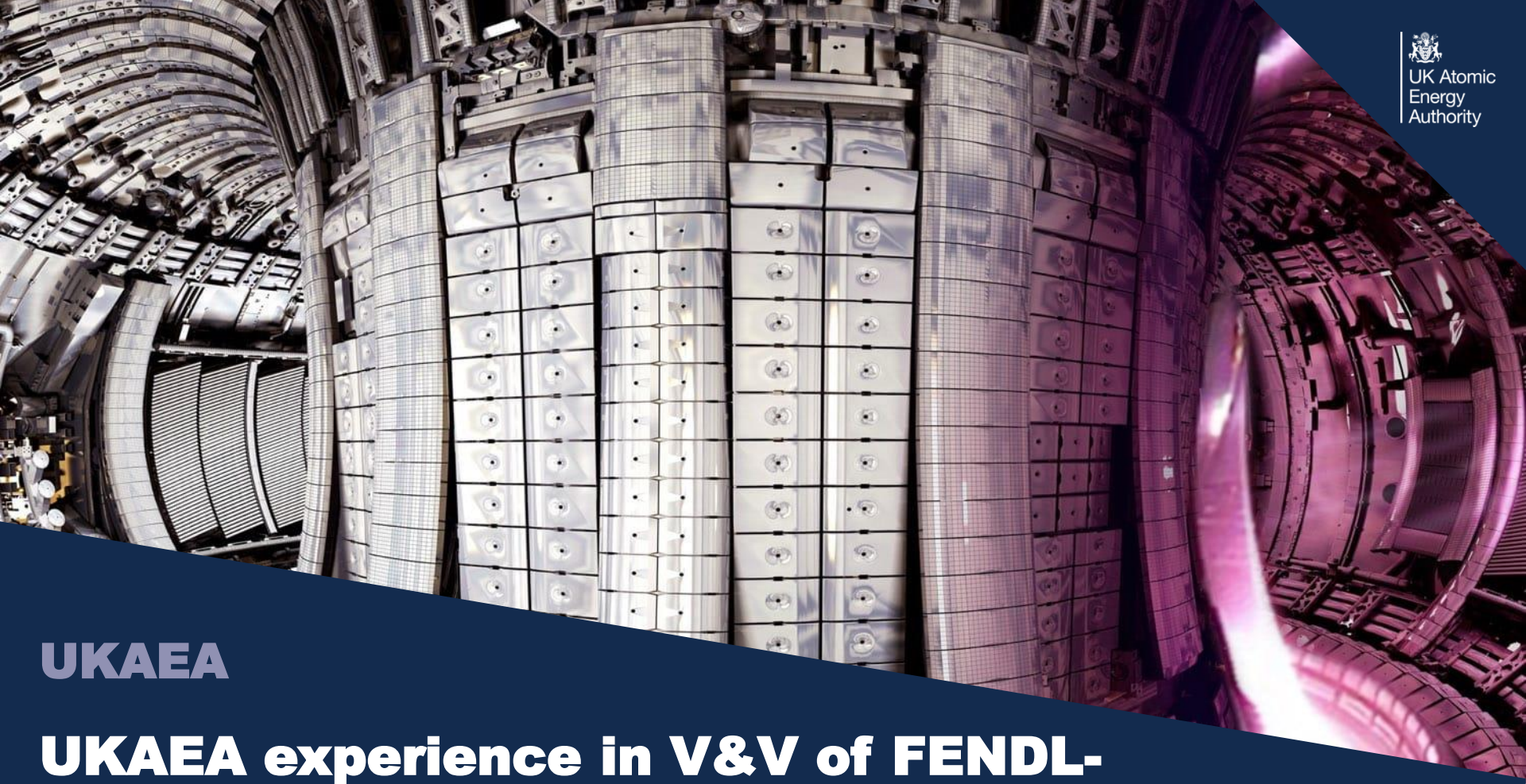


UK Atomic Energy Authority

UKAEA

UKAEA experience in V&V of FENDL-3.2 and proposals for future activities

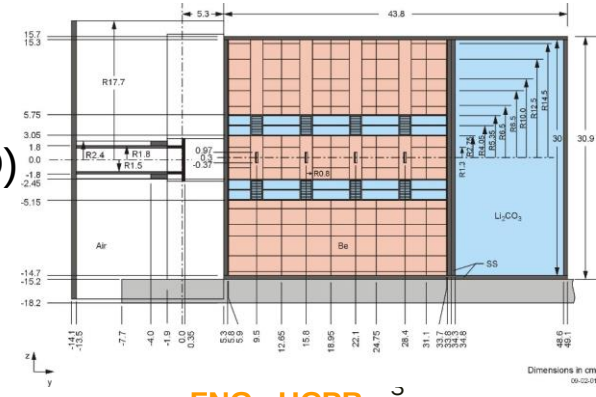
- **Ivo Kodeli**

IAEA FENDL 3.2 Meeting, Oct. 30-Nov. 1, 2023

- **UKAEA interest and V&V activities in FENDL-3.2**
- **SINBAD: Participation of IAEA/FENDL in shielding benchmark databases**
- **SUSD3D/XSUN-2023: experience with FENDL-3.2 neutron and gamma cross sections and covariances data**

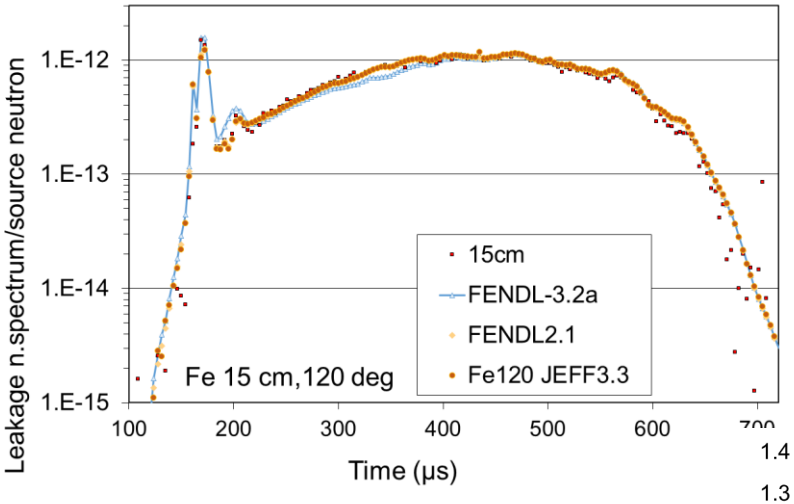
Radiation transport activities at UKAEA

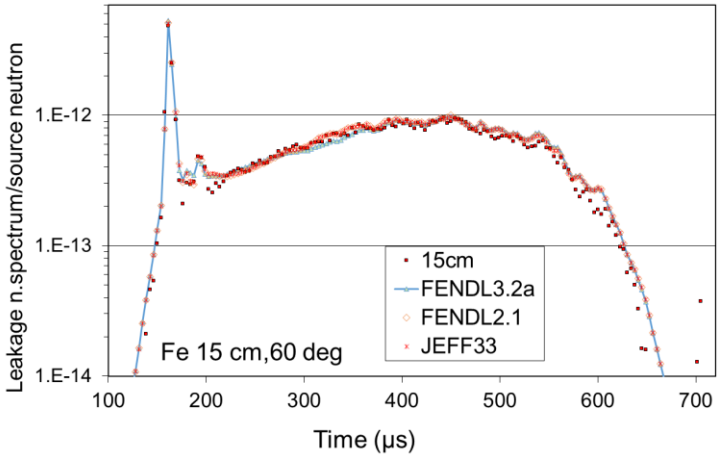
- Focus on nuclear fusion: analyses typically involve large and complex geometries, neutron & gamma source terms, higher energy neutrons than fission.
- Involved in fusion reactor projects such as **JET, ITER, STEP, MAST-U, DEMO**;
- **Licencing needs: V&V, understand and eventually reduce uncertainties**
- **Fusion research** needs (W, Cu, Fe, V, Mo, Cr, Y, Ti, C, Zr, Li, Pb, Be, Si,...)
- Predominantly **MCNP** M/C calculations using acceleration methods, but use of alternative codes is actively studied: **Serpent2, OpenMC, GEANT4, TRIPOLI**, deterministic codes (**THOR, DENOVO, DORT/TORT, PARTISN**)
- SINBAD database serves for validation of transport codes and nuclear data,
- CAD based computational workflows
- Project on automation of benchmark analysis (**JADE**).
- Nuclear data **sensitivity and uncertainty** analysis (**SUSD3D**)
- Activation & nuclear waste studies (**Fispact II**)
- Open to international collaboration: with NEA (SINBAD Task Force), IAEA (Conderc, FENDL), F4E (JADE)



