

**SINBAD new/updated Entries:
KFK γ -ray leakage and ORNL O-broomstick neutron transmission**

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33rd WPEC/SG47 Meeting, 11 May 2021 (via Zoom)



Goal/content = to present the progress/implementation of Actions 2 and 3 from the latest SG47 Meetings:

- actions from Summary records of latest WPEC/SG47 Meetings: [NEA/NSC/WPEC/DOC\(2020\)20](#) 12 May 20 + [NEA/NSC/WPEC/DOC\(2019\)8](#) 24 June 2019
- completion of our work reported at SG47: "KIT contribution to SG-47: progress since June 2019" 12 May 2020 + "Remarks from use of SINBAD" 24 June 2019

Action 2. (S. Simakov, KIT):

"Provide KFK-1977 gamma measurement data for potential SINBAD evaluation",
"SINBAD evaluation of KFK-1977 Fe gamma measurements"

Action is completed, i.e.:

- γ -ray leakage spectra for three Fe spheres (shared by S.H.Jiang in Feb 2019) were after analysis/corrections uploaded (Oct 2020) on <https://nds1.gitlab.io/nds/index.html>
- New SINBAD Entry [NEA-1517/??](#) (since KFK n-leakage entry [NEA-1517/43](#) (KFK_FE) is already exist) is created, which includes:
 - KFK-abs.html, KFK-exp.html, relevant publications ...
 - assembled MCNP model input deck
 - Evaluation Report with necessary details, experiment quality assessment, validation analysis and recommendations what should be done else

NB: Evaluation Report was reviewed by S.H. Jiang in Apr 2021; many thanks to him for his data sharing, communication ...

briefly about all this - next slides 3 - 9

Action 3. (S. Simakov, KIT):

"Quality review of Oxygen ORNL broomstick benchmark (and 91.44 cm liquid O)"
"Contribute models for Oxygen ORNL broomstick benchmark and 91.44cm liquid O data if of interest (sufficient quality) for SINBAD"

Action is completed, i.e.:

- Existing SINBAD Entry [NEA-1517/59 \(ST2\)](#) for ORNL/TSR-II 60" (152.4 cm) O-broomstick was upgraded, which now includes:
 - assembled MCNP model input deck
 - Evaluation Report with necessary details, validation analysis and recommendation what could be done else
- Experimental data for another thicknesses 24" (60.96 cm), 36" (91.44 cm) and probably 72" (182.88 cm) were not found

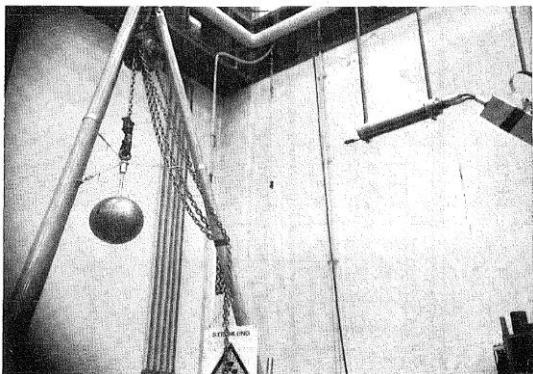
NB: thanks to H.T. Hunter (ORNL/RSICC) for seeking missing experimental data, consultations, discussions ...

briefly about all this - next slides 10 - 17

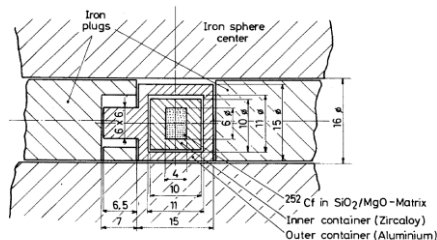
I. KFK Iron spheres Gamma-ray leakage spectra with Cf source in centre

KFK Fe g-ray leakage spectra with Cf source: set-up and experimental results

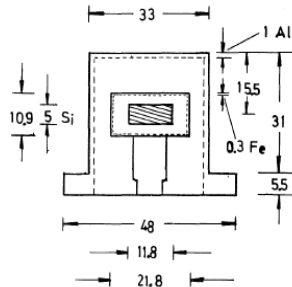
KFK set-up:



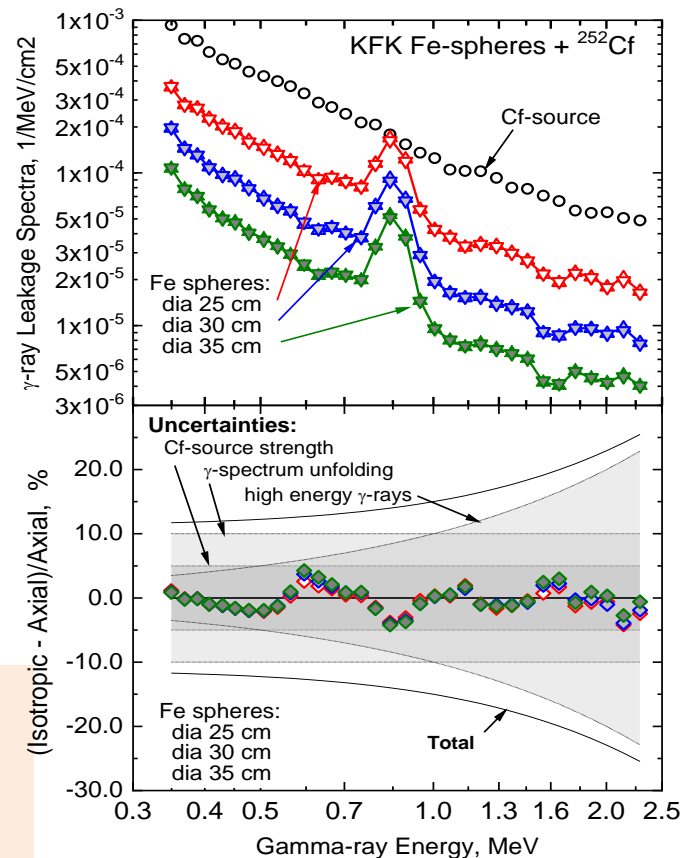
Cf-source:



Si(Li)-detector:



Exp. Results: g-ray leakage spectra and Uncertainties

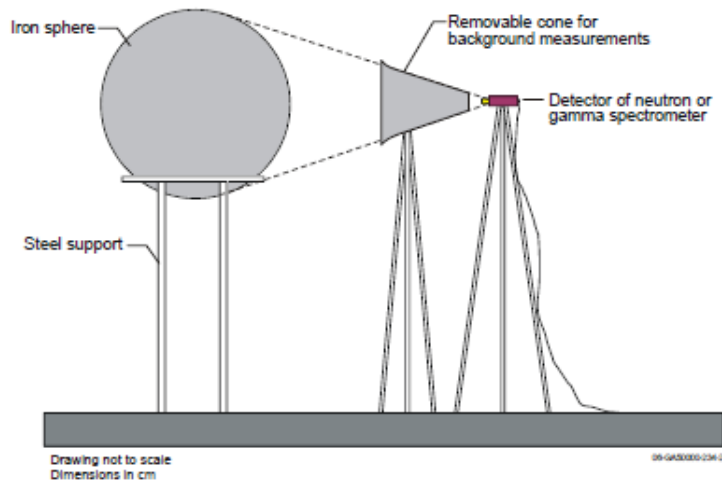


Experimental details and data:

