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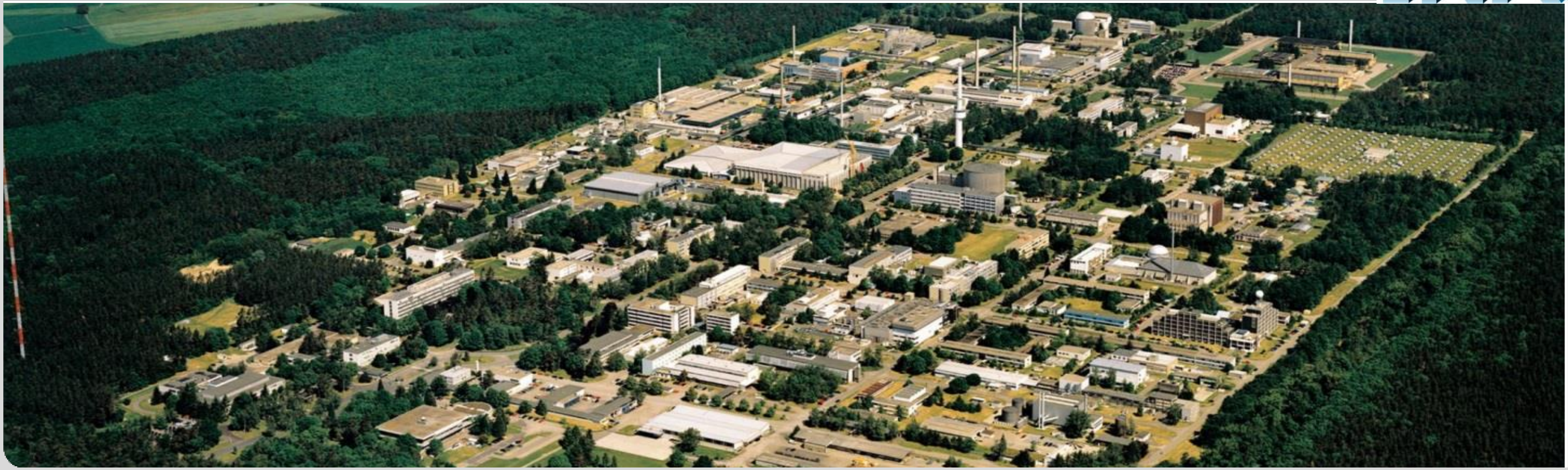
Benchmarking of the latest Neutron and Gamma Transport Cross Sections for Oxygen, Iron and Uranium in clean Benchmarks driven by D-T, ^{252}Cf and Reactor sources

S.P. Simakov and U. Fischer

in collaboration with Experts from CIELO, JEFF, …..:

D. Brown, R. Capote, M. Chadwick, M. Herman, B. Jansky, I. Kodeli, A. Koning, L. Leal, M. Majerle, A. Plompen, D. Rochman, P. Talou, A. Trkov, …

INSTITUTE for NEUTRON PHYSICS and REACTOR TECHNOLOGY (INR)



Content

Nuclei Considered:

I. Oxygen: our *(not completed yet)* **validation results** also presented as *EFFDOC-13XX, NEA Data Bank, Nov 2017*

II. Iron: a) continuation of our recent work *presented as*
JEFFDOC-1851 = EFFDOC-1319, Apr 2017; EFFDOC-1303, Dec 2016

b) MC propagation of TENDL-2017 random files to Covariancies for *n* & *γ*-leakage energy spectra *first time presented at*
TALYS/TENDL Workshop, Nov 2017, Prague; then EFFDOC-13XX, Nov 2017

III. Uranium: revisiting our old validation *presented as a contribution to ND-2004*
AIP Conf. 769(2004)67, Santa Fe, Oct 2004

For these Nuclei following Evaluated Transport Data are under testing:

- ENDF/B-VII.1 and ENDF/B-VIII.0 (= VIII.β4, CIELO)
- JEFF-3.3T4 and "JEFF-4.0T1" (*only ^{56}Fe & ^{54}Fe – L. Leal' work for next JEFF*)
- TENDL-2017 evaluation and BMC random files (*only Fe stable isotopes*)

Tools used:
- File processing by NJOY-2012.82 (from LANL web) or .99 (NEA Data Bank)
- MC simulation of considered benchmarks by MCNP-6.1
  (for TOF measurements: TOF was simulated then transformed to Energy Spectra)
- dedicated *f.95* subroutines for post processing of simulation results

I. Oxygen

I. Oxygen (0): overview of

Experiments with Liquid Oxygen involved in present analysis:

Lab Years	Source: <Energy>	No. of Spheres: Wall Thickn., cm	Methoda	Detector, Threshold	Numerical Data from
FNS 1991	D-T: ≈ 14 MeV	Cylinder: thick = 20 cm	Time of Flight (TOF)	*Leaking Neutrons:* NE-213 > 50 keV	*Y. Oyama et al. SINBAD NEA-1553/61*
LLL 1976	D-T: ≈ 14 MeV	1 sphere: Wall ≈ 10 cm	Time of Flight (TOF)	*Leaking Neutrons:* Pilot B > 1.6 MeV	*L. Hansen et al. NSE 60(1976)27 C. Wong UCRL-51144(1971)*
ORNL 1967	Reactor Fission : ≈ 2.1 MeV	Cylinder: length = 61, 92 cm (?), 152 cm (available)	Pulse Height (PH)	*Uncollided Neutrons (pure transmission):* NE-213: 1.9 - 8.6 MeV	*C .Clifford et al. SINBAD NEA-1517/59*

Additionals/Comments:

- ***liquid Oxygen Transmission experiment (En = 20 - 30 MeV) in progress at NPI/Rez, M. Majele et al. EFFDOC-1323, Apr 2017***
- ***no gamma-leaking measurements ! (then look what we have for water ?)***

I. Oxygen (1): FNS/JAERI, 1991

Neutron scattering benchmark with pure Oxygen, *NEA-1553/61*:

Neutron Leakage Spectra at 0, 12, 25, 42, 67 deg.
from Liquid Oxygen Disc (l = 20 cm × Ø60 cm)
irradiated by pulsed 14 MeV source

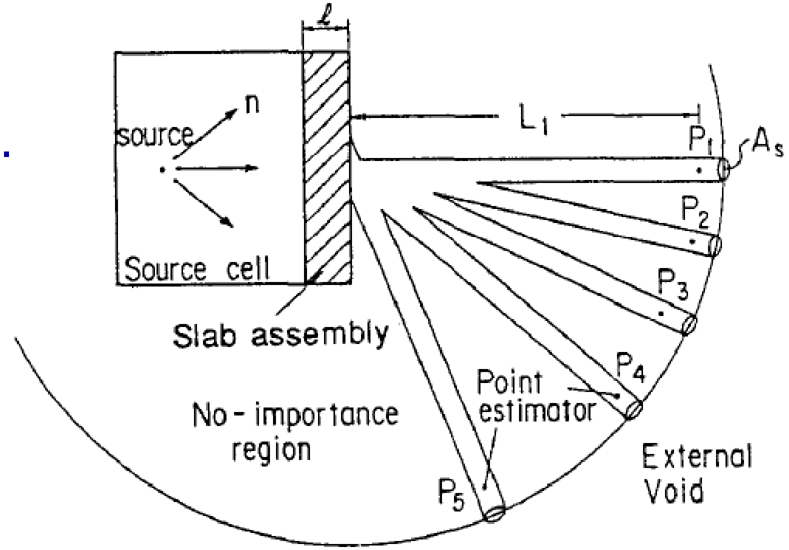


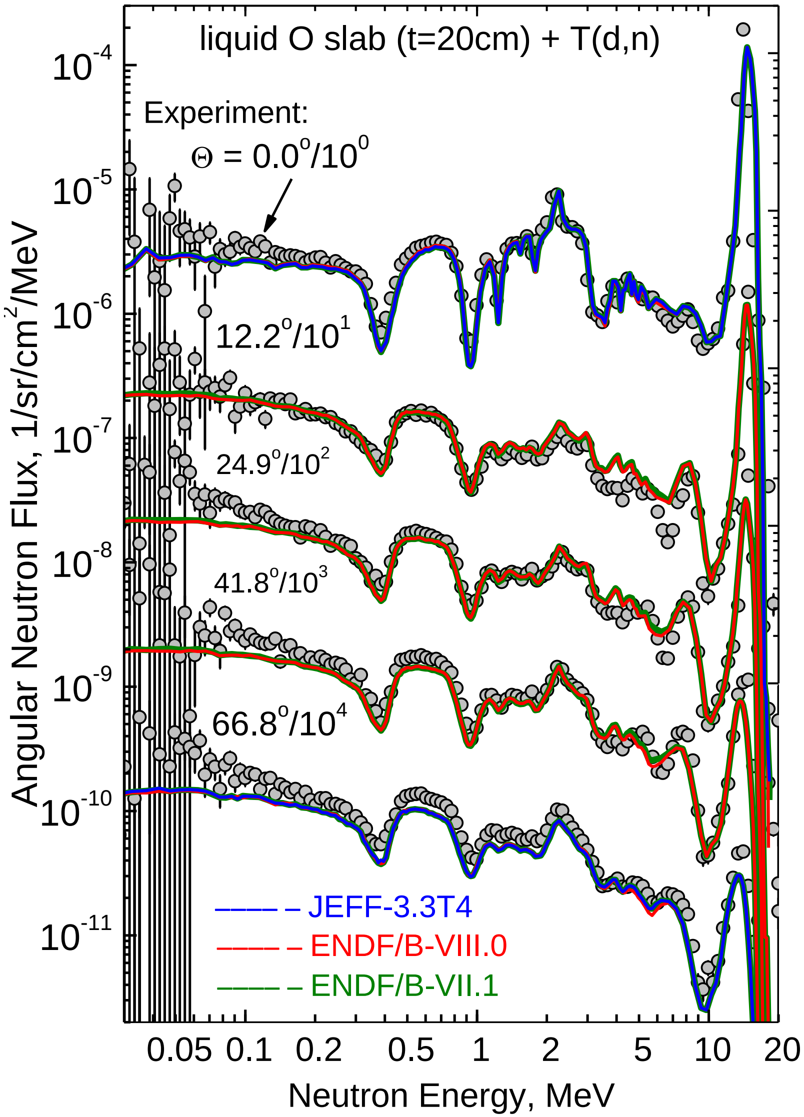
Fig.3 Calculational model for MCNP

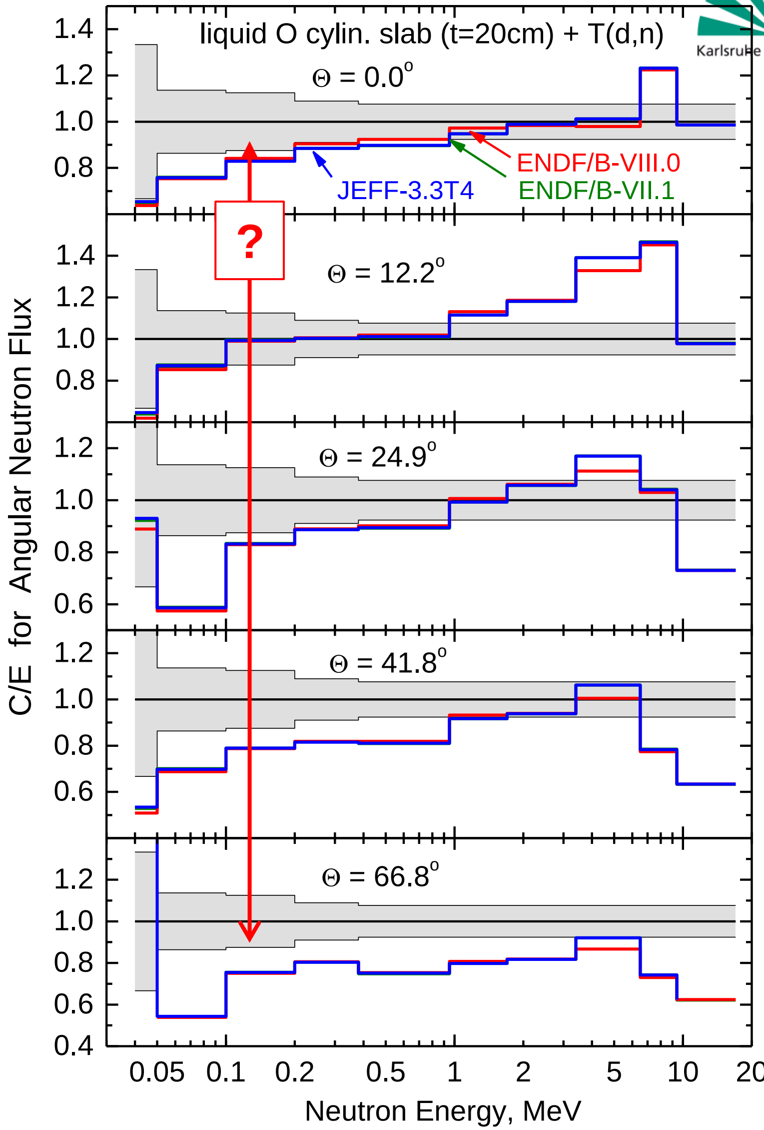
Description of Experiment is available in:
- e.g.: Y.Oyama et al., NDST 1991, p.337; Fig.3 =>
- Details & Numerical Data including author's MCNP input - in SINBAD