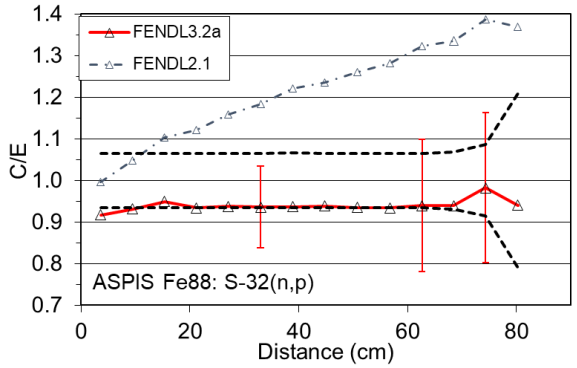
FNG –HCPB

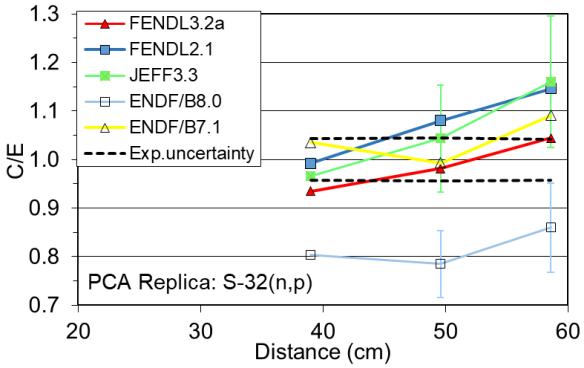
Validation of FENDL-3.2 (ASPIS, FNG, IPPE, CIAE …)

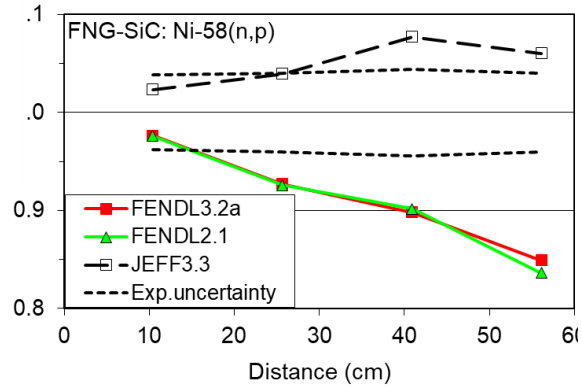


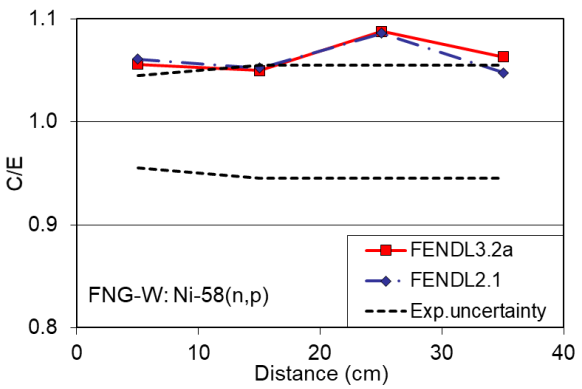


CIAE 15 cm Fe slab, TOA spectra at 60^0/120^0 using MCNP inputs provided by CIAE.

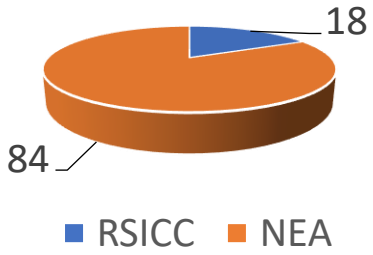






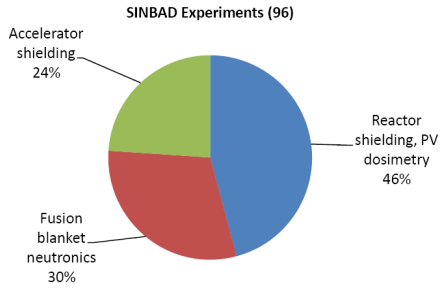


SINBAD - Radiation Shielding Experiments



- Objective: Compilation of high-quality experiments for validation and benchmarking of computer codes and nuclear data used for radiation transport and shielding problems encompassing:
  - reactor shielding, PV dosimetry **(48)**
  - fusion blanket neutronics **(31)**
  - accelerator shielding **(23)**
- **Quality review – 51 benchmarks**

