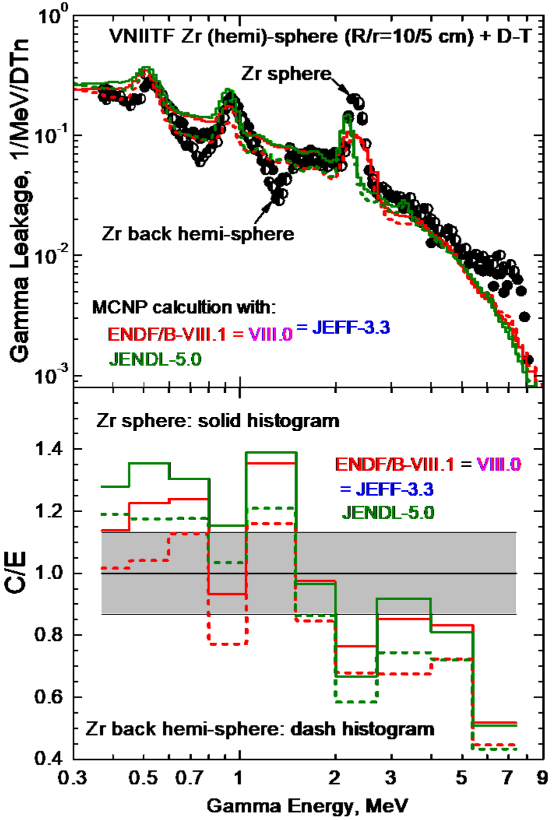
I.3 Evaluated data validation Results: Neutron & Gamma leakage from VNIITF Zr (hemi-)spheres with D-T source

Zr sphere and back hemi-sphere of outer Ø20 cm:

Neutron Leakage



Gamma Leakage



Results of Validation for Zirconium
(note: ENDF/B-VIII.1, ENDF/B-VIII.0 and JEFF-3.3 are identical for Zr isotopes)

Neutron leakage spectra

- ***from Zr sphere:***
  En ≤ 6 MeV – reasonable reproduction (within 1-2 exp. uncertainty or by 6 - 12%) by all tested libraries,
  En ≥ 6 MeV - underestimation by 10 - 25%
- ***from Zr hemi-sphere*:**
  whole energy range - underestimation by ≈ 10 - 25% and by all tested evaluations

Gamma leakage spectra *from sphere and hemi spheres:*

Eg ≤ 5 - 6 MeV (or practically in whole energy range)
- reproduction within 1-2 exp. uncertainties or 13 - 26% by all considered libraries

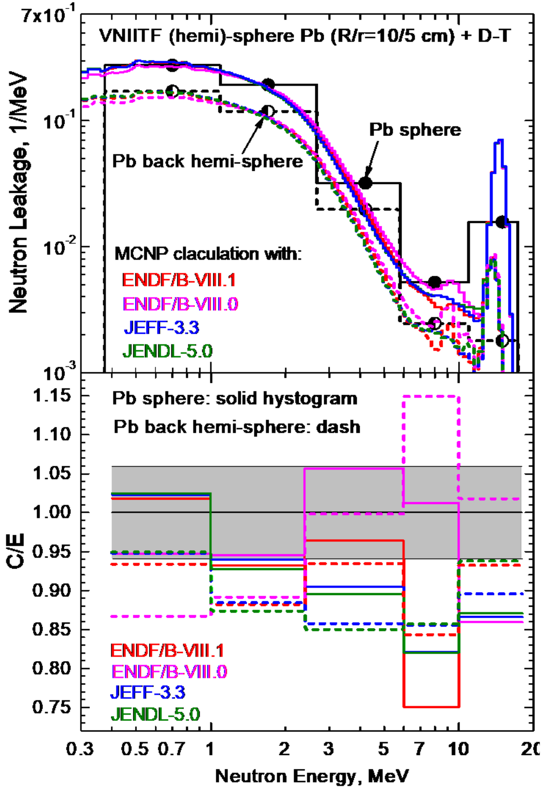
Eg ≈ 5 - 7 MeV - underestimation by ≈ 50%