Essential experimental details which impact on modelling and conclusion:
- measured by TOF which was also represented in MCNP simulations
- background was measured/subtracted by filling collimator hole with iron/polyethylene plugs
- efficiency of NE-213 detector was not measured but was MC-calculated by authors

Our validation results of current evaluations on next slide (all O isotopes are included in MC) =

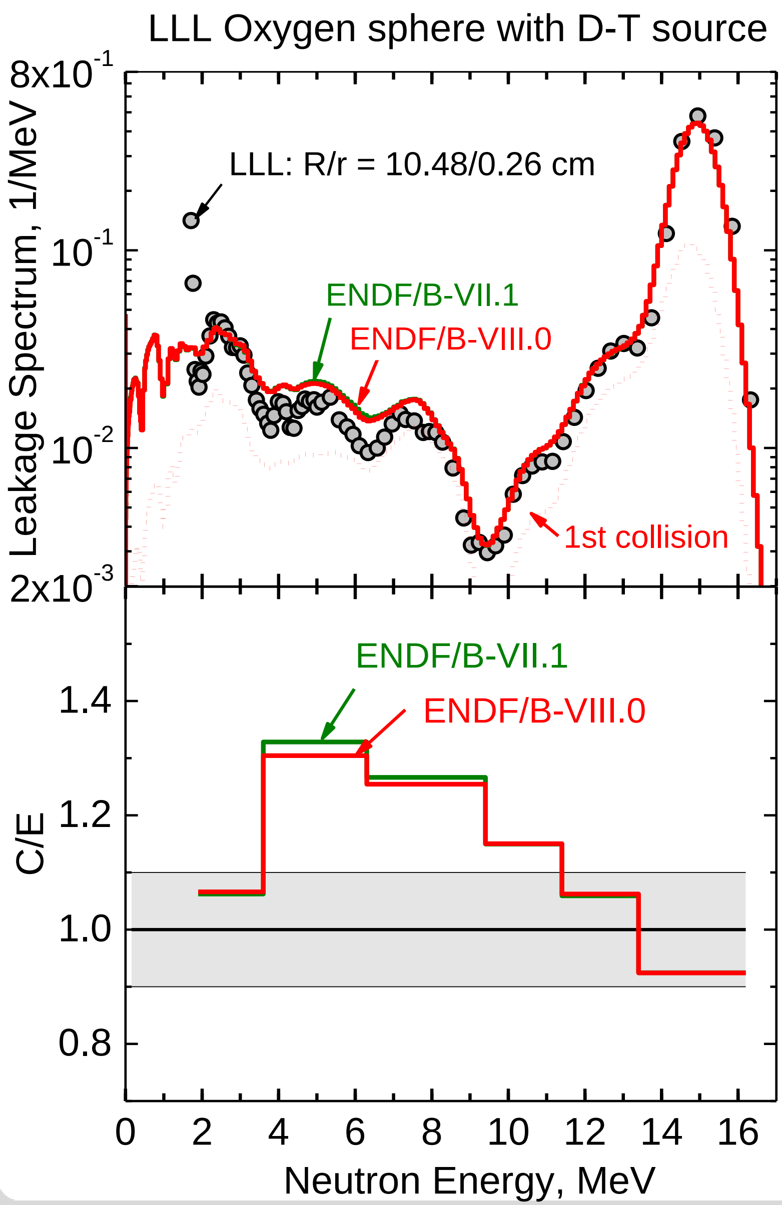
I. Oxygen (1): Neutron Leakage from JAERI cylinder with D-T source





Findings*:** ***- JEFF-3.3T4 = ENDF/B-VII.1 and ENDF/B-VIII.0 are identical
except ≈5% difference only in 3 – 7 MeV, where ENDF/B-VIII.0 trends to unity

I. Oxygen (2): LLL pulsed sphere with D-T source, 1967



Observations :

- ***1st collision dominates***
- ***ENDF/B-VII.1 is practically identical to ENDF/B-VIII.0 however gives ≈2% more only for 4 - 8 MeV (similar to what we saw for FNS/JAERI slab)***
- ***both confirm 14 MeV transmission but overpredict secondary neutrons 4-9 MeV (it similar as FNS shows at 0 - 25 deg)***

I. Oxygen (3): ORNL, Tower Shielding Facility, 1967

Uncollided transmission through Liquid Oxygen

(length: 24in = 60.96 cm & 36in = 91.44 cm; dia: 4in = 10.16 cm)

irradiated by TSR-II reactor spectrum ranged 1.9 to 8.6 MeV

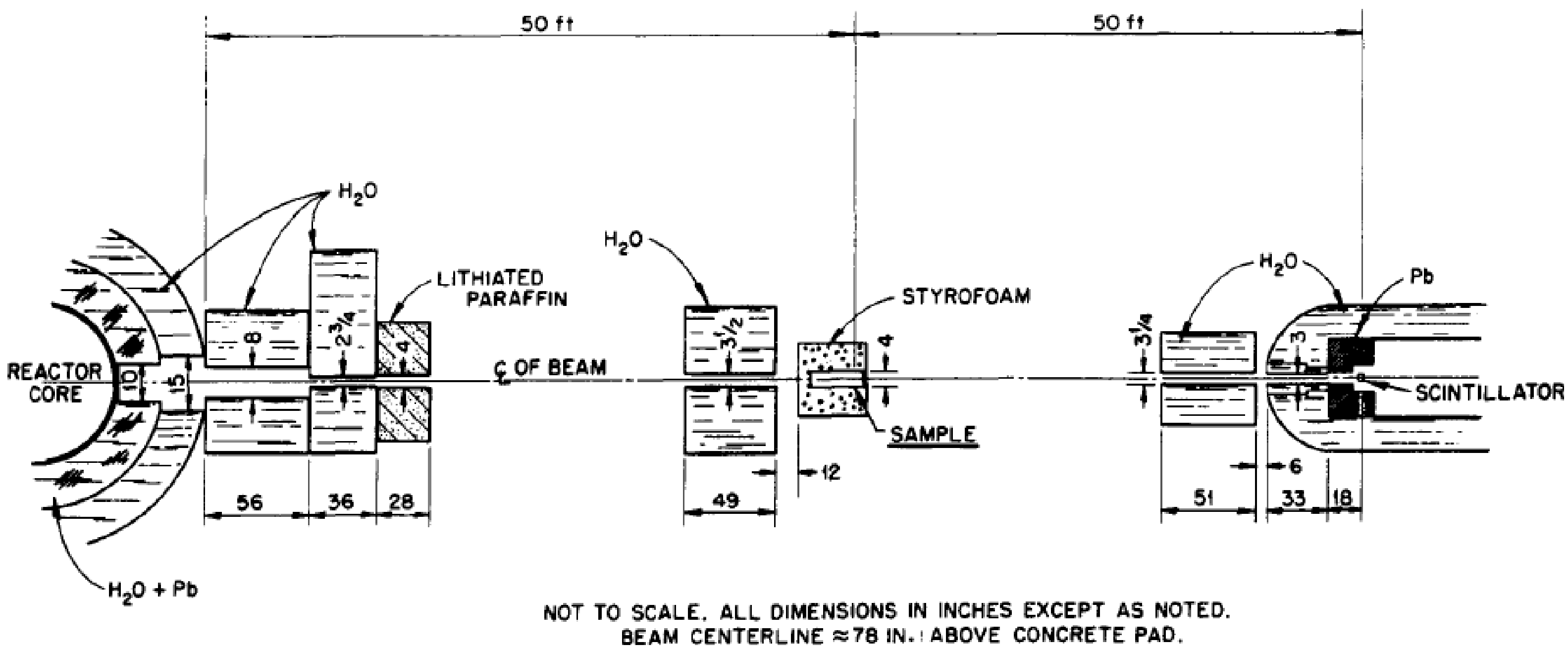


Fig. 1. Schematic diagram of experimental arrangement.

Description of Experiment is available in:

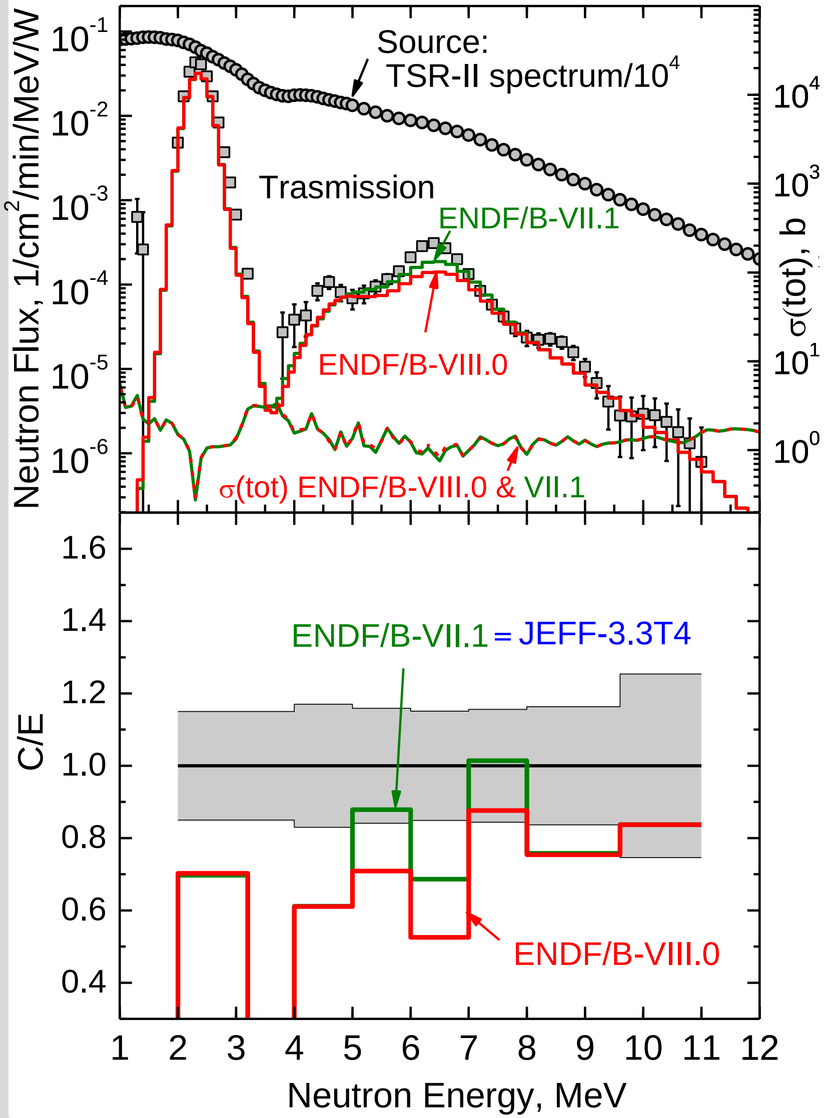
- e.g.: C.Clifford et al., NSE 27(1967)299; E.Straker ORNL-TM-2242(1968), -3868(1972)

- SINBAD NEA-1517/59: description + numerical data (only 60 in. = 152,4 cm), no MCNP model

Our preliminary results on next slide (all O isotopes are included in MC) =>

I. Oxygen (3): ORNL, Tower Shielding Facility, 1967 *(cont.)*

Liquid O broomstick (60in=152cm) + TSR-II



Observations but with preliminary set-up Model:

- ***This Reactor Spectrum Transmission Experiment indeed sensitive only to Uncollided Neutrons, i.e. to σ_{tot}: the fraction of Collided Neutrons seen by detector amounts only ≈ 5 10^{-6}***

- ***It is insensitive to the change of Oxygen Temperature from boiling 90.2°K (-183°C) to room one: σ_{tot} changes only below 1 eV***

- ***152 cm of liquid Oxygen reduce Neutrons by 10^{-4} !,***
  $\Delta\sigma/\sigma = (n\ l\ \sigma)^{-1}\ \Delta T/T = 6.5\ \Delta T/T$!
  e.g.: 10% change of ΔT/T will demand $\Delta\sigma_{tot} \approx 0.65$ b !