Simplicity of use; easy & low-cost maintenance



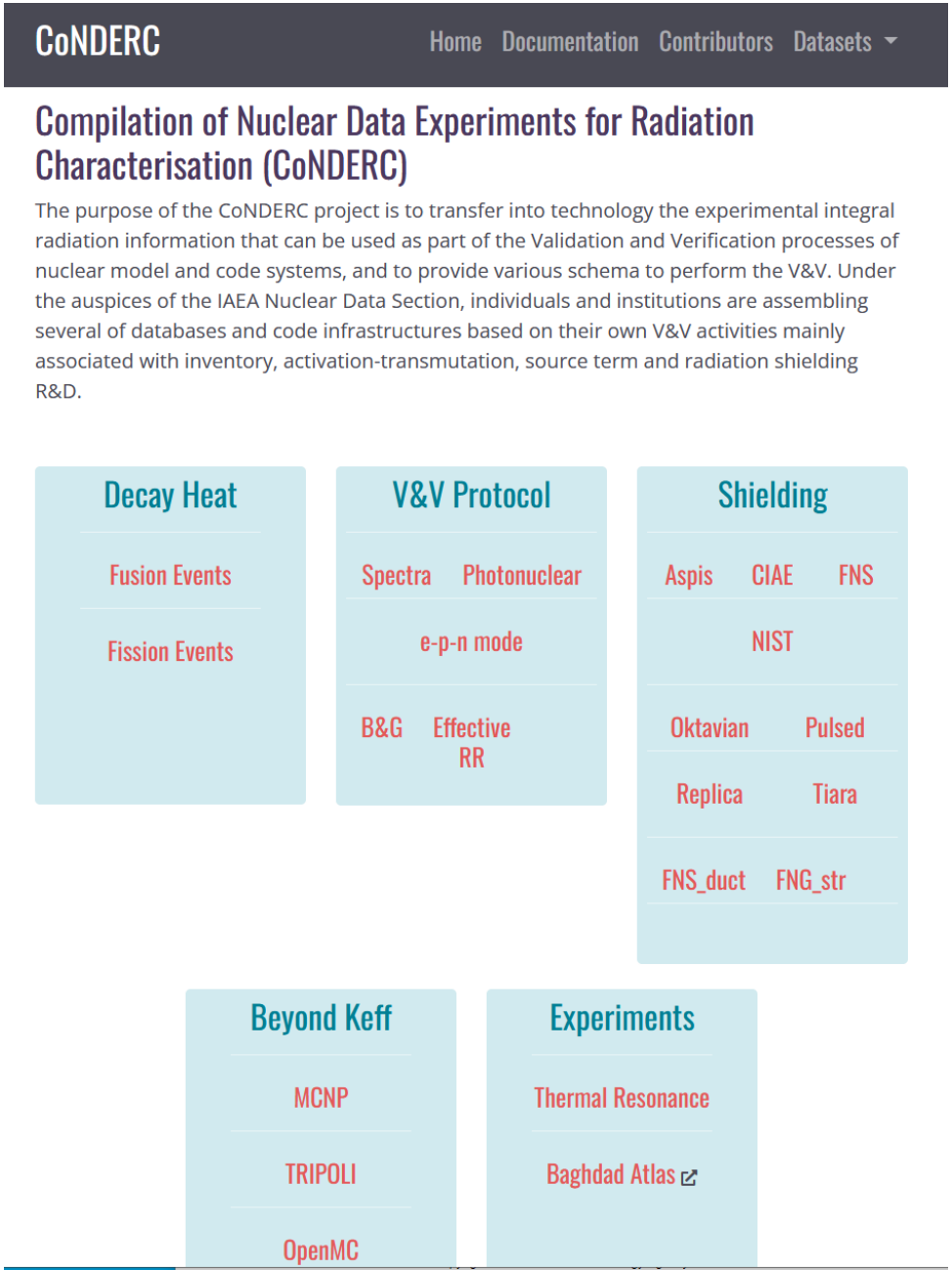
- **OECD/NEA Working Party on Scientific Issues of Reactor Systems (WPRS) Expert Group on Physics of Reactor Systems (EGPRS): monitor, steer and support the continued development of SINBAD (Chair R. Grove, ORNL)**
- **Working Party on Evaluation Cooperation (WPEC) - SG47 "Use of SINBAD for Nuclear Data Validation" 2019 – 2022 (I. Kodeli)**
- **NEA Task Force on SINBAD development (>2022) (O. Buss, NEA, T. Miller, ORNL)**