ENDF/B-VIII.1 slightly better performs than JENDL-5.0

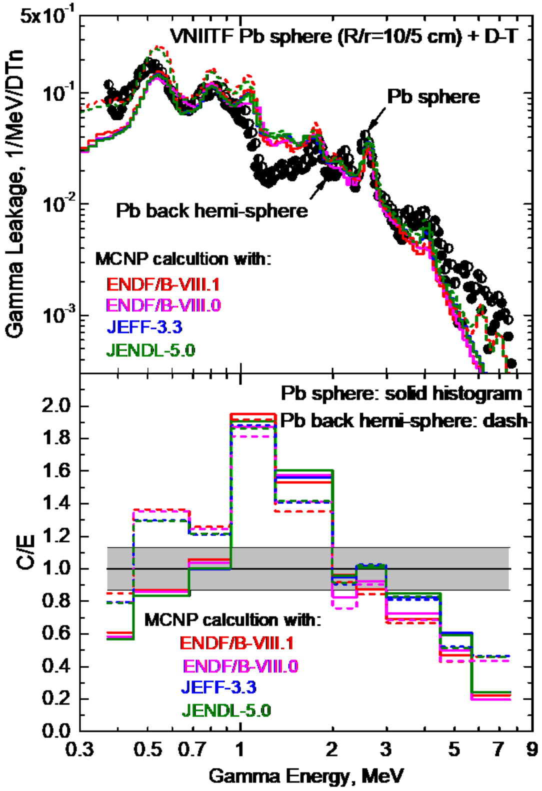
I.3 Evaluated data validation Results: Neutron & Gamma leakage for VNIITF Zr & Pb (hemi-)spheres with D-T source

Pb sphere and back hemi-sphere of outer Ø20 cm:

Neutron Leakage



Gamma Leakage



Results of Validation for Lead

Neutron leakage spectra

- ***from Pb sphere:***
  En ≤ 6 MeV – are reproduced (within 1-2 exp. Uncertainty or by 6 - 12%) by all tested libraries,
  En ≈ (6 – 10) MeV – evaluations are scattered within 25% (ENDF/B-VIII.0 looks better),
  En ≈ 14 MeV – are underestimated by ≈ 15% by all libraries.
- ***from Pb hemi-sphere*:**
  for all En – moderate underestimation by ≤ 5 -15% (En ≈ (6 – 10) MeV ENDF/B-VIII.0 > VIII.1 by 30%)
  En ≈ 14 MeV – all libraries better perform than for whole sphere

Gamma leakage spectra *from Pb sphere and hemi spheres:*

Eg = (1 – 2) MeV – overestimation by 50 - 100%,

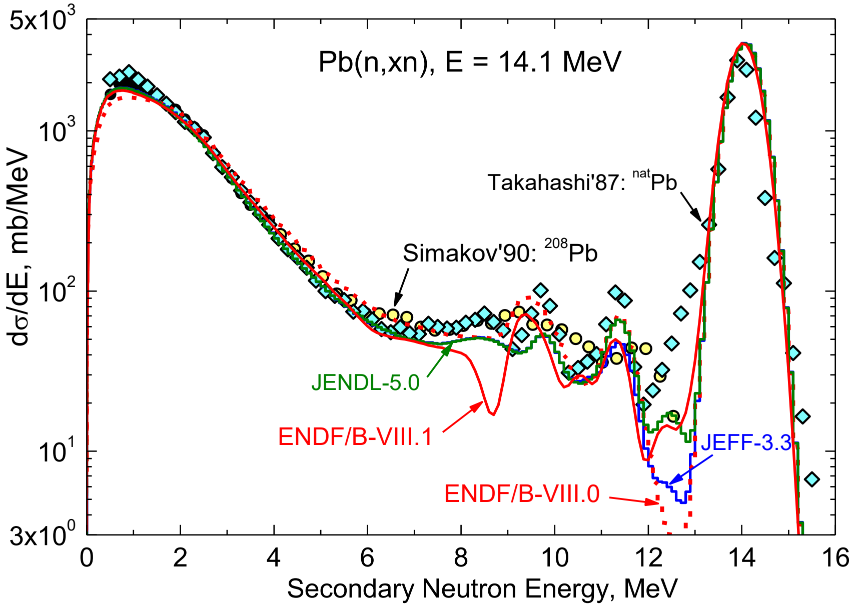
Eg ≥ 5 MeV – underestimation by 40 - 80%,

Eg = (0.37 – 0.9) MeV and (0.37 – 0.9) MeV – agreement within 1 - 2 exp. uncertainties or 13 - 26% by all considered libraries.

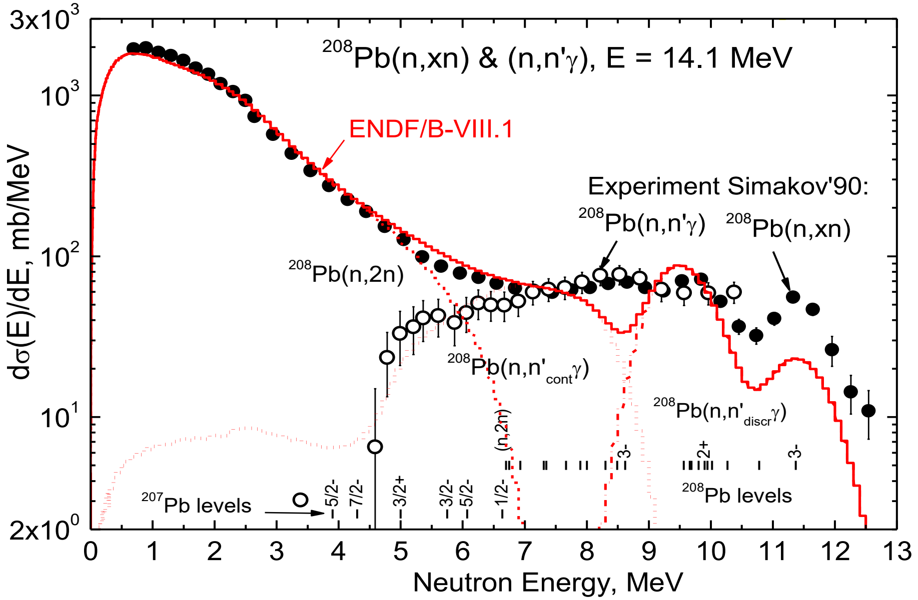
II.1 Performance of tested Evaluations for (n,x)n and (n,x)γ emission cross sections for Pb