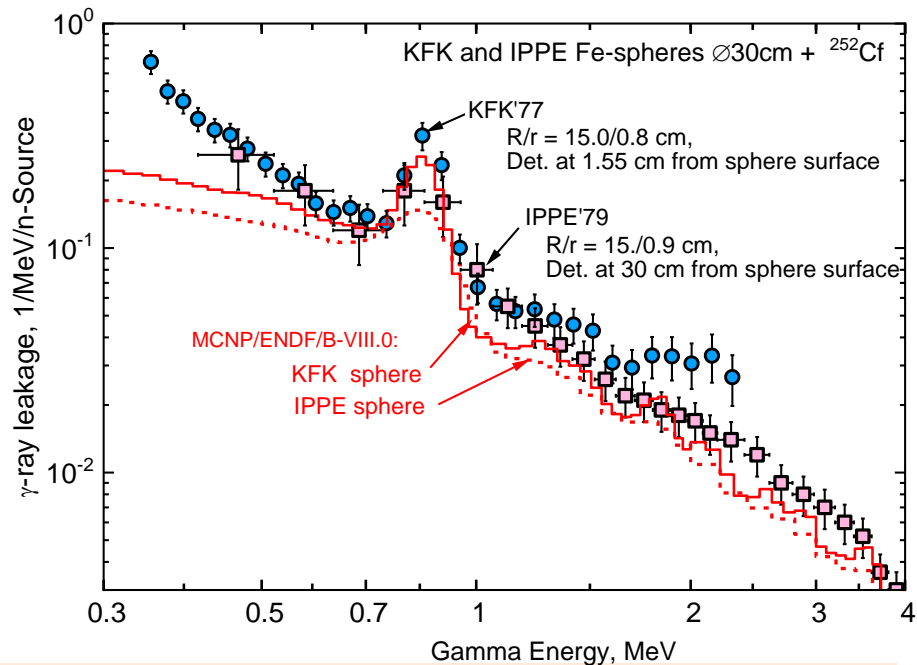
- three soft iron spheres of outer diameters: 25, 30 and 35 cm
- Compton Si(Li) detector on outer sphere surface (background thought to be negligible)
- γ -ray spectra were unfolded from Compton recoil electrons reliably in the energy range between 0.4 and 2.0 MeV
- energy spectra total uncertainties \approx (10 - 20)%, the contributing components are given

(rare case for benchmarks): Two independent experiments = γ -ray leakage spectra from Fe spheres of same $\text{\O}30\text{cm}$: KFK (S.H.Jiang ≈ 1977) vs. IPPE (L.A.Trykov ≈ 1979)

IPPE set-up:



KFK vs. IPPE: γ -ray leakage spectra from Fe $\text{\O}30\text{cm}$ with ^{252}Cf



Set-up difference between IPPE and KFK:

- IPPE has used scintillation (stilbene) detector at larger distance (unfolding of p-recoils) and measured the room returned background

Comparison for Fe sphere of equal outer diameter 30 cm:

- in overlapping interval 0.5 - 2 MeV the both experiment data agree within declared uncertainties 10 – 20%

(NB = you should take into account: MCNP calculations with ENDF/B-VIII.0 shows $\approx 10\%$ difference between KFK and IPPE benchmarks when all specific and slightly different experimental configuration details will be modelled)

Physics & MCNP input: $^{252}\text{Cf}(\text{s.f.})$ and $^{252}\text{Cf}(\alpha)^{248}\text{Cm}$ = source of (prompt & delayed) neutrons and gammas

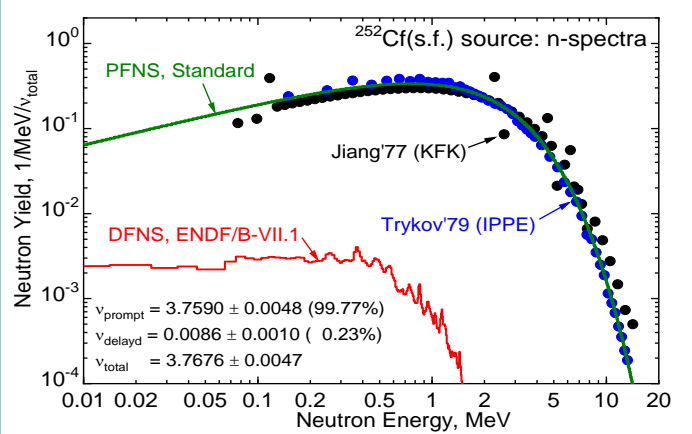
Main parameters of the neutron and γ -ray radiations from disintegration of ^{252}Cf , i.e. spontaneous fission and α -decay
 (Multiplicities are normalized per spontaneous fission event (f); origin of multiplicities energy spectra used in present simulations are referenced)

	Neutrons			Gammas		
	Multiplicity ν , n/f	$\langle E_n \rangle$, MeV	Origin of Spectrum	Multiplicity M_γ , γ /f	$\langle E_\gamma \rangle$, MeV	Origin of Spectrum
	^{252}Cf spontaneous Fission: $P_{sf} = (3.086 \pm 0.008)\%$, $T_{1/2} = (85.76 \pm 0.23)$ y					
Prompt	3.7590 [16]	2.122	Standards [25]	11.0	0.730	present work
Delayed	0.0086 [27,16]	0.464	ENDF/B-VIII [16]	10.7	0.774	Stoddard [28,29]
Total	3.7676 [26,16]			21.7		
	^{252}Cf Alpha Decay: $P_\alpha = (96.914 \pm 0.008)\%$, $T_{1/2} = (2.6470 \pm 0.0026)$ y					
Total				0.0089	0.070	DDEP [24]

← (s.f.) was sampled in MCNP

← α -decay was neglected since $= 0.0089/21.7 \approx 0.04\%$ and $\langle E_\gamma \rangle$ below threshold

Neutron prompt and delayed M and spectra are well known:



MCNP input deck: $^{252}\text{Cf}(\text{s.f.})$ n- and γ -sampling with SDEF card:

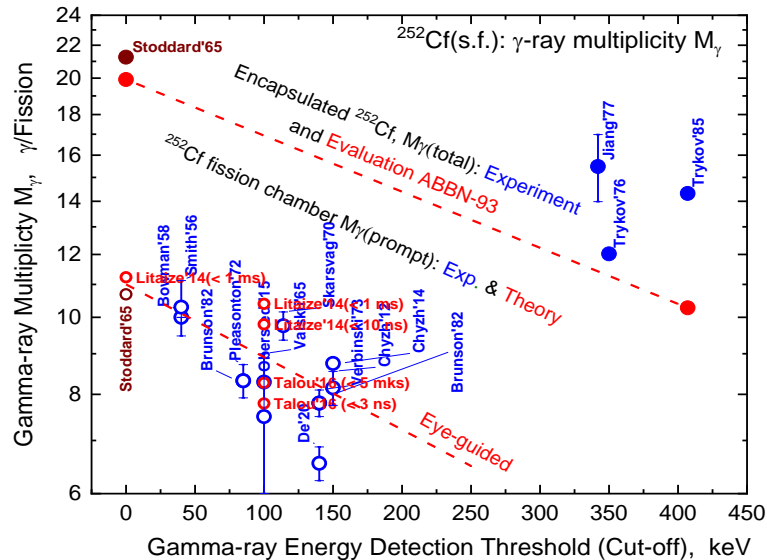
- (i) simultaneously 4 particles (n_p, n_d, Y_p, Y_d) with proper Multiplicity (see Table above)
- (ii) and proper Energy Spectra which are read-in from external files:
 - Cf252_nPrompt_725g.dat - Prompt Fission Neutron Spectrum (PFNS) in 725 groups
 - Cf252_nDelayed.dat - Delayed Fission Neutron Spectrum (DFNS) in pointwise
 - Cf252_gPrompt.dat - Prompt Fission Gamma Spectrum (PFGS) = present work
 - Cf252_gDelayed.dat - Delayed Fission Gamma Spectrum (DFGS) = Stoddard'65

selection of M_γ and γ -spectra for sampling: see next slide



Physics & MCNP input deck (cont.): $^{252}\text{Cf}(\text{s.f.})$ - as a source of prompt and delayed gammas:

Total and prompt γ -ray Multiplicities for $^{252}\text{Cf}(\text{s.f.})$ vs. γ -detection threshold



Observation from existing experimental and compiled/evaluated data for $^{252}\text{Cf}(\text{s.f.})\gamma$:

(I collected/analysed/presented this information during ≈ 4 years:

[TM INDEN 2017](#), [JEFFDOC-1851](#), [EFFDOC-1342](#), [EFFDOC-1373](#), [SG47 2019](#))

- prompt (γ -f coincidence): M_γ & Spectra were rather many measured and theoretically studied

→ at the moment we use a combination of measurement and theory as PFGS

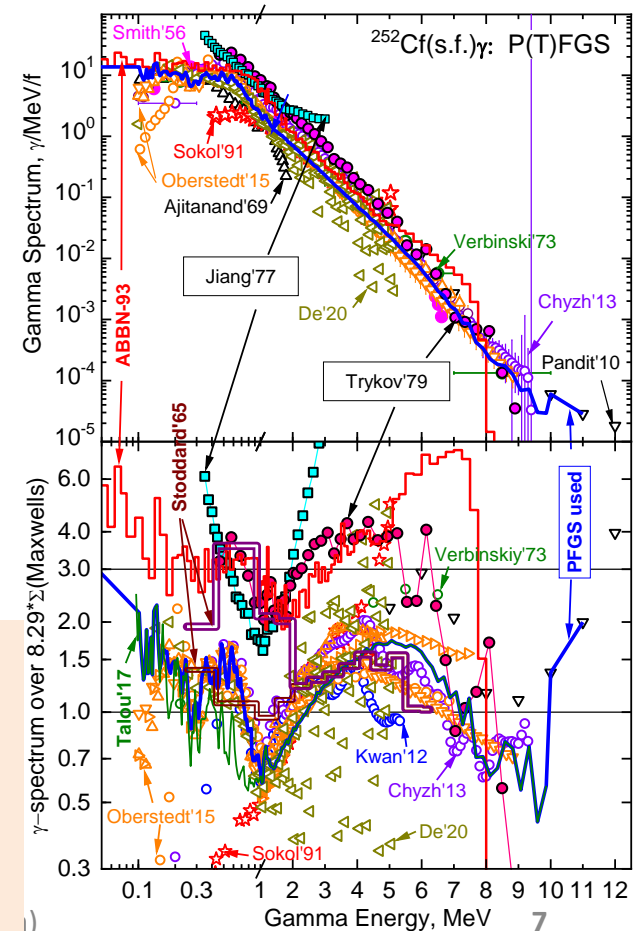
! NB: GLS fit to numerous experimental data can be done to produce a reference PFGS !

- delayed or total (encapsulated Cf): M_γ and Spectra are given by Stoddard'65 and ABBN-93

→ presently we used delayed γ -ray spectra of Stoddard'65 (since β -decay E_γ seems $< 3\text{MeV}$!)

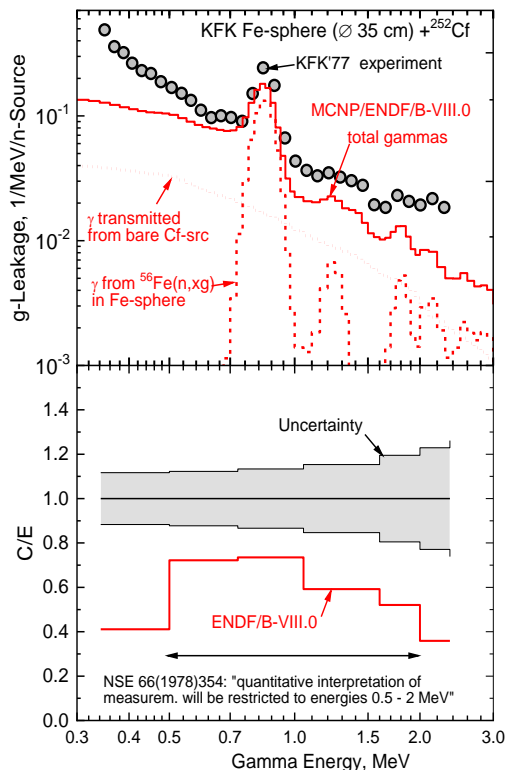
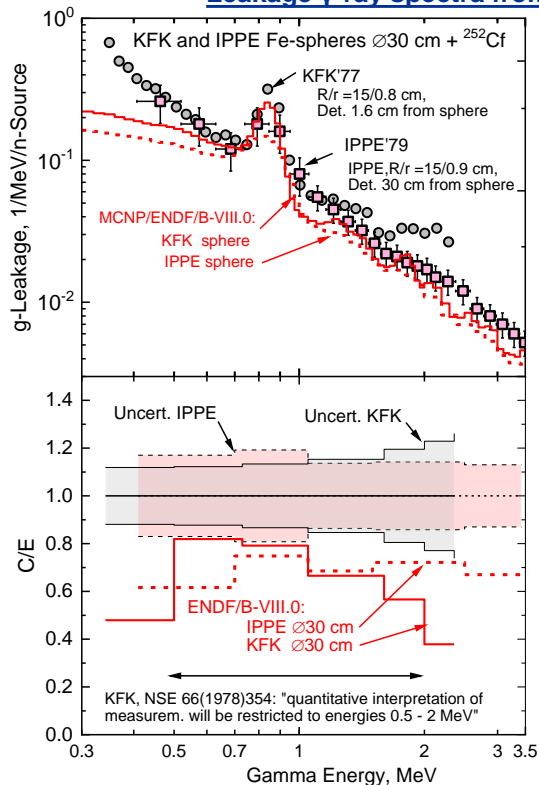
! NB: there are measurements of discrete delay γ - have to be studied to get reference DFGS !