https://www.oecd-nea.org/science/wprs/shielding/sinbad/

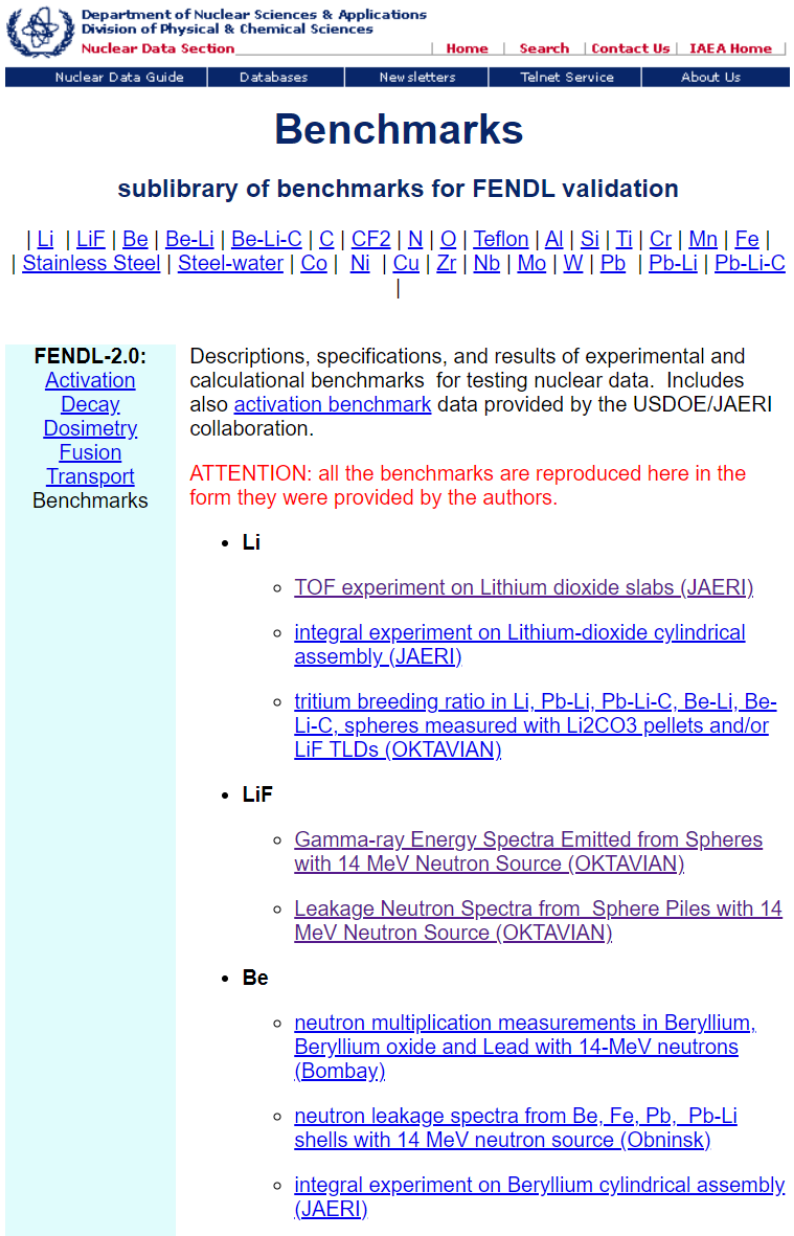
Data received during WPEC SG47 - pending evaluations/updates