^{nat}Pb(n,x)n Secondary Energy Distribution (SED) of Neutrons at E ≈ 14 MeV

^{nat}Pb(n,x)n



^{208}Pb(n,x)n and ^{208}Pb(n,n'γ) (n' coincident with Eγ = 2.615 MeV)



^{nat}Pb(n,x)n SED at 14 MeV (relevant for D-T benchmarks):

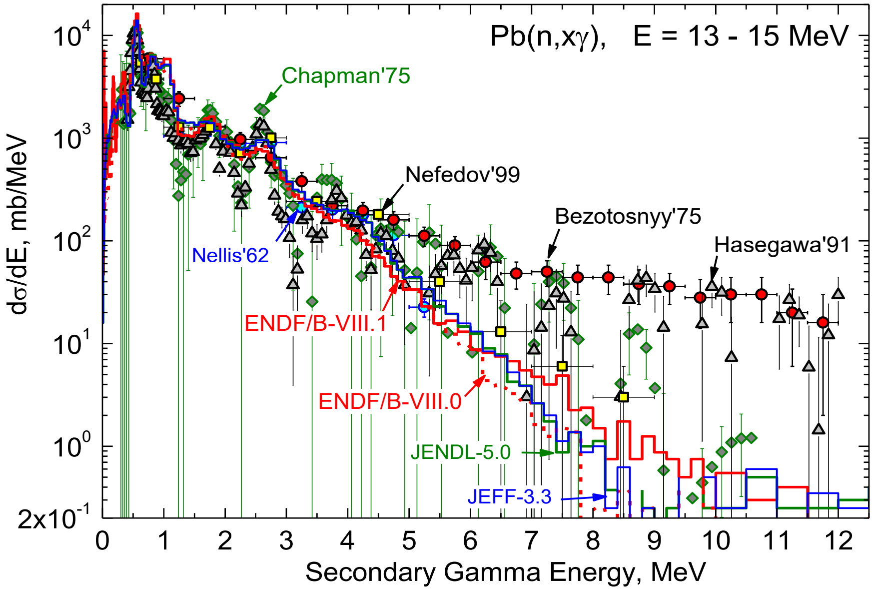
En ≤ 6 MeV – all tested libraries equally well represent SED (ENDF/B-VIII.0 > VIII.1 for En = 4 - 12 MeV - also seen in TUD Pb benchmark, *slide 13*)

En ≥ 6 MeV – all tested libraries more differ each other and, as a rule, underpredict measurements (could be a reason for moderate ≈ 10 – 20% underprediction of neutron leakage in energy interval 7 - 12 MeV observed in TUD and VNIITF benchmarks, *slides 13 and 17*)

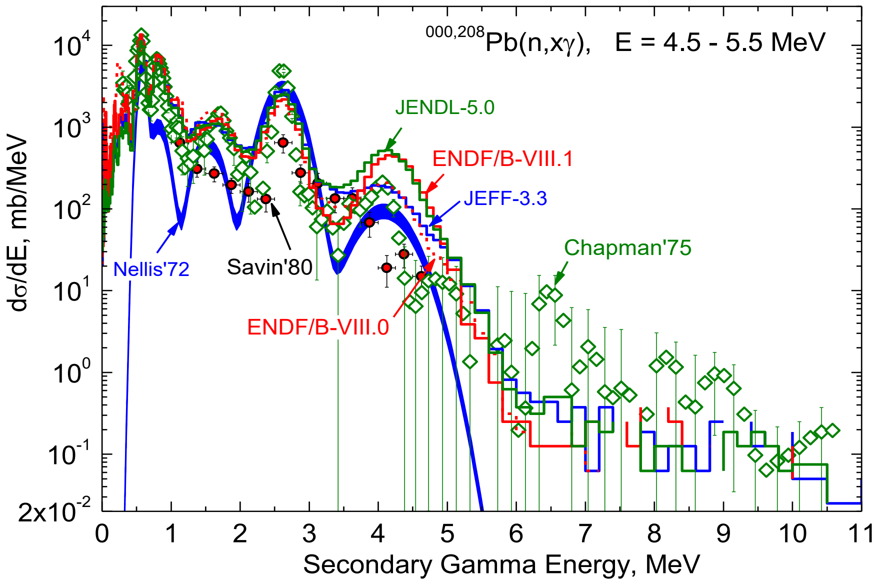
II.1 Performance of tested Evaluations for (n,x)n and (n,x)γ emission cross sections for Pb