Total and prompt γ -ray Spectra from $^{252}\text{Cf}(\text{s.f.})$

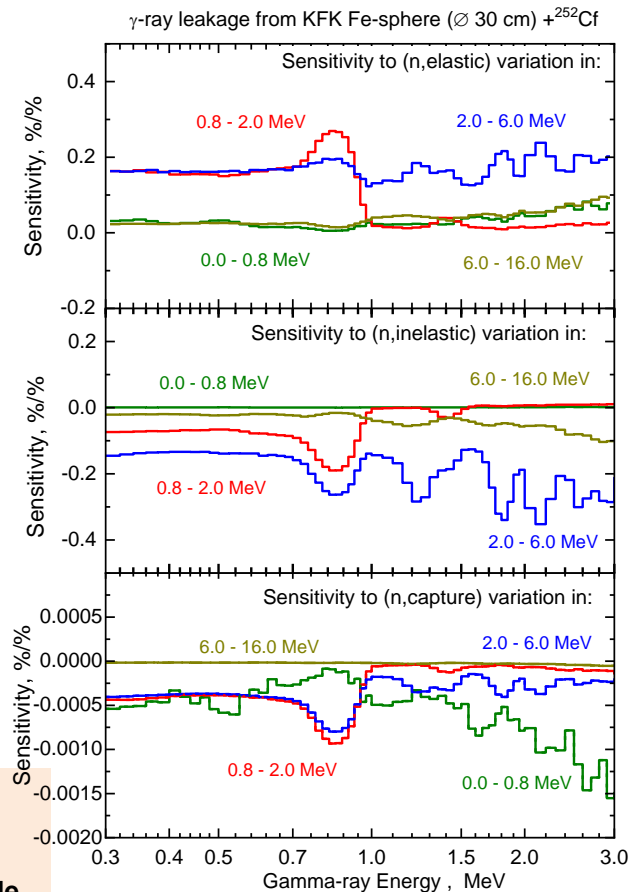


Validation example of ENDF/B-VIII.0: Fe sphere γ -leakage with $^{252}\text{Cf}(\text{s.f.})$ source (both KFK and IPPE):

Leakage γ -ray spectra from Fe spheres $\varnothing 30\text{cm}$ and $\varnothing 35\text{cm}$ and C/E



Sensitivities of KFK leakage γ -ray spectra to n+Fe XS



Validation conclusion:

- ENDF/B-VIII.0 underestimates γ -ray leakage by (20 – 40)% in energy interval 0.5 – 2.0 MeV
- it is highly likely a truth since is observed in two independent benchmarks (KFK and IPPE) and since for larger thickness ($\varnothing 35\text{cm}$) the direct contribution from Cf(s.f.) γ becomes negligible
- sensitivity profiles can probably help to find a reason

Conclusions and **what could be done else**

The new entry for the SINBAD database was created. It comprises the KFK measurements of the γ -ray leakage spectra from three iron spheres of the outer diameter 25, 30 and 35 cm with spontaneously fissioning ^{252}Cf source in the center

Following the SINBAD requirements, the present entry includes the short (abstract) and more detailed descriptions of facility, methods and final numerical results with uncertainties which are necessary to validate the evaluated nuclear data in this benchmark.

To facilitate benchmarking the MCNP input deck was created and included in SINBAD entry. The specific (and new) feature of the proposed input deck is the modelling of $^{252}\text{Cf}(\text{s.f.})$ as a source of neutrons and γ -rays, both from prompt and delayed emission. It allows to get gamma and neutron responses in one MCNP run.

The modelling of ^{252}Cf as a source of neutrons is straightforward since the prompt neutron spectrum is a standard, whereas a contribution of the delayed neutrons is relatively small.

The challenge in the Cf-source modelling is the energy distributions and multiplicities of the γ -rays. Fortunately the prompt gamma emission was already measured in dozens of experiments and also theoretically studied. This information was used in present work to assess the prompt γ -ray spectrum and multiplicity. The situation is much worse for the delayed γ -ray emission: presently we manage to find and use the relevant data produced back in 1965.

For the nuclear data validation and other Cf-applications (e.g., medicine) it would be very useful to establish a reference prompt and delayed γ -ray spectra and multiplicities - I would like to finish this study and produce such reference data

Created MCNP input deck was used for sampling radiation transport calculations with ENDF/B-VIII.0 neutron reaction cross section data. It was shown that this library underestimate the γ -ray yield within 0.5 – 2.0 MeV by 20 - 40%. Such conclusion becomes more reliable for the Iron shell wall thickness more than ≈ 15 cm, when transmitted (maybe questionable) $\text{Cf}(\text{s.f.})\gamma$ -ray spectrum becomes already negligible in comparison with gammas produced by $\text{Fe}(n,x)\gamma$ reactions in Iron sphere.