- ***JEFF-3.3T4 is practically identical to ENDF/B-VII.1***

- ***ENDF/B-VIII.0 gives 10% less then VII.1 only for 5-8 MeV or similar trend which we observe for FNS/JAERI slab and LLL sphere***

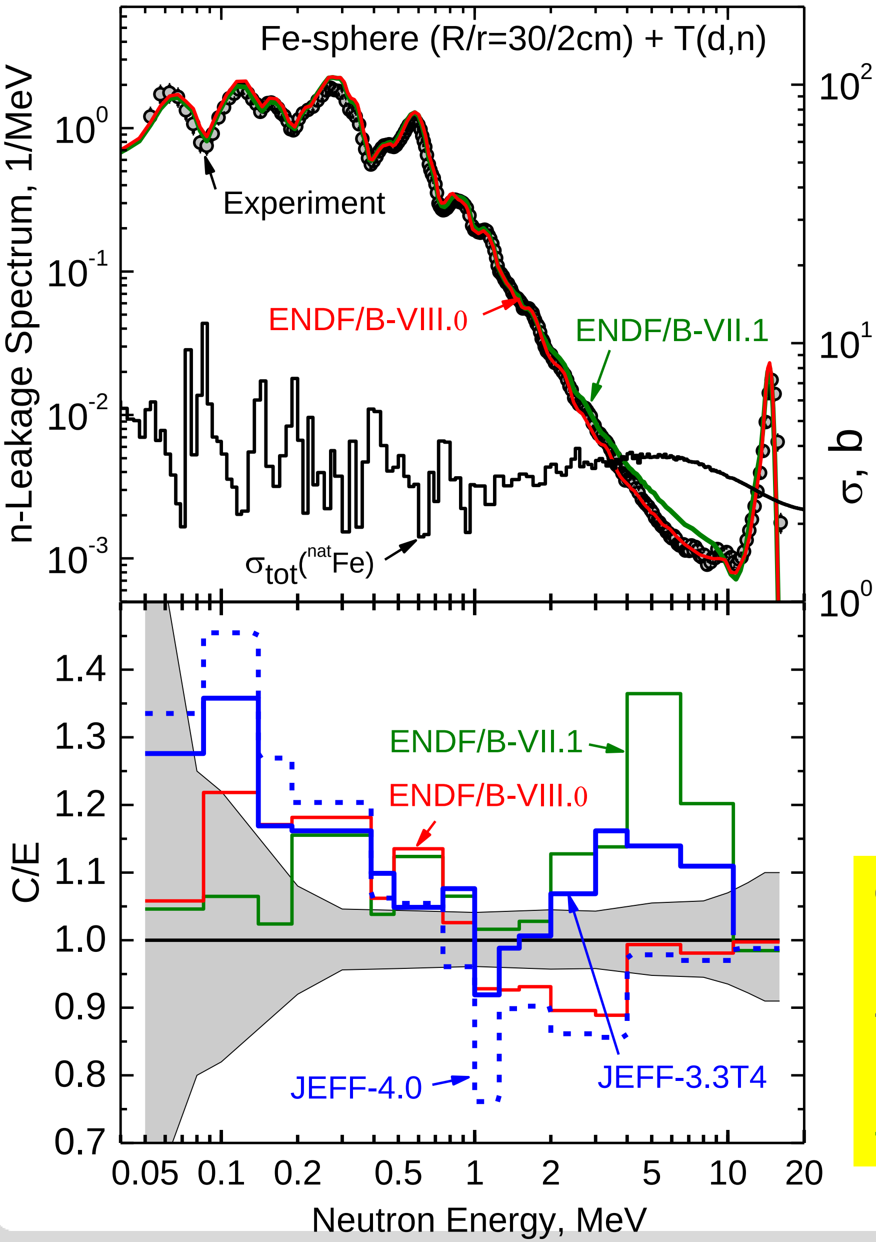
II. Iron, *the first part:* Secondary Neutron Validation

II. Iron (0): overview of

Experiments involved in the present analysis:

Lab Years	Source: <Energy>	No. of Spheres: Wall Thickn., cm	Method	Detector, Threshold	Numerical Data from
IPPE 90-98	D-T: ≈ 14 MeV	5 spheres: Wall = 2.5, 7.5, 10.0, 18.1, 28 cm	Time of Flight (TOF)	*Neutrons:* p-Ter.scint. > 50 keV	*S.Simakov et al.* SINBAD Fusion: *NEA-1553/75*
IPPE 1985	^{252}Cf: ≈ 2.1 MeV	6 spheres: Wall = 4, 9, 19, 23, 29, 34 cm	Pulse Height (PH)	*Neutrons:* H-prop. 5 – 700 keV Stilben 0.2 - 17 MeV *Gammas:* Stilben 0.4 - 10 MeV	*L.Trykov et al.* *ICSBEP/DICE*: *ALARM-CF_FE-SHIELD-001*
LLL 1976	D-T: ≈ 14 MeV	3 spheres: Wall ≈ 4, 13, 22 cm	Time of Flight (TOF)	*Neutrons:* NE-213 > 1.6 MeV	*L.Hansen et al. NSE 60(1976)27 C.Wong UCRL-51144(1971)*
LLL 1990	D-T: ≈ 14 MeV	1 sphere: Wall ≈ 4 cm	Time of Flight (TOF)	*Neutrons:* NE-213 > 1.6 MeV *Gammas (e-Recoils):* NE-213 > 0.255 MeV	*E.Goldberg et al. NSE105(1990)319*
VNIITF 1991	D-T: ≈ 14 MeV	1 sphere & 1 semi-sphere: Wall = 5 cm	Time of Flight (TOF)	*Neutrons:* Stilben > 0.25 MeV *Gammas (e-Recoils):* Stilben > 0.35 MeV	*A.Saukov et al.* SINBAD Fusion: *NEA-1517/74*

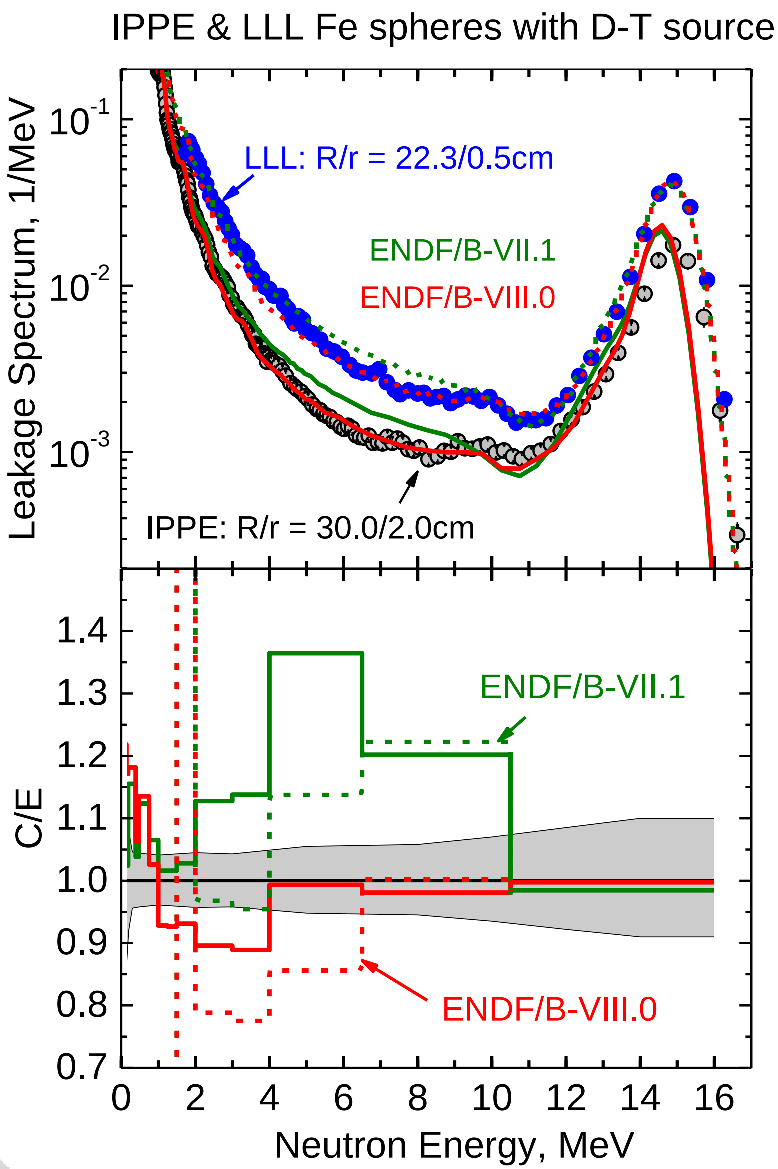
II. Iron (1): Results for IPPE D-T pulsed sphere (Wall=28cm), Neutron leakage



Observations for 14 MeV pulsed and thickest (Wall = 28 cm) sphere:

- JEFF-4.0T1 (Geel) is different from EFF-3.3T4 but comparable with it from view abs(C/E -1)
- ENDF/B-VIII.0 looks better than ENDF/VII.1

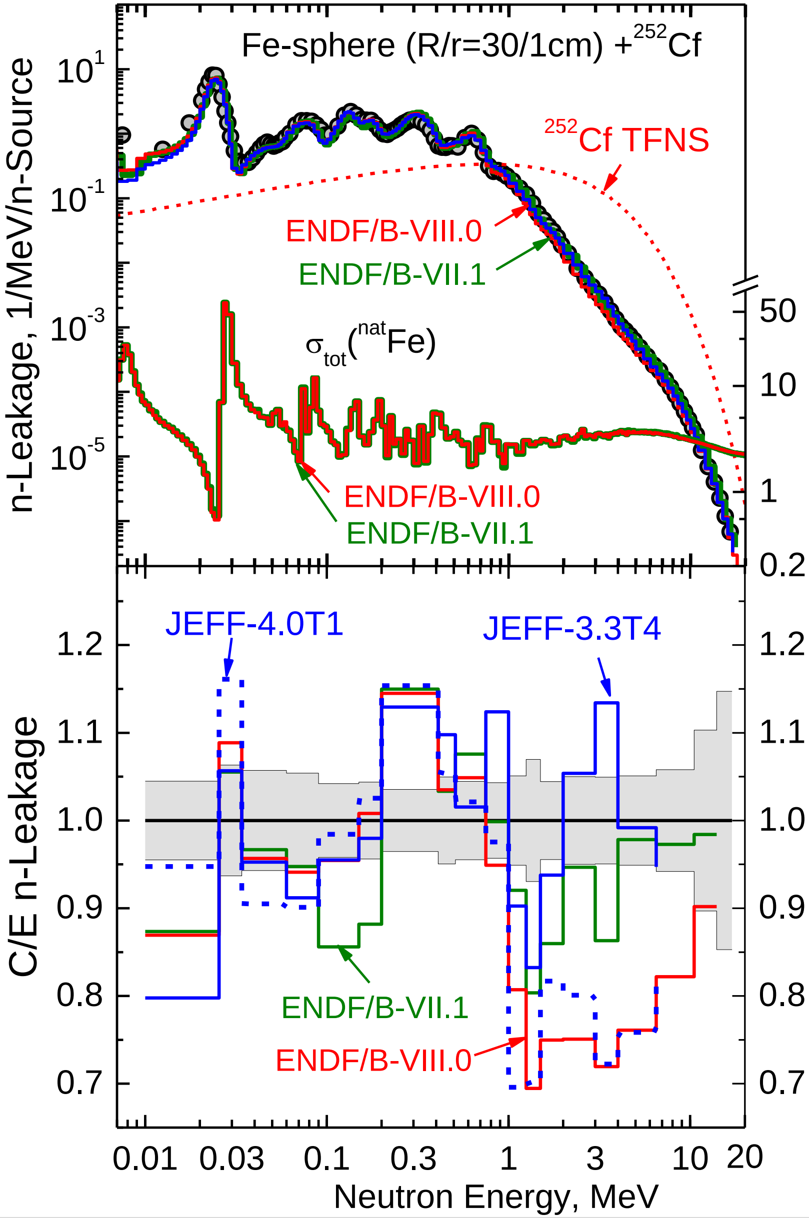
II. Iron (2): Comparison of IPPE (28cm) and LLL (22cm) spheres with D-T pulsed source: Neutron leakage