^{nat}Pb(n,x)γ Secondary Energy Distribution (SED) of Gammas at E ≈ 14 MeV and lower E

^{nat}Pb(n,x)γ at E ≈ 14 MeV



^{nat,208}Pb(n,x)γ at E ≈ 4.5 - 5.5 MeV



^{nat}Pb(n,x)γ SED at 14 MeV (relevant for D-T benchmarks):

Eγ ≤ 5 MeV – all tested libraries equally and reasonably represent gamma emission spectra

Eγ ≥ 5 MeV – all tested libraries tend to follow the lowest measurements, which start to scatter up to order of magnitude

(underestimation for Eγ ≈ (5 - 7) MeV was also observed in VNIITF Ø20cm Pb (hemi-)spheres with all tested evaluations, *Slide 17*)

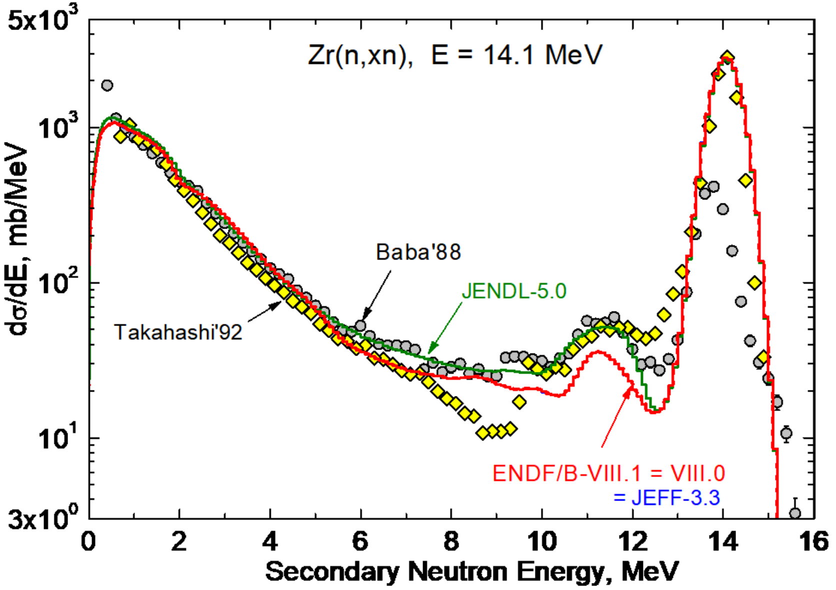
^{nat}Pb(n,x)γ SED at 4.5 -5.5 MeV (relevant for Cf benchmarks):

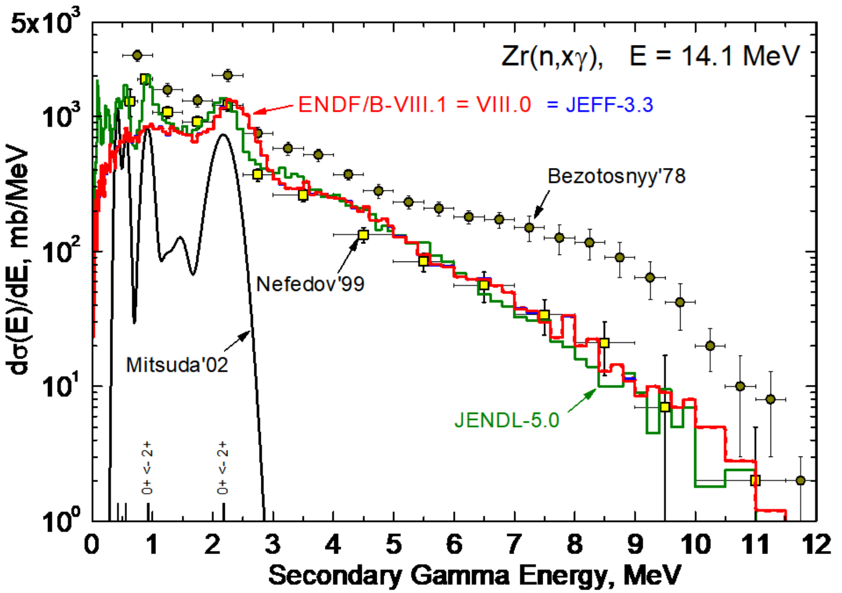
Eγ ≤ 6 MeV - tested evaluated libraries generally agree with experimental results (but pay attention to their large scattering)

Eγ ≈ (6 - 11) MeV - we probably can state that all evaluations still underestimate the single (!) existing experiment

II.2 Performance of tested Evaluations for (n,x)n and (n,x)γ emission cross sections for Zr