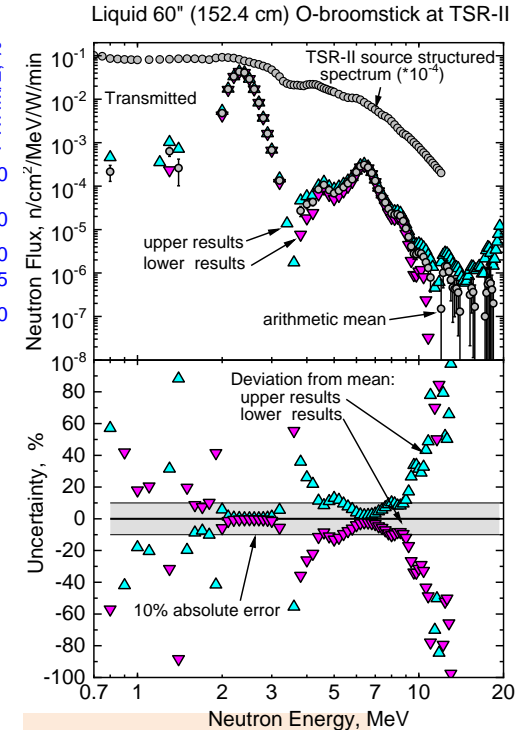
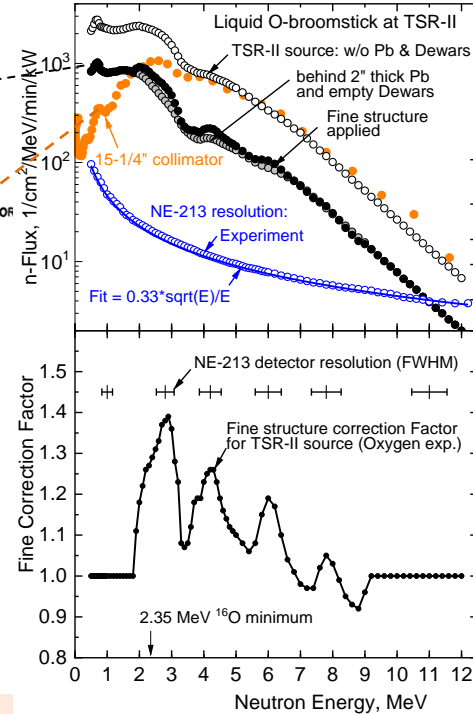
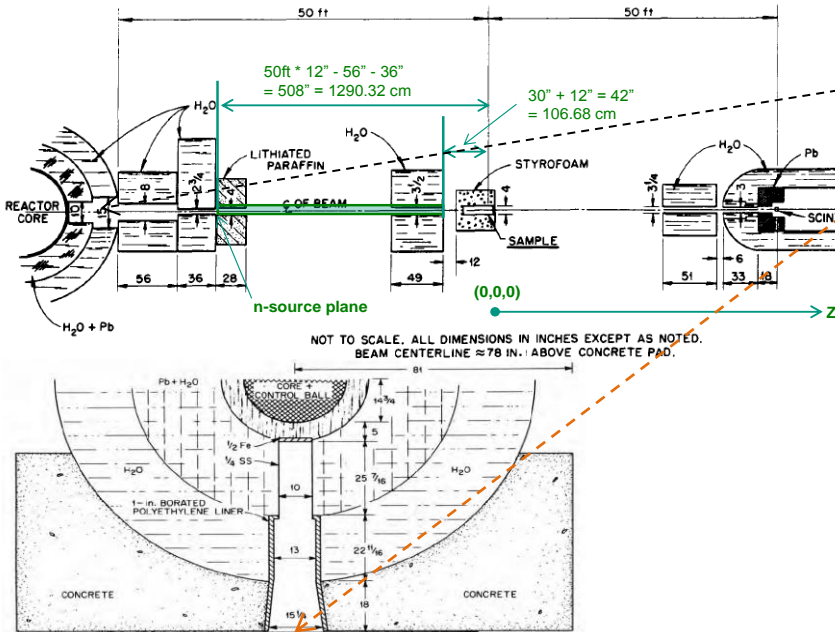
It turns out that KFK and IPPE have measured the γ -ray leakage spectra from Iron spheres of the same outer diameter 30 cm. It gave us a unique option to compare directly (as well as through C/E analysis) two independent measurements and confirm the agreement between them. This valuable fact increases the reliability of conclusions derived from validation analysis of both benchmarks.

II. ORNL/TSR-II 60" (152.4 cm) long liquid Oxygen broomstick neutron transmission

ORNL/TSR-II 60" liquid O-broomstick: Set-up, TSR-II source and transmitted neutron spectra

ORNL/TSR-II transmission set-up and MCNP model:

Exp. Results: TSR-II neutron source and transmitted spectra



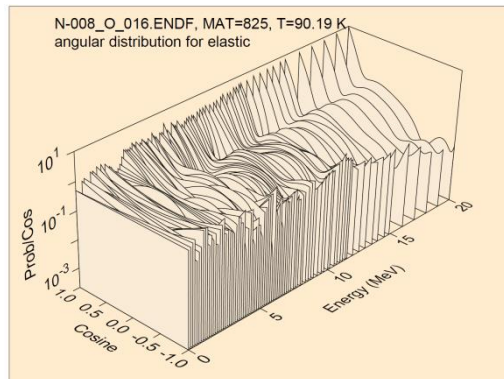
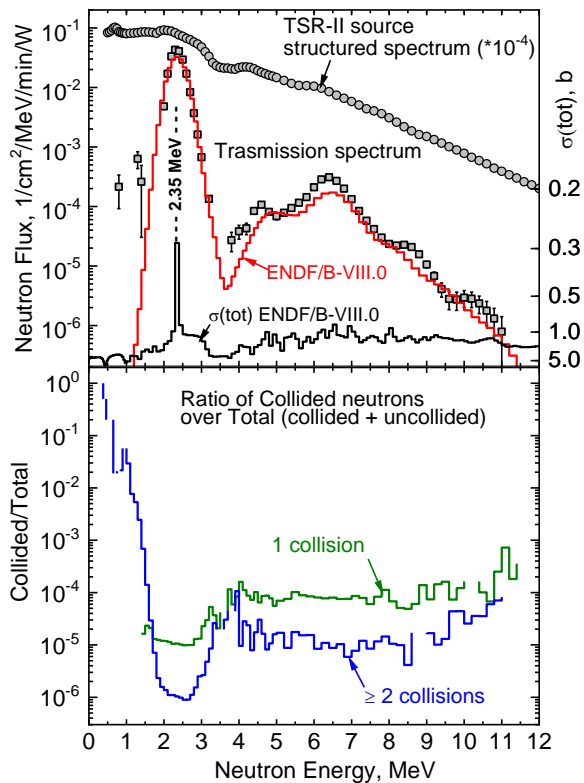
Experimental data:

- 60" (152.4 cm) liquid ($T = 91^\circ\text{K}$) Oxygen in two 24" + 36" Dewars
- shielded NE-213 detector with 4" Pb in front to suppress γ -rays
- n-spectra were measured between 0.7 and 14 MeV, however reliable data only in 2.0 - 3.2 MeV and 3.8 - 8.0 MeV with uncertainty $\approx (5 - 10)\%$
- 40% (!) calculated (!) fine corrections for beam transmission through 5" (12.7cm) H₂O core shield since O(n,tot) resonances/valleys will indeed express themselves in spectrum (as was shown for ≈ 5 cm of water layer in VR-1 reactor, Fig. 6 in M.Kostal et al. [Ann.Nucl.Ener.158\(2021\)108268](#))

ORNL 60" liquid O-broomstick: uncollided approximation is valid

Transmitted n-spectra and Uncollided/Collided fraction by MCNP and Analytically:

60" (152.4cm) liquid O-broomstick at TSR-II



Angular and Collisions issue:

MCNP: probability of ≥ 1 collisions is $\leq 1.E-4$

Analytically: Angle subtended by detector

$$\Theta = \arctan(0.5 \cdot \varnothing / \text{Distance}) = 0.19^\circ$$

The fraction of elastically scattered neutrons

$$= (1 - \cos \Theta) \cdot \sigma_{el}(0) / (\sigma_{el} / 4\pi) \approx 1.E-4$$

Thus the Uncollided approximation works!