Observations from comparison of LLL (Wall = 22cm) and IPPE (Wall= 28 cm):

- **LLL: Neutrons > 1.6 MeV** *(for convenience of comparison I converted original ToF spectra in Energy ones and folded with Gauss)*
- **IPPE: Neutrons > 0.1 MeV**
- **both: show similar C/E in overlapping energies, e.g. 4 - 10 MeV is overestimated by ENDF/VII.1, where ENDF/B-VIII.0 performs better**

II. Iron (3): Results for IPPE Fe sphere (Wall=29 cm) + ^{252}Cf(s.f.), Neutron Leakage



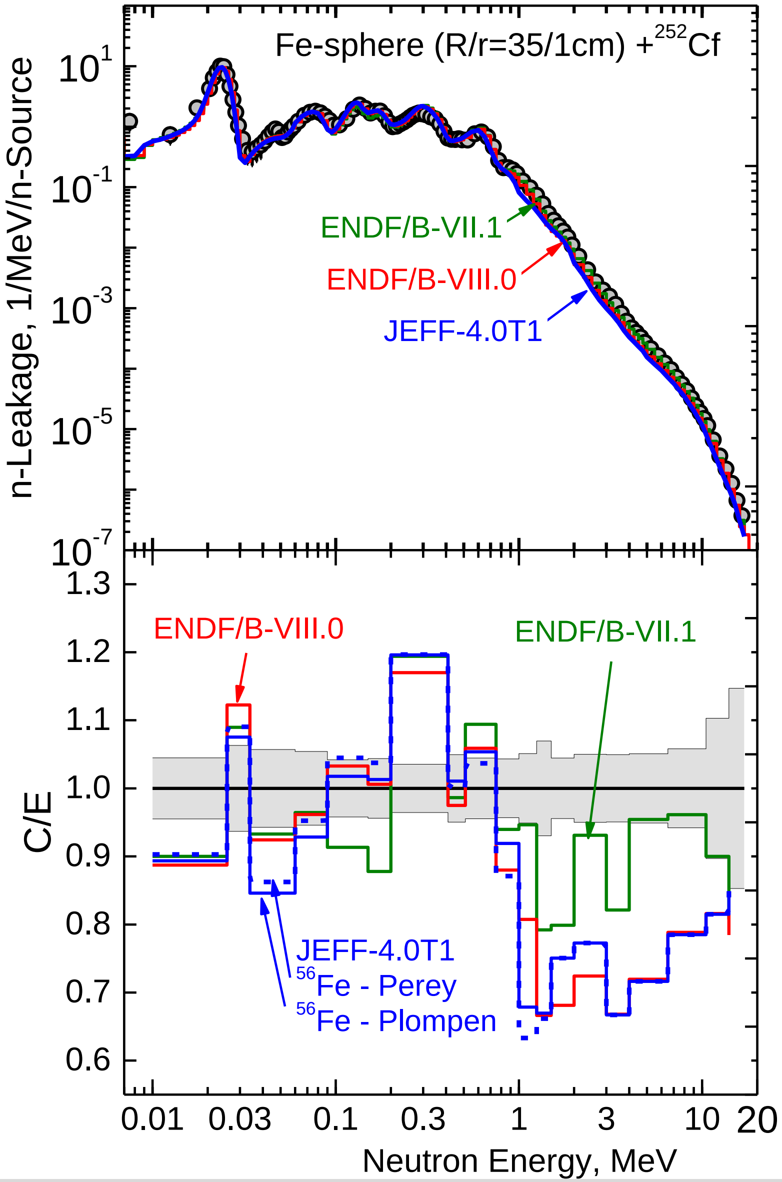
Before MCNP simulation we modified MCNP input given in ICSBEP/Alarm-Cf_Fe-Shield-001:

- **^{252}Cf(s.f.) source neutron spectrum (given as *Watt with Froehner parameters)* was replaced by PFNS Standard *(Mannhart evaluation), vp = 3.7590***
- **and we added delayed neutrons (*vd = 0.0086*) with DFNS spectrum from ENDF/B-VII.1**

Observations from C/E comparison:

- **JEFF-3.3T4 looks even more better than others**
- **possible reasons for underestimation (*σtot, angular distribution …*) by ENDF/B-VIII.0 were studied**

II. Iron (4): IPPE Fe thckest sphere (Wall=34 cm) with ^{252}Cf source, <u>Neutron Leakage</u>



Observations:

JEFF-4.0T1 which adopts ^{56}Fe(n,n') either Perey'71 (ORNL) or Plompen'13 (Geel) are hardly distinguished by this benchmark

II. Iron, *the second part*:

- Secondary Gammas Validation and
- problem of L.Trykov' Benchmark (*ALARM-CF_FE-SHIELD-001)*

L. Trykov et al. Atom Energy, 98(2005)50 (*highlighting by couloirs is my*):
"*The experimental fluxes of >0.8 MeV neutrons are, for the most part, greater than the computed values, and the fluxes of >0.35 MeV photons are also greater than the computed values. The differences reach a factor of 2–3***":**

TABLE 2. Characteristics of the Neutron and Photon Spectra from Spherical Iron Models with a ^{252}Cf Source at the Center

Diameter of spherical model, cm	Flux of >10 keV neutrons/source neutron		Flux of >0.35 MeV photons/source neutron		Average energy of the photon spectrum, MeV	
	Experiment	Calculation	Experiment	Calculation	Experiment	Calculation
20	0.98	0.995		0.482		
40	0.97	0.988	0.112	0.0657	1.10	1.21
50	0.96	0.982	0.086	0.0310		
60	0.94	0.975	0.049	0.0186	1.59	1.34
70	0.91	0.965	0.035	0.0120	1.91	1.57
10	0.85	0.908	0.0165	0.00651	3.13	2.61

What could be a reason for differences between L.Trykov experiment and calculations *by factor 2–3 for leaking Gammas, when for leaking neutrons - it is within 10%* (*???*)

II. Iron (1): IPPE bare ^{252}Cf source of <u>Gammas</u> vs. others

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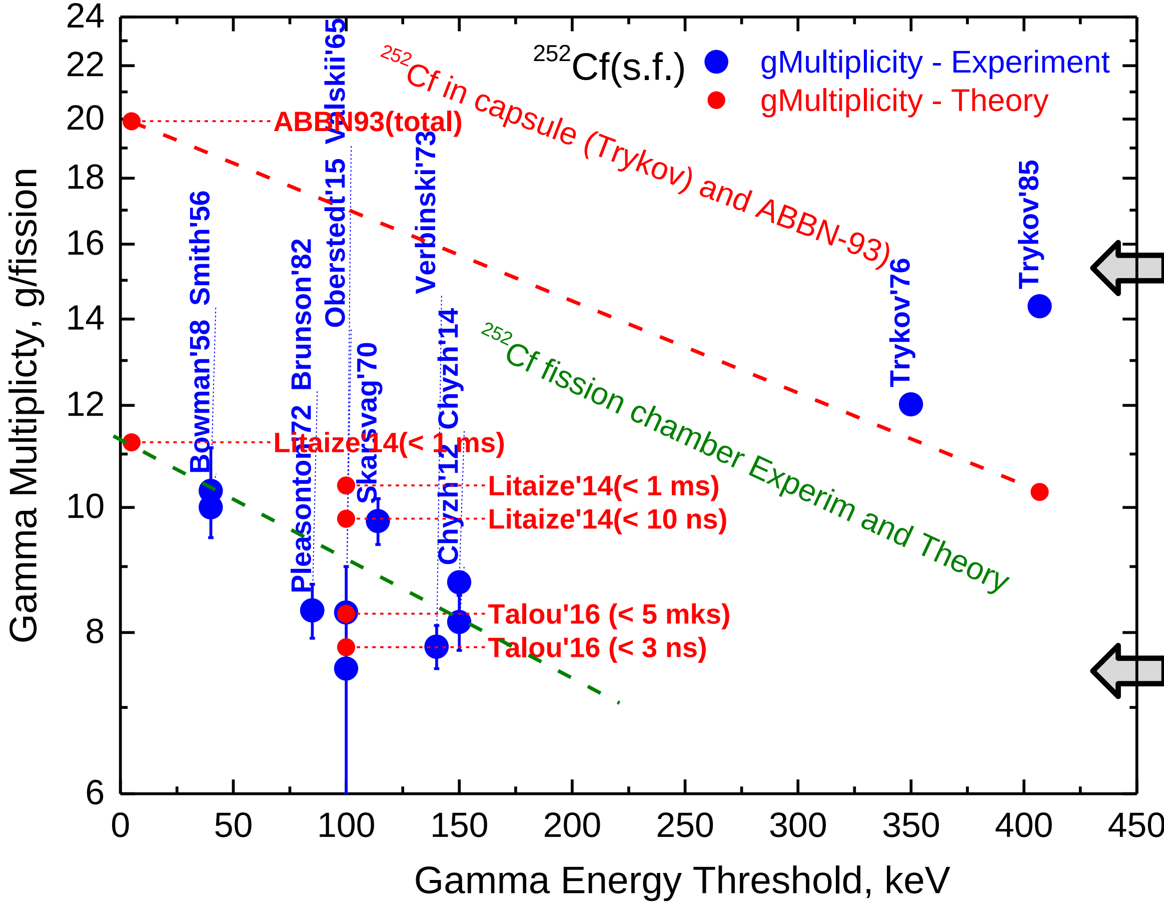
^{252}Cf(s.f.) <u>Gamma Multiplicity</u>: L.Trykov (ICSBEP, …) vs. other known data



Bare ^{252}Cf source encapsulated in 3.2mm thick Fe + 2.3mm Cu:

- Trykov'85 (FEI-1730) = 3.8 g/n *then* *3.7676 = 14.3 g/f

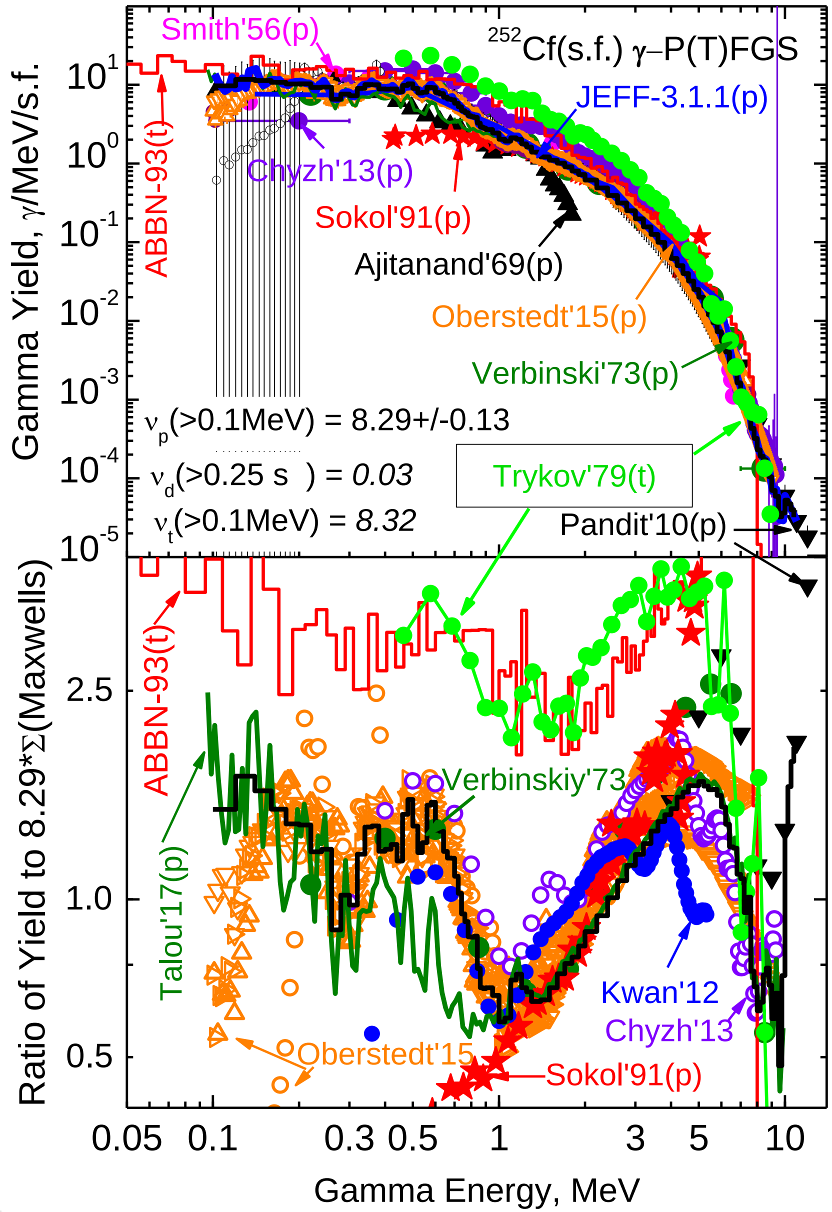
^{252}Cf from ABBN'93 = 5.287 g/n *then* *3.7676 = 19.9 g/f