^{nat}Zr(n,x) Secondary Energy Distribution (SED) of Neutrons and Gammas at E ≈ 14 MeV





^{nat}Zr(n,x)n SED at 14 MeV (relevant for D-T benchmarks, neutron leakage):

En ≤ 5 MeV – JENDL-5 and ENDF/B-VIII.1 reasonably represent measured neutron spectrum
En ≥ 5 MeV – JENDL-5 is higher than ENDF/B-VIII.1 and probably better agrees with measurements (however only two measurements which scatter)
JENDL-5.0 is also more preferable for VNIITF Ø20cm Zr sphere leakage spectrum in range En ≈ (6 - 10) MeV, Slide 16

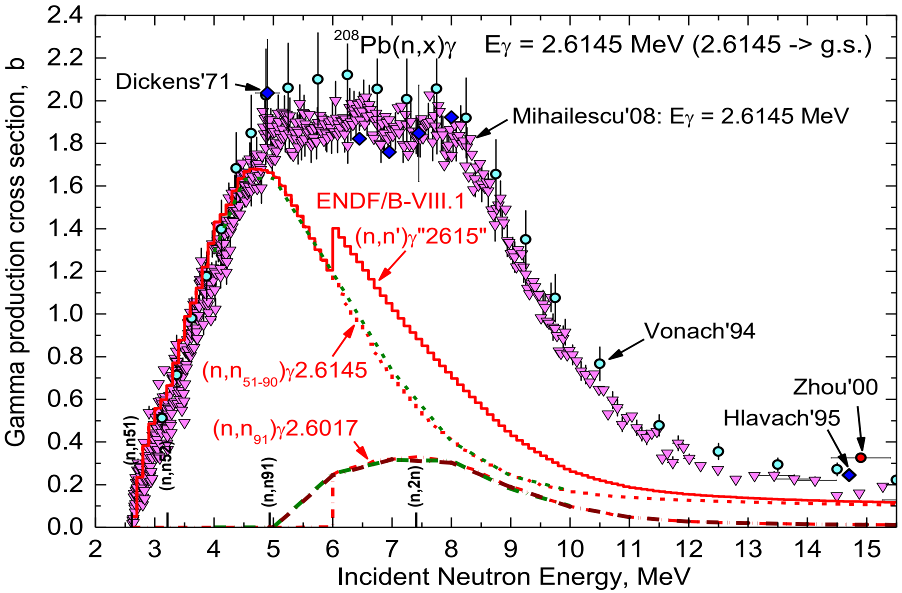
^{nat}Zr(n,x)γ SED at 14 MeV (relevant for D-T benchmarks, gamma leakage):

Eγ ≤ 5 MeV – JENDL-5 and ENDF/B-VIII.1 are similar, except E < 1 MeV (the lower ENDF/B-VIII.1 γ-SED is more preferable to VNIITF Ø20cm Zr γ-leakage spectrum)
Eγ ≥ 5 MeV – JENDL-5 and ENDF/B-VIII.1 follow the lowest measurement, which is systematically lower than the second (only two experiments were done !)
(underestimation in Eγ ≈ (5 - 7) MeV was also observed in VNIITF Ø20cm Zr (hemi-)spheres (*Slide 16*) => require increasing of SED(Eγ ≥ 5 MeV)

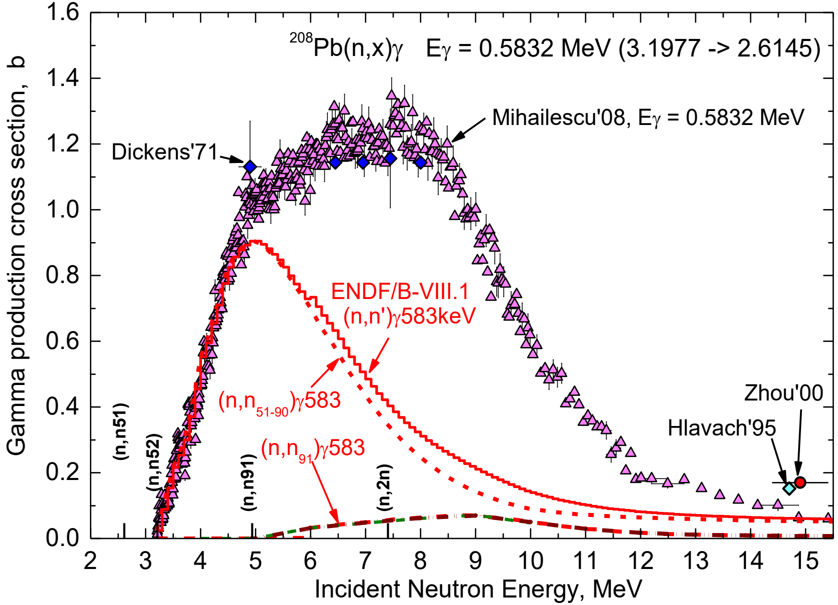
II.3 Performance of ENDF/B-VIII.1 for (n,x)γ discrete gamma cross sections for ^{208}Pb: XS vs. incident Energy