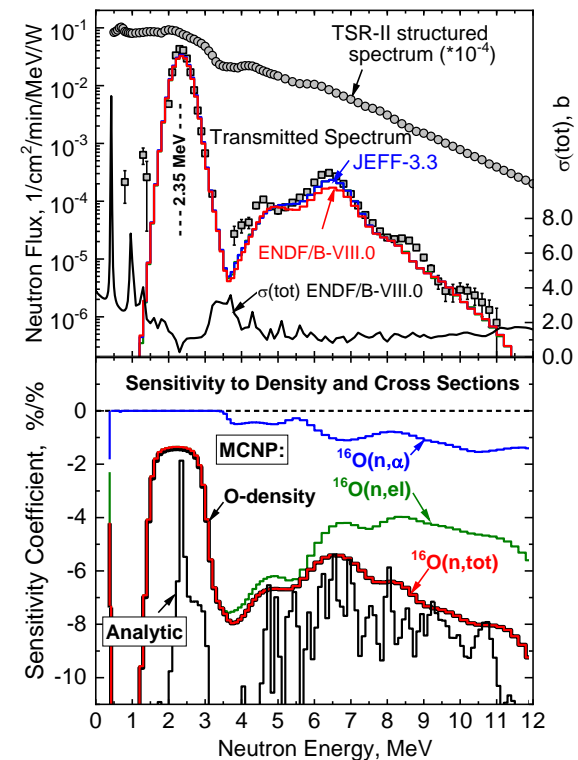
Sensitivities to atom fraction and XS were calculated:

- by MCNP (with NE-detector resolution) and Analytically (w/o resolution) - **similar results**
- sensitivity to (n,tot) varies between -2 and -8 reaching maximum at $^{16}\text{O}(n,\text{tot})$ resonance peaks (as Analytic calculation shows it could be even > 10 (!) at facilities with improved energy resolution)

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Transmitted neutron spectrum and Sensitivities

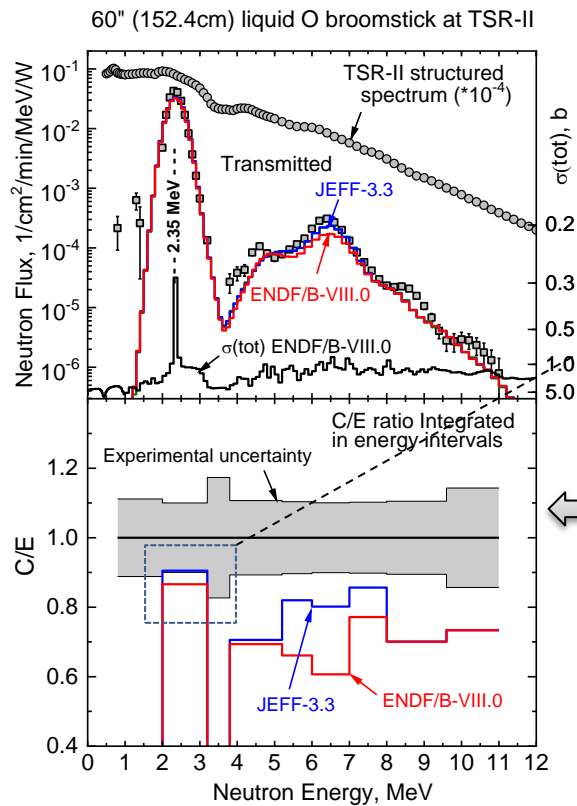
60" (152.4cm) liquid O broomstick at ORNL/TSR-II



ORNL/TSR-II 60" liquid O-broomstick: validation example with ENDF/B.VIII.0 and JEFF-3.3

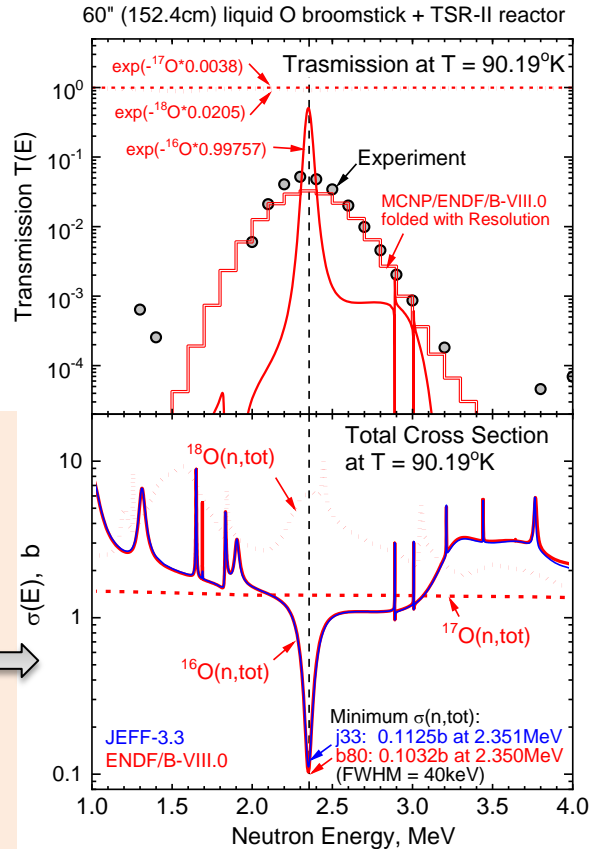
Transmitted n-spectra and C/E between 1 and 10 MeV:

Validation of 2.35 MeV $^{16}\text{O}(n,\text{tot})$ minimum:



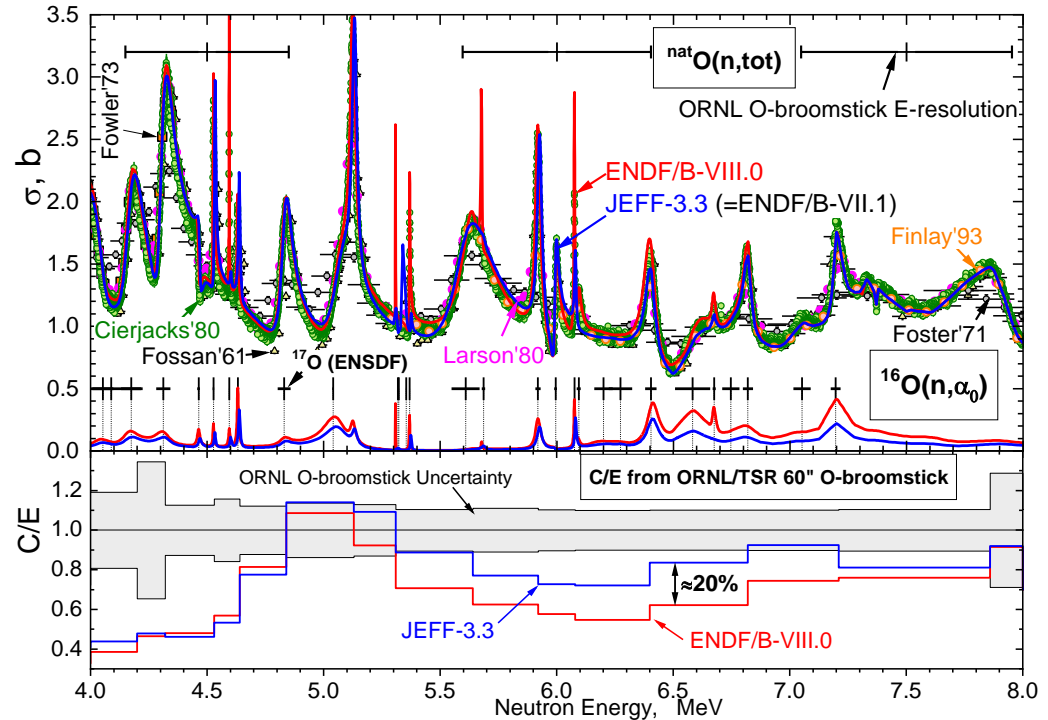
Validation outcomes:

- (i) at 4 - 10 MeV:
 - JEFF-3.3 underestimates by $\approx 30\%$ (≈ 2 exp. error)
 - ENDF/B-VIII.0 even worse between 5 and 8 MeV
- (ii) at 2.35 MeV:
 - ^{16}O $\sigma(n,\text{tot})$ minima = **0.1125 (JEFF-3.3)**
 - looks better than **0.1032 (ENDF/B-VIII.0)**
 - i.e. 60"-broomstick sees this difference $\approx 9\%$
 - Transmission through ^{17}O and ^{18}O is flat and ≈ 1.0
 - Experimental Resolution ≈ 10 times exceeds the FWHM = 40keV of $^{16}\text{O}(n,\text{tot})$ valley at 2.35 MeV and boiling temperature $T = 90.19^\circ\text{K}$



ORNL/TSR-II 60" liquid O-broomstick: impact on $^{16}\text{O}(n,\text{tot})$

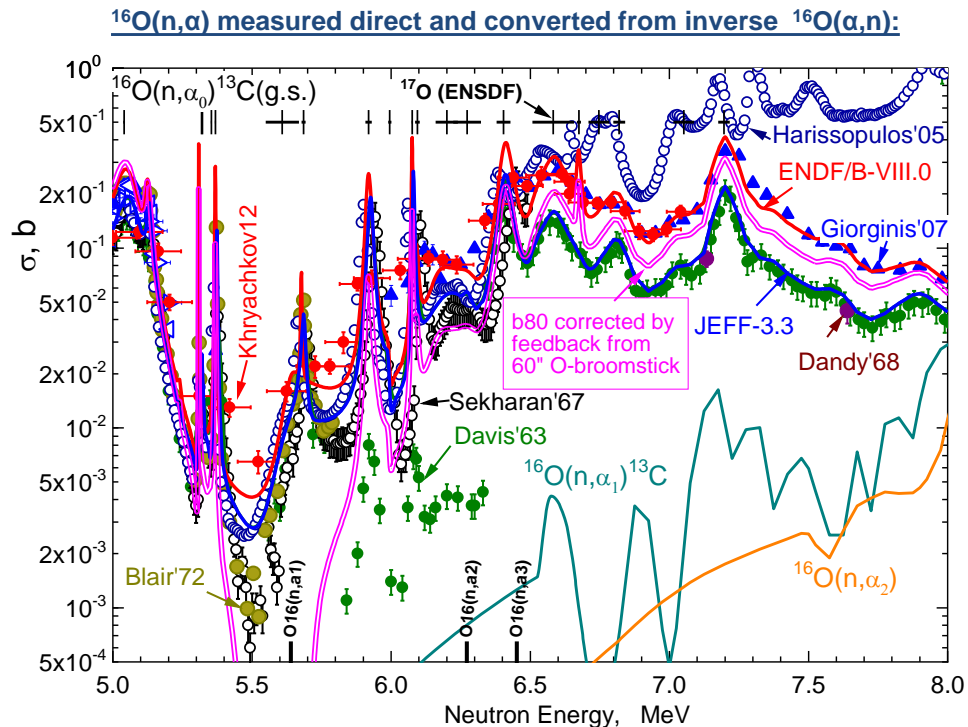
$^{\text{nat}}\text{O}(n,\text{tot})$ cross sections and C/E from ORNL/TSR-II transmitted n-spectra:



Validation impact of 60" O-broomstick on $\text{O}(n,\text{tot})$:

- it demands **decreasing of ENDF/B-VIII.0** between 5.5 and 7.2 MeV, **JEFF-3.3 looks practically OK there**
- using calculated sensitivity for ORNL experiment to $\sigma(n,\text{tot}) \approx -6$
we roughly estimate (n,tot) cross section correction = $\Delta\sigma_{\text{tot}}(E)/\sigma_{\text{tot}}(E) = (\Delta T(E)/T(E))/S(E) \approx 20\%/(-6) = -3.3\%$ (should be applied to min & acceptable)
- since total cross section in interval 5 - 8 MeV is a sum of (n,elast) and (n,α) we may also consider the propagation of observed 20% underestimation by ENDF/B-VIII.0 also to $^{16}\text{O}(n,\alpha)$ with sensitivity to $\sigma(n,\alpha) \approx -1$:
we estimate (n,α) cross section correction = $\Delta\sigma(n,\alpha) / \sigma(n,\alpha) \approx (\Delta T(E) / T(E)) / (-1) \approx -20\%$

ORNL/TSR-II 60" liquid O-broomstick: impact on $^{16}\text{O}(n,\alpha)$



Experimental and evaluated cross sections for $^{16}\text{O}(n,\alpha)$ reactions:

- Closed Symbols – Direct measurements [4 Experiments]; Open Symbols - Converted cross sections from Inverse reaction $^{13}\text{C}(\alpha,n_0)^{16}\text{O}$ [3 Exp.]; for latter we used Detailed Balance: $^{16}\text{O}(n,\alpha_0)^{13}\text{C}(\text{g.s.}) \leftrightarrow ^{13}\text{C}(\alpha,n_0)^{16}\text{O}$ is valid exactly $< E_{n1} = 5.640$ MeV but practically $< 7.5 - 8.0$ MeV ($E_{\alpha} < 6.32 - 6.94$)
- between 5 and 8 MeV the measured and evaluated data **ENDF/B-VIII.0** and **JEFF-3.3 (= ENDF/B-VII.1)** do visibly scatter
- if **ORNL 60" O-broomstick** observed C/E will be propagated, then it demands decreasing of **ENDF/B-VIII.0** by $\approx 20\%$ - **could it be a truth ? => next slide**

ORNL/TSR-II 60" liquid O-broomstick impact on $^{16}\text{O}(n,\alpha)$: whether it agrees with $\text{C}(\alpha,n)$ TTY benchmark ?