Measurements which employ ^{252}Cf fission chambers and coincidence/counting FF as well as Theory/Modelling

Observations on Gamma to Neutron Multiplicities ratio Mg/Mn for ^{252}Cf(s.f.), Eγ > 100 keV:

- **all known measurements (Cf fission chamber) and theory ≈ (8 - 10)/3.7676 = (2.1 - 2.7) – it's truth !**
- **Trykov/Alarm-Cf-Fe-Schield-001 (encapsulated Cf) ≈ (18 - 20)/3.7676 = (4.7 - 5.3) – why ?**

II. Iron (1): IPPE bare ^{252}Cf source of Gammas vs. others (cont.)



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^{252}Cf(s.f.) Gamma Energy Spectra: Trykov (ICSBEP, …) vs. other known data

Looking on these spectral data I did following:

***1. from comparison of g-spectra** (Eg = 0.5 - 3 MeV)*
from L.Trykov' bare Cf source
(corrected for attenuation in CuFe capsule)
and known PFGS
there was found Normaliz. Factor = 0.33 ± 20%

2. this Factor was applied to all Iron g-leakage spectra measured by L.Trykov
(all slides on next slides show his data after correction)

3. in MCNP input file the ABBN-93 g-spectrum was replaced by one derived from independent measured PFGS (< 1 MeV) and P.Talou' modelling (> 1 MeV)

NB. Additional verifications of such correction against independent measurements of g-leakage from encapsulated Cf source and Fe spheres are highly needed

II. Iron (1): Results for IPPE bare ^{252}Cf(s.f.) source: <u>Gamma Spectrum</u>

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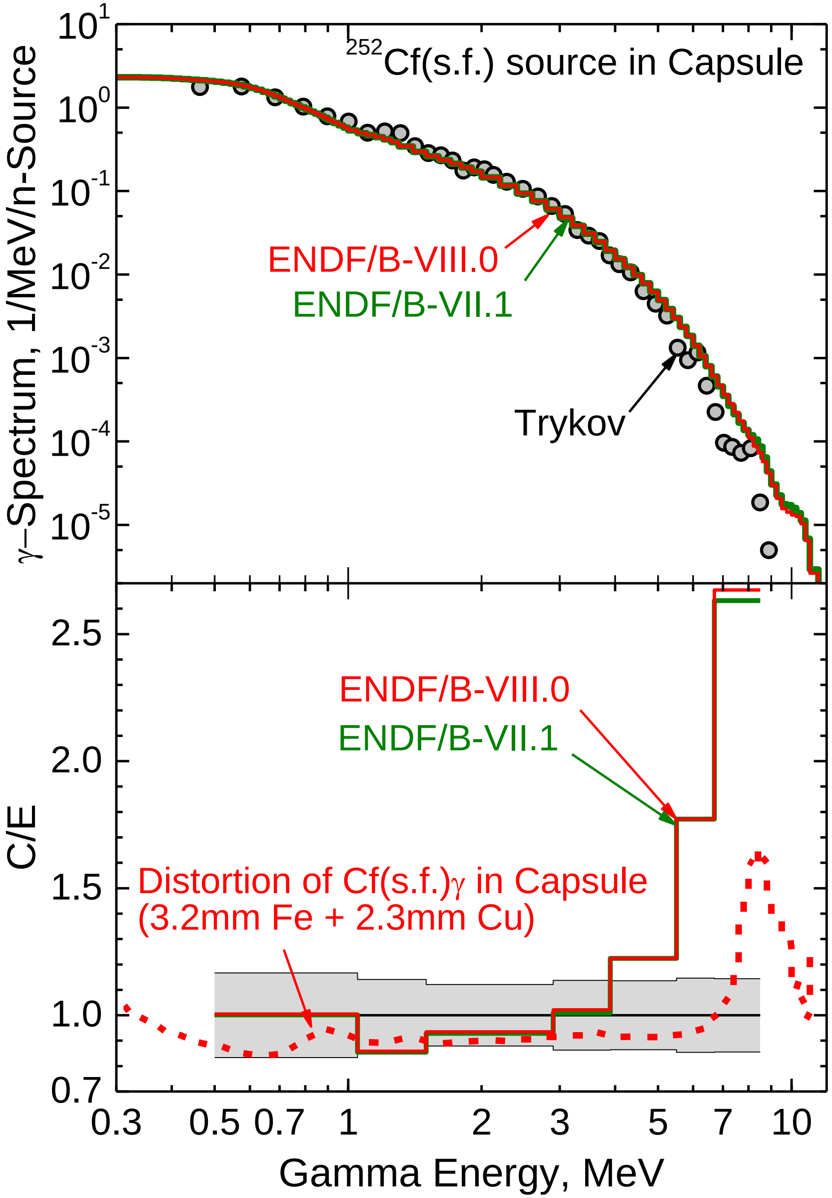


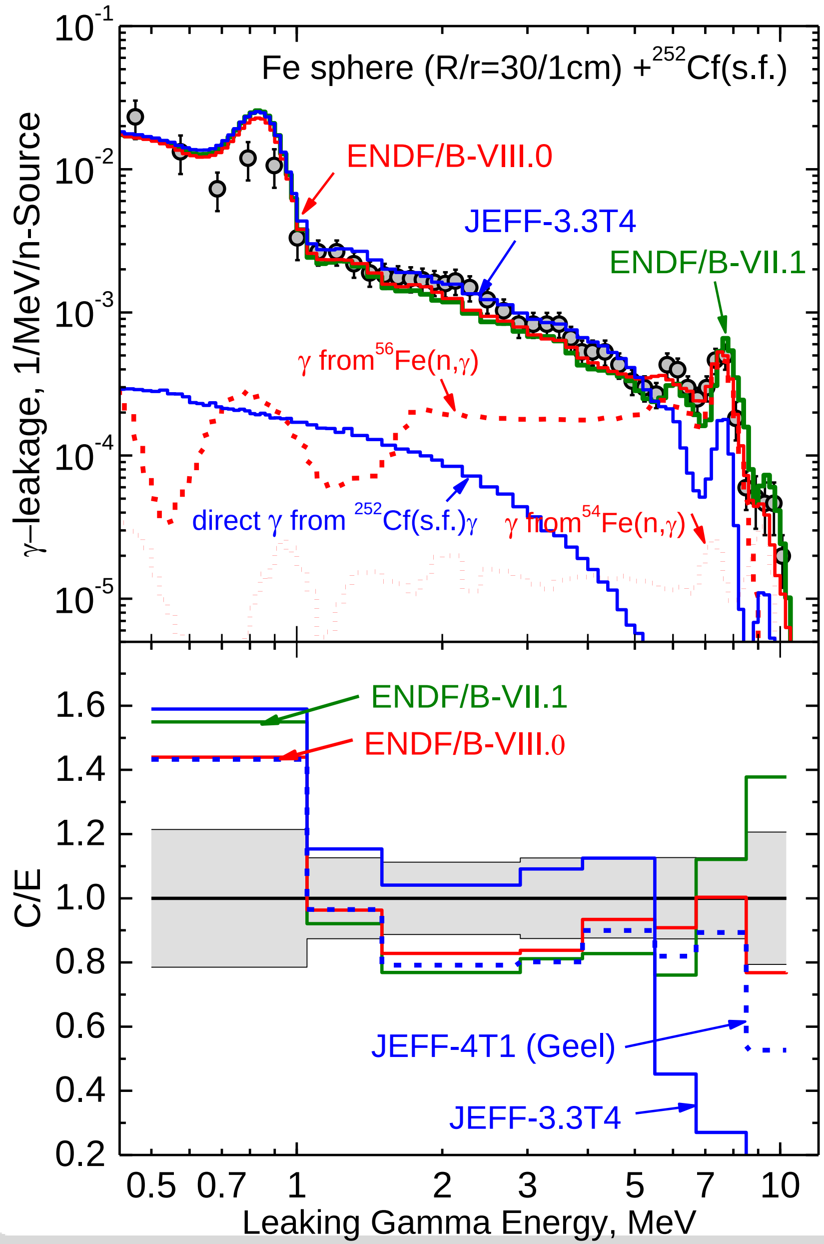
Observations/Comments on:

1. Distortion of Cf(s.f.) Gamma Spectrum in Fe/Cu capsule:

- below 7 MeV – attenuation by ≈ 10%
- above 7 MeV – increasing by up to 50% due to (n,γ) on Fe and Cu

2. above 5 MeV the Cf(s.f.) γ-spectrum or L.Trykov' bare source data seem are not so reliable - there we used P.Talou' modelling since existing experimental PFGS data are controversial

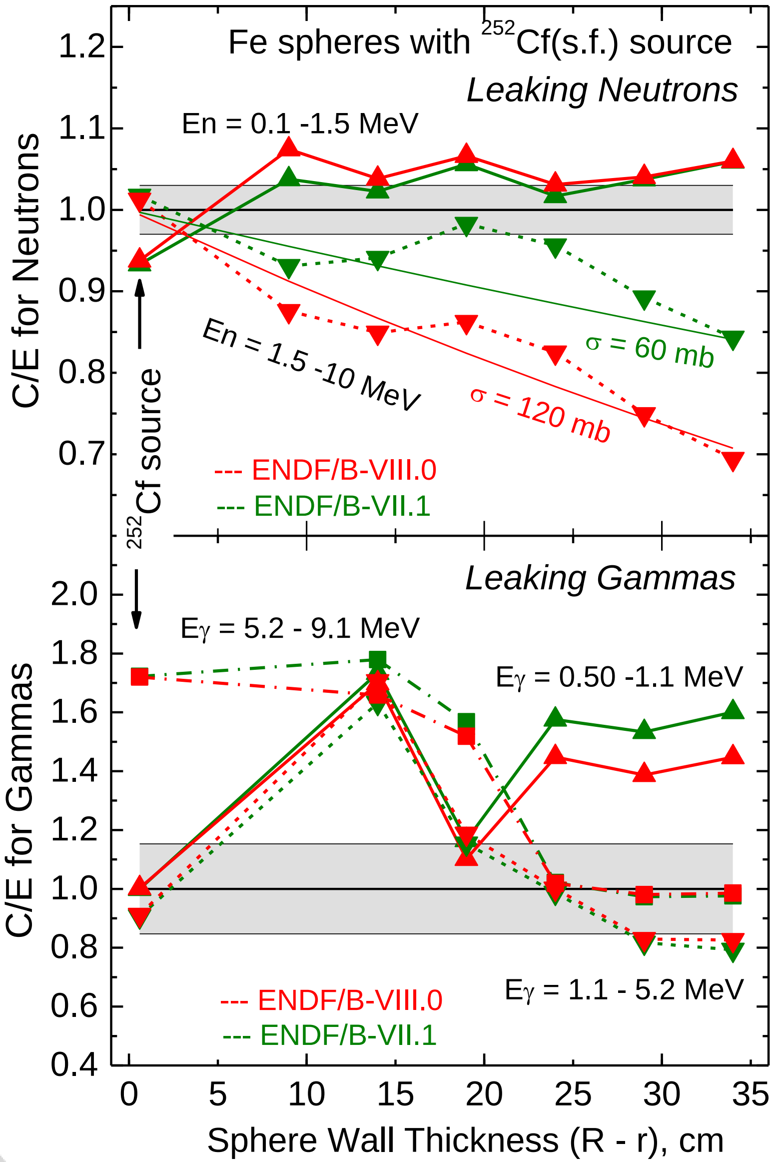
II. Iron (1): Results for IPPE Fe sphere (Wall=29 cm) with ^{252}Cf(s.f.): Gamma Leakage