^{208}Pb(n,x)γ Production Cross Section of Discrete Gammas from threshold to E ≈ 15 MeV (relevant for IPPE Pb sphere with Cf source)

^{208}Pb(n,x)γ: Eγ ≈ 2.6145 MeV



^{208}Pb(n,x)γ: Eγ ≈ 0.5832 MeV



FYI: discrete γ cross sections were extracted from ENDF/B-VIII.1 by: NJOY (red dash curve), directly from endf-file (red point-dash) or by MCNP (green dash)

For dominant isotope ^{208}Pb and strongest discrete gammas Eγ = 2.614 and 0.583 MeV from ^{208}Pb(n,n')γ, ENDF/B-VIII.1 performs as:

Eγ ≤ 5 MeV, or up (n,n91) threshold – well represents production XS as a sum of de-excitation of 40 levels populated by (n,n51 - 90)

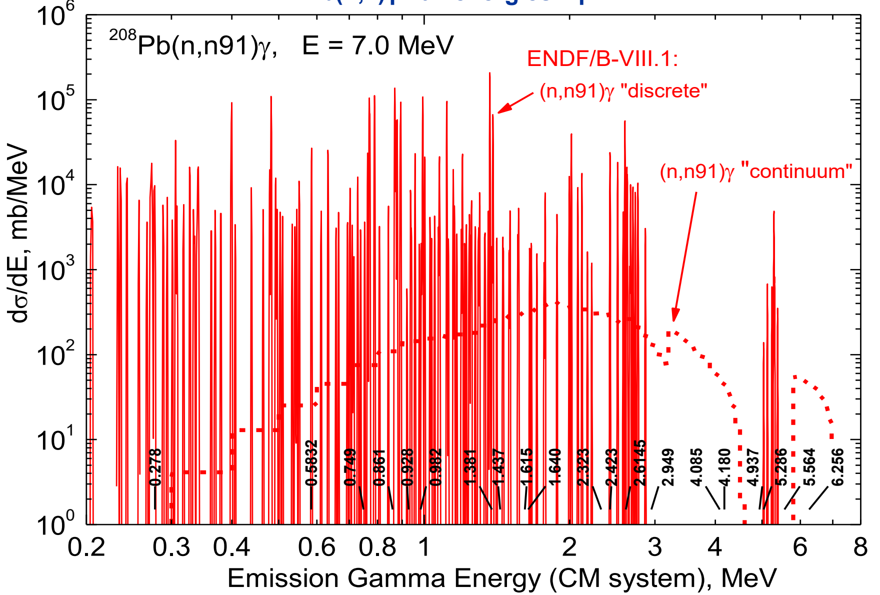
Eγ ≥ 5 MeV – underpredicts by several times (NB: may improve underestimation for Eγ ≤ 3 MeV observed in IPPE Ø20-60cm Pb spheres (?!), see *Slide 9*)

Why ENDF/B-VIII.1 is too low above (n,n91) threshold ? - consider gamma-continuum representation in ENDF/B-VIII.1 on next slide →

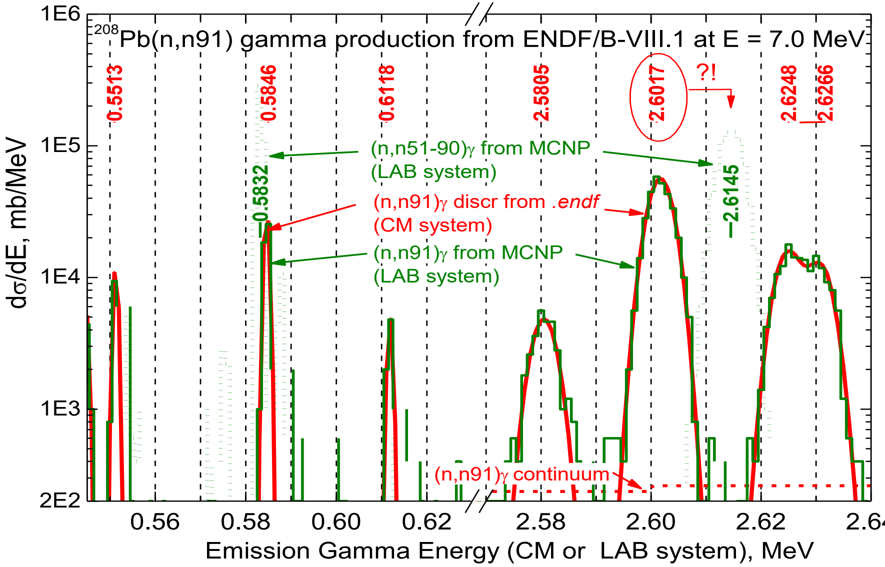
II.3 Performance of ENDF/B-VIII.1 for (n,x)γ discrete gamma cross sections for ^{208}Pb: Gammas from Continuum