$^{\text{nat}}\text{C}(\alpha,n)$ TTY neutron yield measured and computed but employing the XS inverted from $^{16}\text{O}(n,\alpha)^{13}\text{C}$:

As was recently shown, e.g. by

M.Pigni, S.Croft [Phys. Rev C102 \(2002\) 014618](#) and

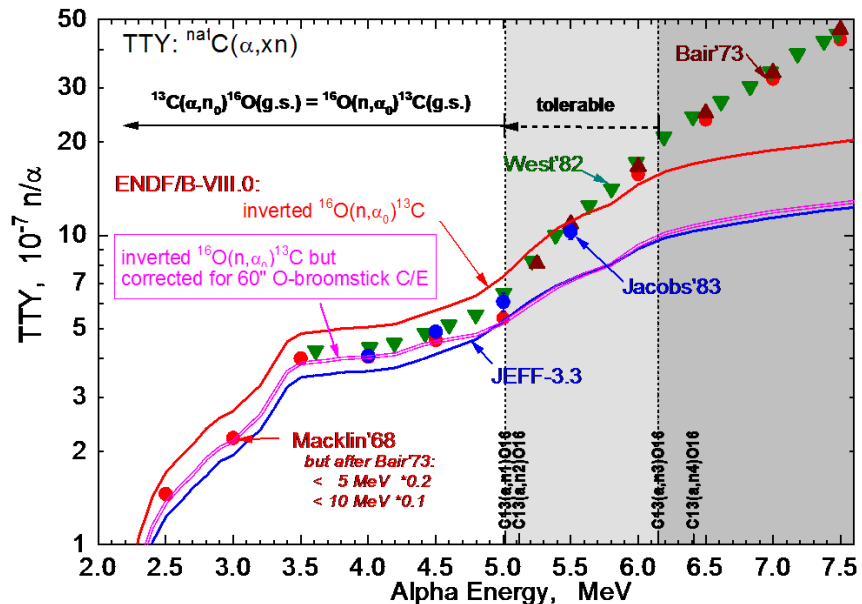
A.Plompen [JEFFDOC-2034, 29 Apr 2021](#):

carbon (α,n) thick target data (TTY) are rather consistent and useful for fixing of discrepant measured $^{13}\text{C}(\alpha,n)^{16}\text{O}$ cross sections

? Could $\text{C}(\alpha,xn)$ TTY be also useful for the cross-checking of the ORNL 60" O-broomstick validation message/outcome ?

For this we:

- converted ENDF/B-VIII.0, ENDF/B-VIII.0 corrected for C/E & JEFF-3.3 XS for $^{16}\text{O}(n,\alpha)^{13}\text{C}(\text{g.s.})$ into $^{13}\text{C}(\alpha,n)^{16}\text{O}$ (using detailed balance relation)
- folded XS $^{13}\text{C}(\alpha,n)^{16}\text{O}$ with α -particle energy losses in reactor graphite (taken from NIST/ASTAR)
- used ^{13}C abundance in graphite = 1.0866% \pm 2.4% (from CIAAW)
- compared with 4 known experiments for $^{\text{nat}}\text{C}(\alpha,n)$ TTY in this Figure



Observations from inter-comparison of the O-broomstick neutron transmission and $^{\text{nat}}\text{C}(\alpha,n)$ TTY benchmarks:

- propagation of underestimation observed for 60" O-broomstick transmission to the $^{16}\text{O}(n,\alpha)$ cross section which demands XS decreasing by $\approx 20\%$ between 6 and 8 MeV seems is confirmed by TTY neutron yield induced in Carbon by α -particles with $E_\alpha < 5 - 6$ MeV
- Note that below $E_\alpha \approx 3.5$ MeV there are no other n-TTY data except Macklin'68 which requires 5-10 times (!) decreasing

Conclusions and **what could be done else**

The existing entry SINBAD NEA-1517/59 (SDT2) = the measured neutron spectra from the TSR-II reactor source and transmitted through 60" thick liquid oxygen broomstick) was upgraded.

The actual upgrade additionally includes the MCNP model input deck assembled for this experiment and Evaluation report which describes the necessary details of experiment , quality assessment and validation analysis.

Communication with RSICC at ORNL was undertaken to seek the numerical data for the neutron spectra transmitted through O-broomsticks of the 24" and 36" (and probably 72") length - **no success.**

Completeness and quality of experimental data:

- **TSR-II neutron source spectrum, measured with energy resolution $\approx 10\%$, not allowed to see fine energy structure caused by H₂O shield of core. Authors have recommended to correct the spectrum incident on O-broomstick by oscillating function which reaches up to 40%.**
- **To increase the benchmark representativeness for oxygen cross sections validation, the transmission of the core neutron through the water shield could nowadays be re-simulated with higher precision at least to show how 13 cm of water impact on smooth U(n,f)PFNS.**
- **Spectrum of neutrons transmitted through 60" thick O-broomstick is given as upper and lower limits resulting from unfolding of recoil pulse distribution in NE-213 detector. The negative values and more than 100% difference between upper and lower limits restrict the usage of experimental data only to energy intervals (2.0 - 3.2) MeV and (3.8 - 8.0) MeV.**
- **Uncertainty of the atom density in the liquid oxygen and chemical admixtures are not explicitly given, that forced us to guess these values.**

Analysis and validation outcome:

- The fraction of the collided and uncollided neutrons was found to be at level $\approx 1.E-4$ that proves the usage of uncollided approximation
- Due to such negligible contribution of the collided neutrons the analytical and Monte Carlo analysis deliver practically identical results. However the use of MCNP makes easier to imply detector resolution, calculate contribution of collided neutrons, sensitivity etc.
- Sensitivity of 60" O-benchmark to the oxygen total cross section varies between -2 and -8 (even the larger value up to -10 could be reached, if the facility energy resolution will be improved).
- Monte Carlo validation simulation evidences that $^{16}\text{O}(n,\text{tot})$ from JEFF-3.3 (= ENDF/B-VII.1) behaves better than ones from ENDF/B-VIII.0
- Propagation of underestimation observed for 60" O-broomstick transmission to $^{16}\text{O}(n,\alpha)$ cross section demands decreasing of this XS by $\approx 20\%$ between 6 and 8 MeV.
- The latter is shown do agree with TTY neutron yield induced by α -particles with energies up to 5 - 6 MeV in elemental carbon.