Observations/Comments for Gamma leakage:

- **No essential difference between JEFF-4.0T1, ENDF/B-VII.1 or ENDF/B-VIII.0**
- **but JEFF-3.3T4 lacks of high energy gammas from "thermal" (n,γ) on Fe-56 and Fe-54 as TENDL-2015/2017 do**

II. Iron (1): Results for IPPE Fe sphere with ^{252}Cf(s.f.), Neutron and Gamma Leakage vs. Wall Thickness

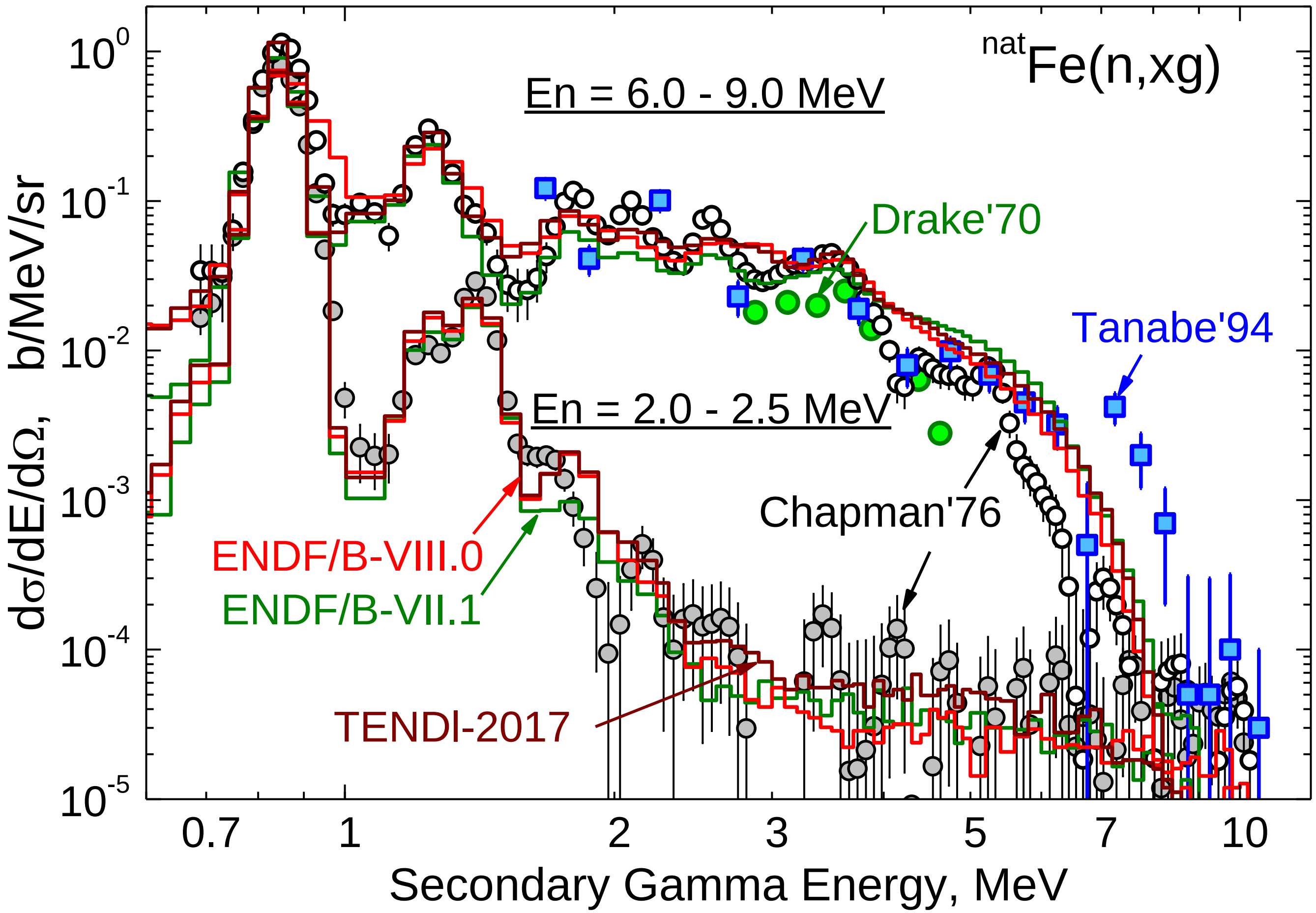


Observations:

- **Leaking Neutrons**
  0.1 - 1,5 MeV – both ENDF/B-VII.1 and ENDF/B-VIII.0 are doing well
  1.5 – 10 MeV – both lack removal XS
  = 60 mb (ENDF/B-VII.1)
  = 120 mb (ENDF/B-VIII.0)
- **Leaking Gammas**
  status is worse than for neutrons

Long Terma Int. Collaboration, 18 - 21 Dec 2017, IAEA, Vienna

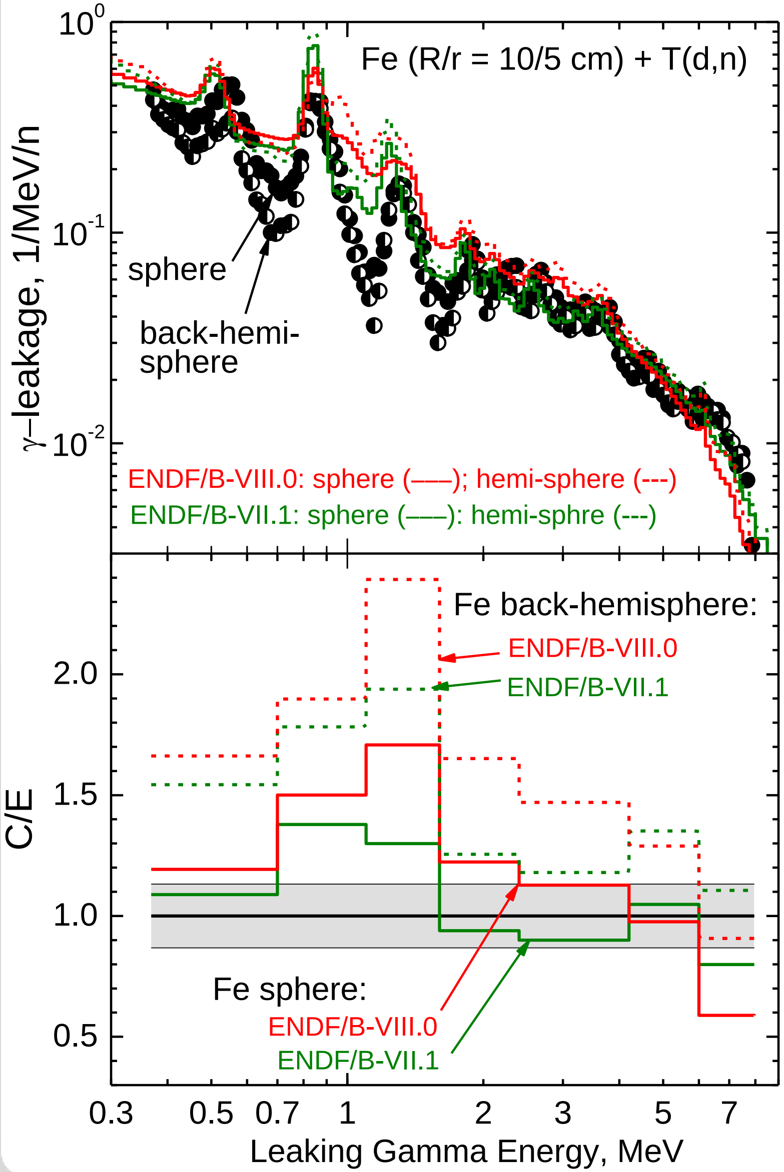
II. Iron (2): Independent DDX Measurements: Fe(n,x) γ-production spectra at ≈2 and ≈7 MeV



Observation for differential Gamma spectra:

- **Differential Experimental γ-ray production spectra for Fe(n,xγ) reaction at neutron energies typical for Cf(s.f.) transmission benchmark do support the latest evaluations ENDF/B-VII.1, -VIII.0 and TENDL-2017**

II. Iron (3): Independent Experiment for <u>Gamma leakage</u>: VNIITF hemi- and spheres with D-T source



Observations for VNIITF' Fe-sphere (Wall = 5 cm), Leaking Gammas:

- **whole sphere: ENDF/VII.1 looks almost perfect and better than ENDF/B-VIII.0**
- **back hemi-sphere: both ENDF/VII.1 and ENDF/B-VIII.0 overpredict by 30-150%**

II. Iron, *the third part:*

straightforward Monte-Carlo propagation of Cross Section Uncertainties to Clean Benchmark Response Covariances

II. Iron: from TENDL-2017 random files to Covariancies for Energy Spectra of Neutrons and Gammas leaking from Iron Spheres fed by ^{252}Cf(s.f.) source

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- ***Propagation Method implemented:***

- 1 + 500 TENDL-2017 Bayesian Monte Carlo (BMC) random files for each stable Fe isotope were provided by *A.Koning and D.Rochman*

- all were processed to ACE files by NJOY2012.82

- MCNP-6 simulation of neutron-gamma transport was re-run 1 + 500 times

each run *(1.E+9 events to reduce statistical uncertainty well below 1%)* takes ≈ 3 min on 300 CPUs of KIT server

total Wall time consumed was ≈ 16 hours (*i.e., it is a feasible task !)*

- neutron and gamma leakage spectra have been read-in from 501 MCNP output files to compute Covariancies Matrices

- ***Example of Application:***

- IPPE Iron sphere (R/r = 30/1cm, dia = 60 cm) with ^{252}Cf(s.f.) source:

results - on the next 2 slides =>

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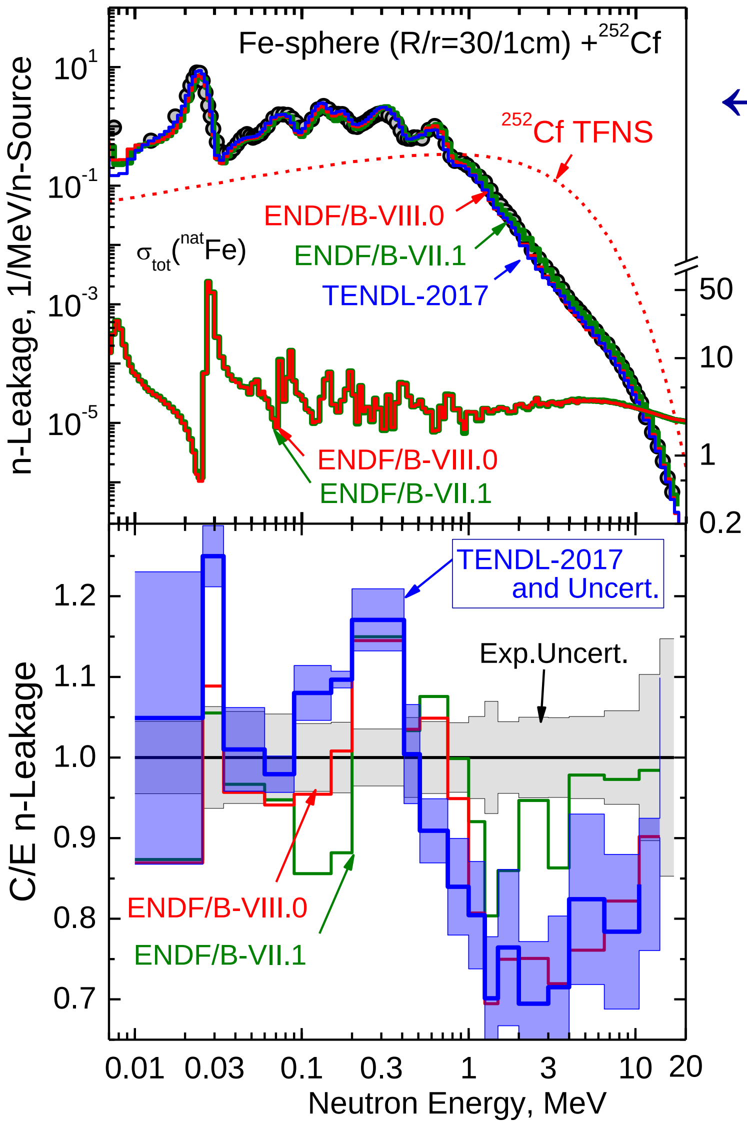
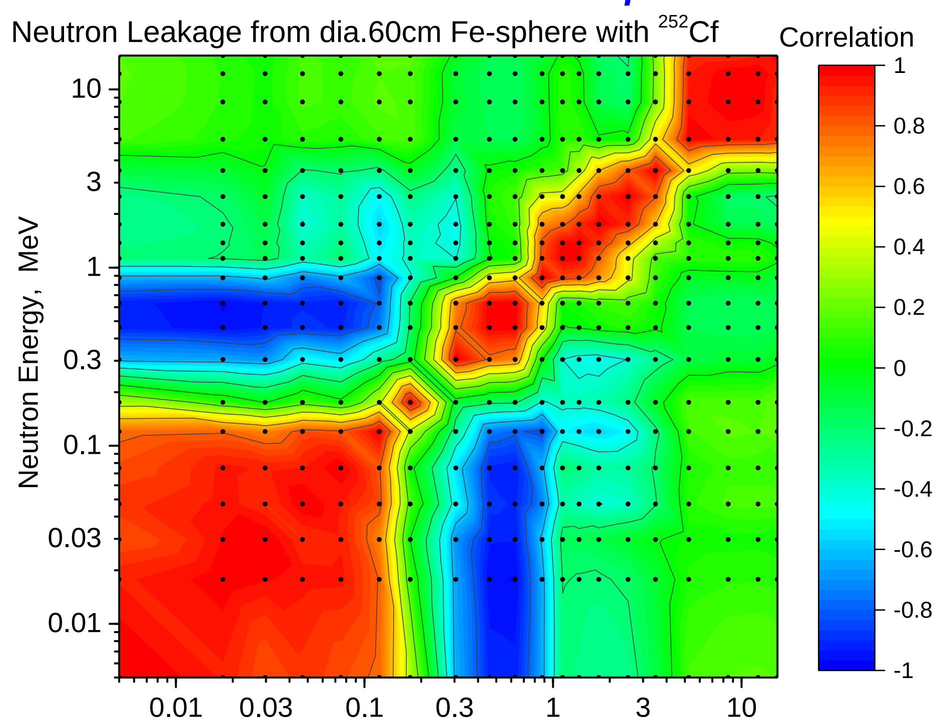
II. Iron: TENDL-2017 and Covariance propagation for IPPE Fe sphere with Cf source: Neutron Leakage



← ***n*** **Leakage and Uncertainties ≈ 2 - 20%**

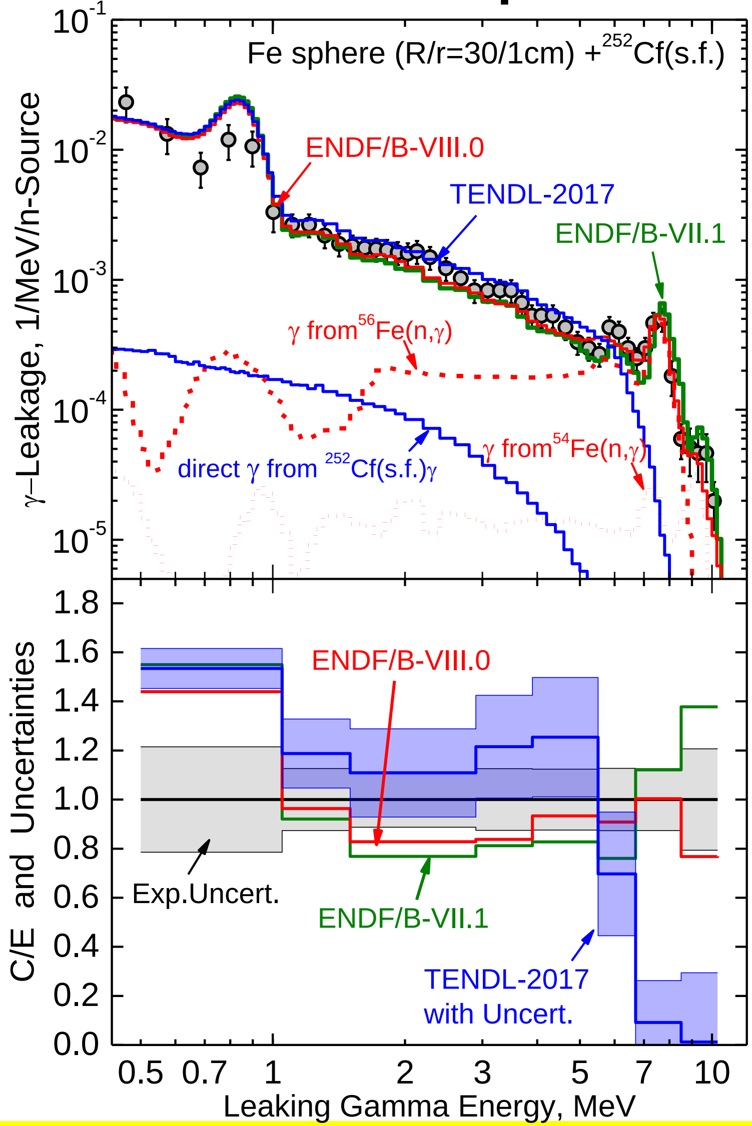
↓ ***n*** **E-E Correlation Matrix: from strong correlation (≈ 1) to anti-correlation (≈ -1)**

NB: Please note: original values are discrete points, colours are continuum interpolation between them!



Findings for n-Leakage: - Uncertainties (≈ 2-20%) from TENDL-2017 are comparable with Experimental
- E-E correlations will play role below 100 keV, above 1 MeV – no correlation

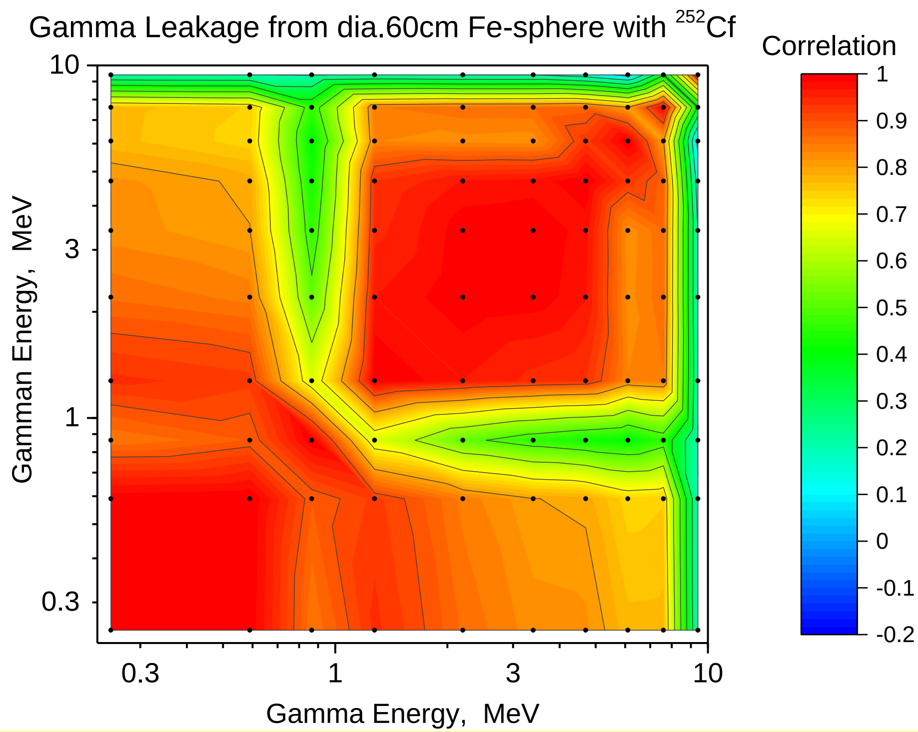
II. Iron: TENDL-2017 and Covariance propagation for IPPE Fe sphere with Cf source: Gamma Leakage



← γ Leakage and Uncertainties ≈ 20 - 40%

↓ γ E-E Correlation Matrix: practically everywhere strong correlation (≈ 1)

NB: Please note: original values are discrete points, colours are continuum interpolation between them!



Findings for γ-Leakage: - Uncertainties (≈ 20-40%) from TENDL-2017 are comparable with Experimental
- TENDL-2017 underestimates Measurements: seem it lacks (n,γ) to ground state
- E-E correlations will play role in whole energy range 100 keV - 10 MeV

III. Uranium:

Secondary Neutrons and Gammas Validation

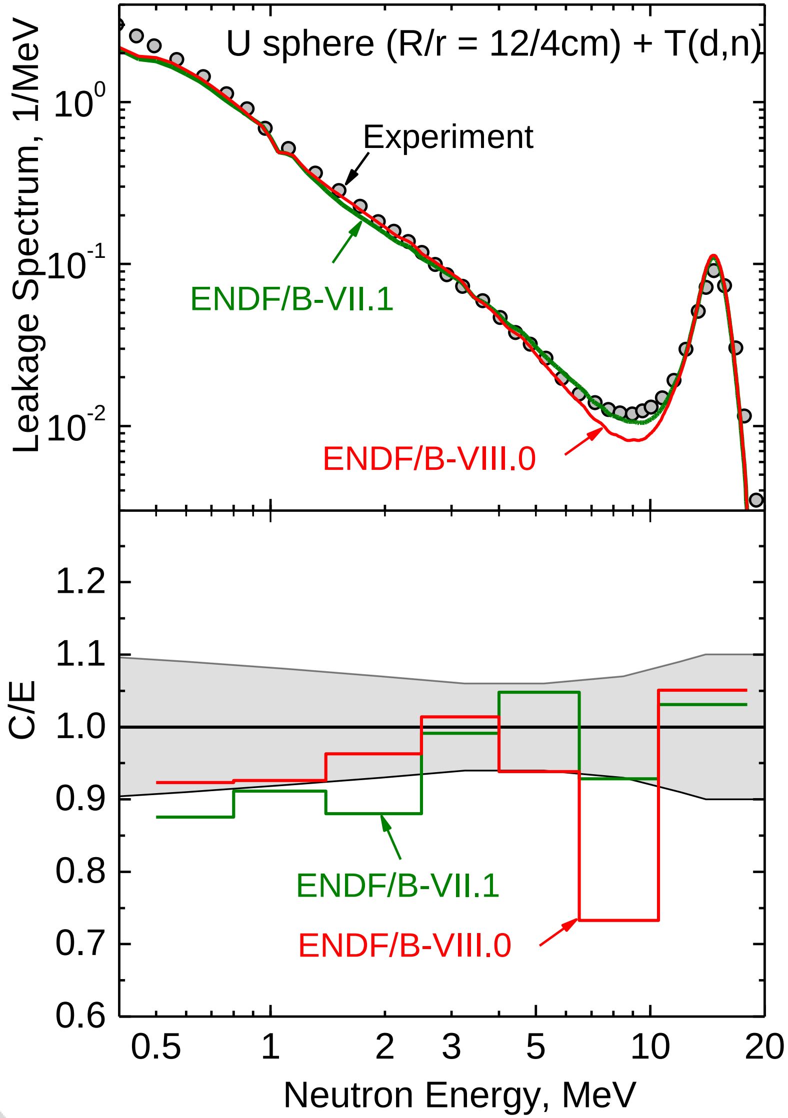
III. Uranium (0) – overview of

Experiments involved in the present analysis:

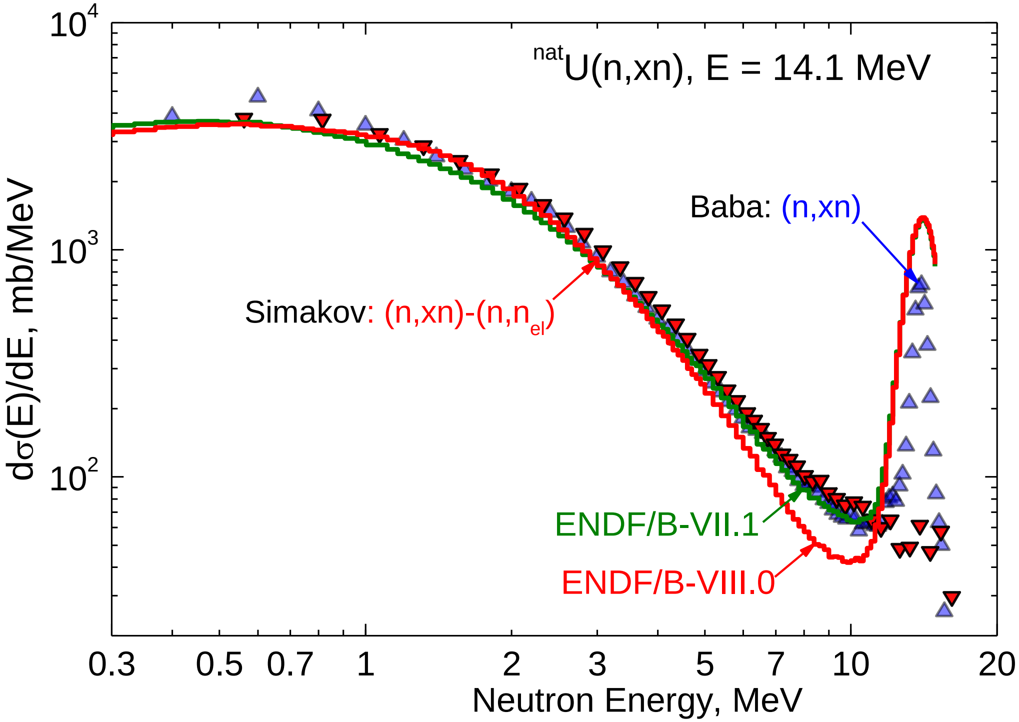
Lab Years	Source: <Energy>	No. of Spheres: Wall Thickn., cm	Method	Detector, Threshold	Numerical Data from
IPPE 90-91	D-T: ≈ 14 MeV	1 sphere: Wall = 8.0 cm	Time of Flight (TOF)	*Neutrons:* Stilben > 0.5 MeV	*S.Simakov et al.* *AIP Conf. 769(2004)67*
IPPE 1998	^{252}Cf: ≈ 2.1 MeV	1 sphere: Wall = 8.0 cm	Time of Flight (TOF)	*Neutrons:* Stilben 0.5 - 17 MeV	*S.Simakov et al.* *AIP Conf. 769(2004)67*
LLL 1976	D-T: ≈ 14 MeV	2 spheres: Wall ≈ 3.2, 10.4 cm	Time of Flight (TOF)	*Neutrons:* NE-213 > 0.010 MeV Li-glass 10keV - 1MeV	*L.Hansen et al.* *N.Tech 51(1980)70* *C.Wong UCRL-76263(1971)*
LLL 1990	D-T: ≈ 14 MeV	1 sphere: Wall ≈ 3.2 cm	Time of Flight (TOF)	*Neutrons:* NE-213 > 1.2 MeV *Gammas (as e-recoils):* NE-213 > 0.255 MeV	*E.Goldberg et al.* *NSE105(1990)319*
VNIITF 1991	D-T: ≈ 14 MeV	1 sphere & 1 semi-sphere: Wall = 5 cm	Time of Flight (TOF)	*Neutrons:* Stilben > 0.25 MeV *Gammas:* Stilben > 0.35 MeV	*A.Saukov et al.* SINBAD Fusion: *NEA-1517/74*

III. U (1): Results – Neutron Leakage from IPPE Sphere with D-T source

Neutron Leakage at 14 MeV



dσ/dE at 14 MeV

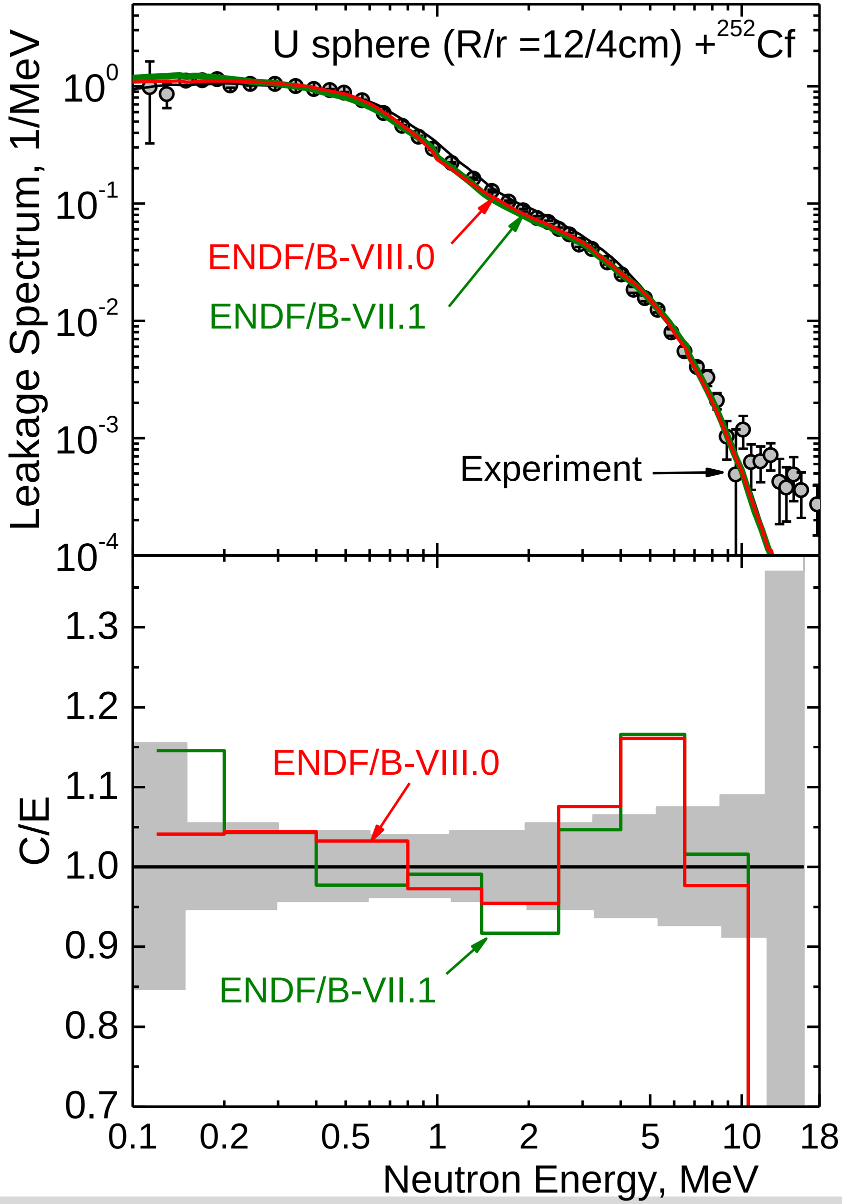


Observations:

Both Spherical Benchmark and SED (dσ/dE) discover very similar trend:

- ***ENDF/B-VIII.0 underestimate 6-12 MeV interval***
- ***ENDF/B-VII.1 looks better***

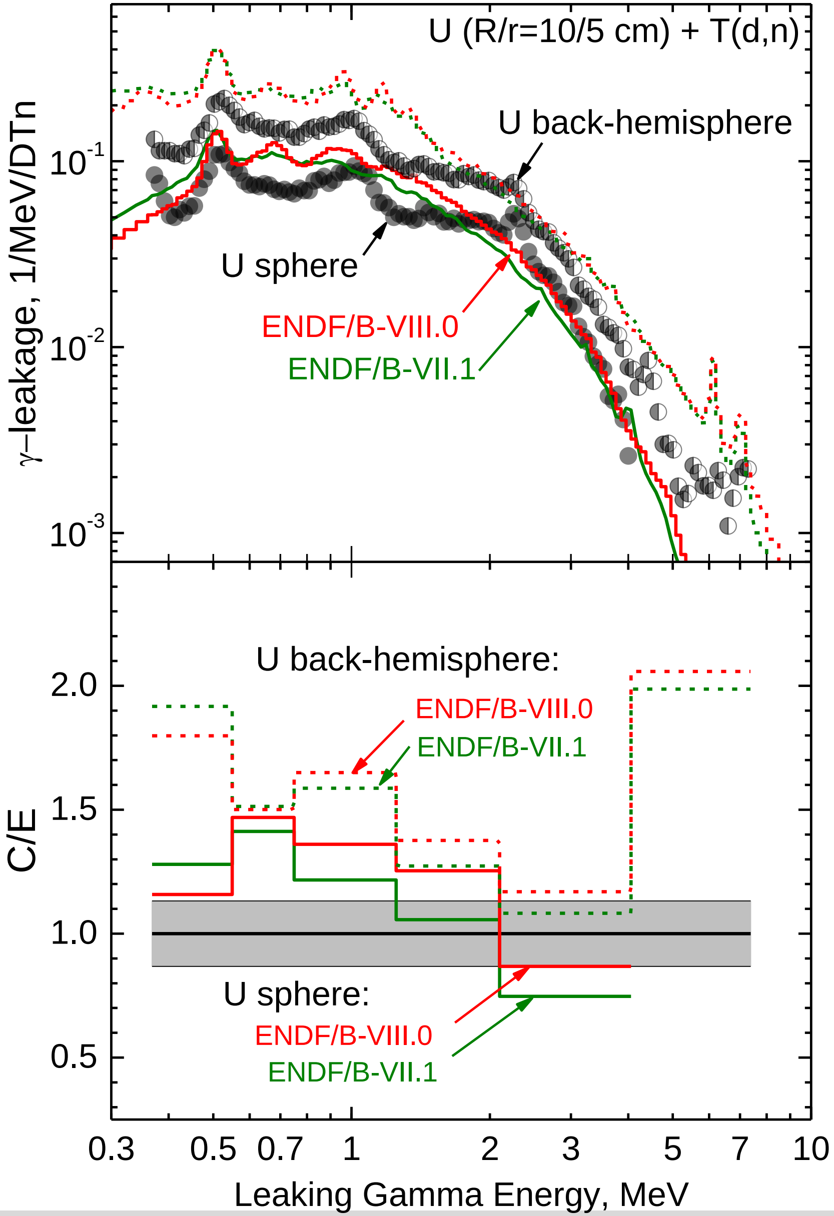
III. U (2): Results - Neutron leakage from IPPE sphere with ^{252}Cf source



Observations:

- ENDF/B-VIII.0 and ENDF/B-VII.1 perform similarly well

III. U (3): Results - <u>Gamma</u> leakage from VNIITF hemi- and whole spheres with D-T source



<u>Observations</u>:

- first results – no conclusion yet, the experiment set-up models has to be checked

General Summary (*details for each Nuclei - in proper sections*)

- **latest versions of ENDF, JEFF, TENDL evaluations for O, Fe and U are currently under validation against known clean benchmarks driven by neutron sources D-T, Cf and fast fields created at reactors**
- **quantities analyzed/tested are neutron and gamma leakage, uncollided neutron transmission**
- **relevant experimental benchmarks are available in SINBAD, ICSBEP or literature; however in some cases the complete information about measurements are not presented in these resources that prevent the correct modelling and concluding nowadays**
- **the main purposes of this work was to check <u>whether independent benchmarks as well as differential XS indicate the similar trend for potential corrections/adjustments</u>**
- **we generally saw this however excepting the case of L.Trykov' measurements of γ-leakage from Iron spheres with Cf-source: γ-spectra seem have to be downscaled by factor ≈3 to reach agreement with other differential and integral measurements *(? - still need confirmation ! - additional independent measurements will be decisive)***
- **XS uncertainties (presented as TENDL-2017 randoms) were MC propagated to Covariancies of *n*- and *γ*-leakage spectra from Fe sphere fed by ^{252}Cf**