^{208}Pb(n,x)γ Energy differential emission Cross Section of discrete and continuum Gammas at E ≈ 7.0 MeV (plateau of XS)

^{208}Pb(n,x)γ: all energies Eγ



^{208}Pb(n,x)γ: 2 fragments around Eγ ≈ 0.5832 and 2.6145 MeV



***<u>Left-hand Figure: Photons from (n,n91) are stored in MF/MT=6/91 as energy-angle distribution (CM) for</u>*:**

(1) discrete photons (delta functions) tabulated in decreasing energy order

(2) continuum distribution tabulated in increasing energy order (negligibly contribute to strongest discrete 2.6145 or 0.5832 MeV)

<u>Right-hand Figure: Spectrum two fragments 0.560 - 0.620 MeV and 2.570 – 2.640 MeV:</u>

(discrete γ were extracted from endf-file directly (red histogram) or by MCNP (green histogram) and were folded with typical HPGe rel. energy resolution 0.2%):

Eγ = 2.6017 MeV (MF6/MT=6/91, CM) is shifted by 12.8 keV (!!?) from "real" 2.6145 MeV (LAB) (note that HPGe resolution ≈ 5 keV)

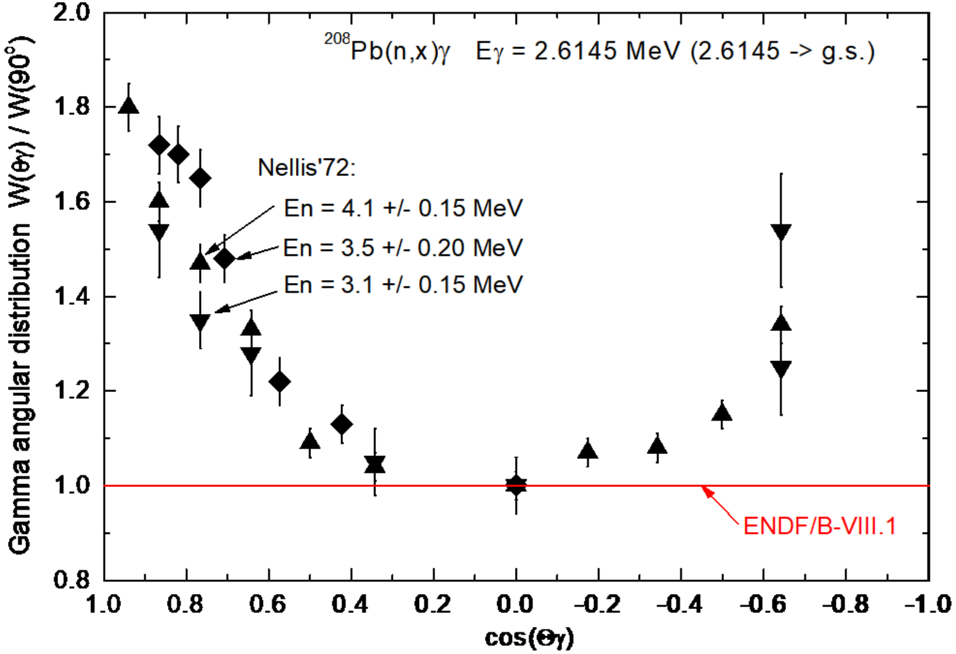
Eγ = 0.5846 MeV (MF6/MT=6/91, CM) is shifted by 1.4 keV (OK) from "real" 0.5832 MeV (LAB) (note that HPGe resolution ≈ 1 keV)

<u>Summary</u>: Shift of discrete gammas Energies and Absolute Yields should be corrected (i.e., adjusted to measurements shown in previous Slide)

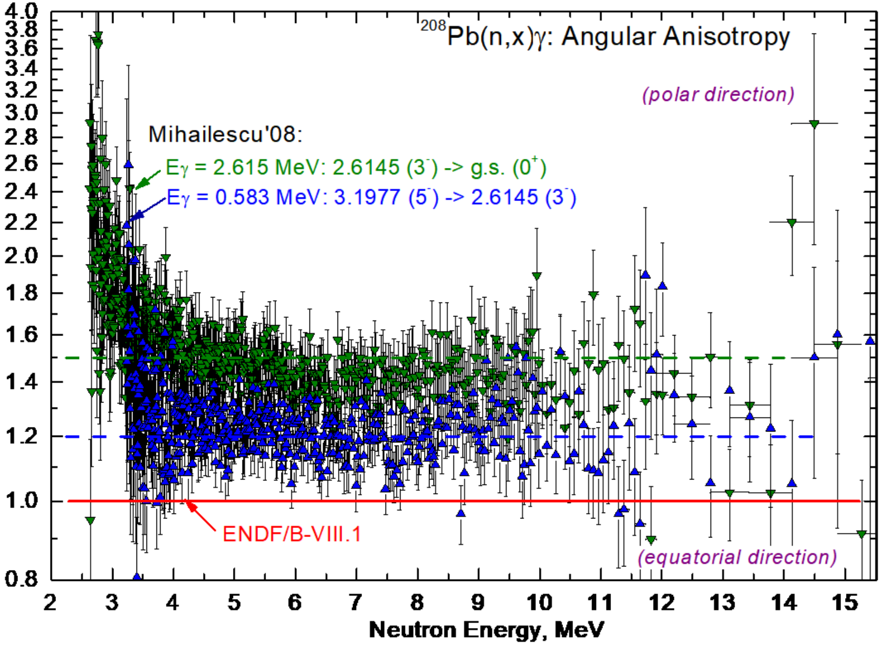
II.4 Performance of ENDF/B-VIII.1 for (n,x)γ discrete gamma cross sections for ^{208}Pb: Gamma Angular Distribution

^{208}Pb(n,x)γ Angular Distributions of strongest Discrete Gammas

^{208}Pb(n,x)γ: W(Θ) for Eγ = 2.6145MeV at E = 3.1, 3.5, 4.1 MeV



^{208}Pb(n,x)γ: W(Θ) for Eγ = 0.5832 and 2.6145 MeV from threshold to 15 MeV



^{208}Pb(n,x)γ: W(Θ) for discrete 2.615 and 0.583 MeV gammas from threshold to 15 MeV (relevant for sphere benchmarks with Cf source):

- **ENDF/B-VIII.1: isotropic angular representation of (all) gamma emission**
- **Experiment: polar directed at all relevant incident neutron energies, W(Forward Angles) / W(90) ≈ 1.5 – 1.2**

Conclusion: ENDF/B-VIII.1 isotropy could be an additional source of underestimation of gamma leakage for Pb spheres with Cf source, since polar anisotropy will result to increasing of gamma emission in first neutron collision towards escaping from sphere (for at least γ-energies ≤ 2.615 MeV)

III. Conclusions

1. IPPE Ø20,40,60cm Pb spheres with Cf source = most well documented/compiled (in ICSBEP) benchmark among considered here
   - we modified/improved sample 1-D MCNP input deck provided by IPPE authors:
     - more detailed 3-D set-up: Cf containers, cavity in spheres, all impurities in Pb;
     - physics: ^{252}Cf(s.f.) is represented as source of PFNS + DFNS and PFGS + DFGS or TFGS (preliminary GMA fit)

       => measurements of γ spectra are required to get reliable T(D)FGS and to explain why TFGS/PFGS(Eγ ≥ 2MeV) ≈ 2 ?
   - MC simulation show: underestimation of (i) neutron leakage by ≤ (30 - 50)% and (ii) gamma leakage - by factor (0.7 – 10) in whole energy range
   - Analysis of ENDF/B-VIII.1 for ^{208}Pb show: (i) underestimation of production of strongest discrete gammas 2.615 and 0.583 MeV by factor (2 – 3) and (ii) isotropic angular representation instead of polar directed observed experimentally
2. TUD Ø50 Pb sphere with D-T source = documented/compiled on dedicated IAEA/FENDL site
   - since no MCNP input deck was found we elaborated/verified our 3-D (and also 1-D):
     - set-up: thick T target in holder tubes for d-beam and associated alphas, Pb sphere with dock hole;
     - physics of D-T source: angular dependence of neutron Energy and Yield,

       and verification against measured angular energy distributions for bare D-T source.
   - MC simulation show: (i) underestimation of neutron leakage by ≈ (40 - 10)% below 1 MeV and by 10 - 30% in (6 – 10) MeV

     (ii) SACS which have Emean ≈ (2 – 14) Me V confirm this but with two exceptions
   - Analysis of Pb(n,x)n SED show: (i) tested libraries in high energy part of SED, 6 to 12 MeV, as a rule, underpredict measurements
3. VNIITF Ø20 cm Pb and Zr (hemi-)spheres with D-T source = documented in SINBAD (only gamma but no neuron leakage spectra)
   - since only 1-D MCNP input deck for Fe sphere was found we elaborated/verified our 3-D:
     - set-up: thick T target in holder tubes for d-beam, Pb sphere with dock hole, SS rode between D-T source and detector;
     - physics of D-T source: angular dependence of neutron Energy and Yield, with minor verifications
   - MC simulation show: (i) neutron leakage - agreement within 1-2 std at most energies with tendency to underestimate in (6 - 10) MeV

     (ii) gamma leakage - underestimation of high energy part Eg ≥ 5 MeV by 40 - 80%
   - Analysis of Pb and Zr(n,x)n SED show: (i) tested libraries in high energy part of n-SED, 6 to 10 MeV, as a rule, underpredict measurements

     Analysis of Pb and Zr(n,x)γ SED show: (i) tested libraries in high energy part of γ-SED, Eγ > 5 MeV, follow the lowest measurements, which are significantly scattered and scarce