- **New and updated SINBAD evaluations**
  - **FNG-Copper (Kodeli)**
  - **KFK Fe spheres g-leakage (S. Simakov)**
  - **ORNL O broomstick (S. Simakov)**
  - **CIAE Iron slab (Y. Ding, H. Wu)**
  - **TIARA benchmark (Y. Iwamoto)**
  - **ASPIS Iron88, JANUS (L. Buiron, A. Hajji, I. Kodeli, G. Rimpault)**
  - **ASPIS PCA Replica & NESDIP 3 (David Hanlon, Jacobs, Responses to Quality Assessment Concerns)**
  - **LLNL spheres (S. Kim, D. Neudecker, O. Cabellos)**
  - **BALSAC/MASURCA (CEA Cadarache 1988): internal storage for fast reactors A. Hajji, G. Rimpault, L. Buiron**
  - **PETALE program in CROCUS on stainless steel (Vincent Lamirand, EPFL)**
  - **FNS Liquid Oxygen flux definition/effective area (A. Milocco, S. Simakov, I. Kodeli)**
- **New computer code inputs:**
  - **MCNP, ADVANTG, SuperMC/INEST Hefei, TRIPOLI, SERPENT, OpenMC, GEANT, DORT & TORT, FLUKA, PHITS, MARS, MCBEND**

CoNDERC

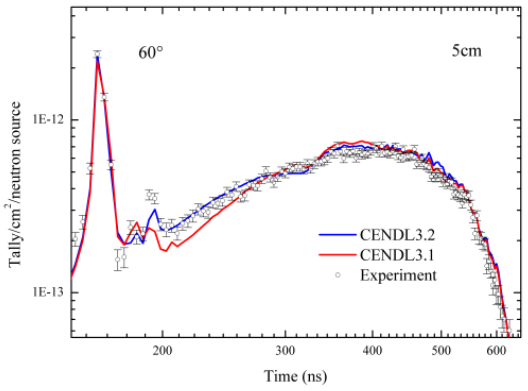


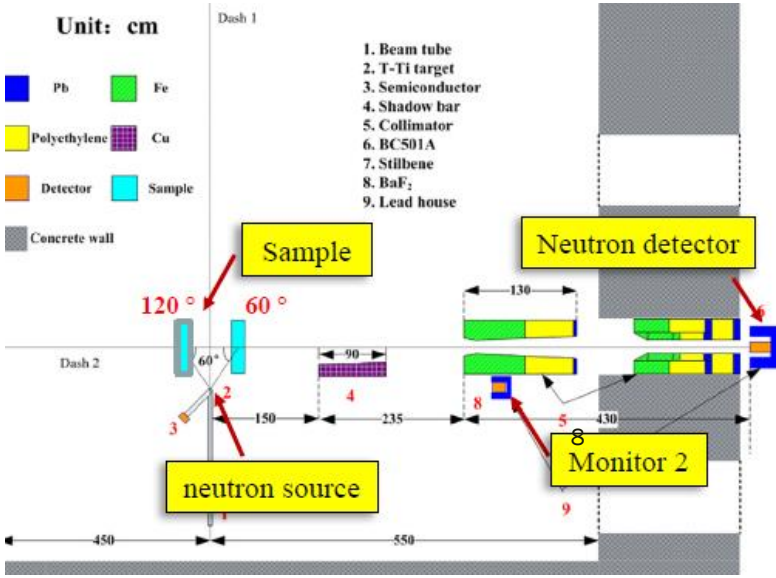
Collection of benchmarks for FENDL-2.0 validation



Yanyan Ding et al.: Benchmark experiment on iron with D-T neutrons at CIAE

- CIAE Neutron leakage spectra measurements from iron slab with D-T neutrons were presented, including the uncertainty quantification (systematic, random) and computational models. TOF spectra were measured at 60^0 and 120^0. C/E for CENDL-3.1, ENDF/B-VIII.0, JENDL-4.0 and JEFF-3.3 were shown and discussed.
- SINBAD evaluation in preparation to be presented at ICSBEP/IRPhE/SINBAD TRG meeting.
- CIEA performed benchmarks on ^{238}U, Be, Fe, Ga, W, C, SiC, Pb, Pb-Bi, ThO_2, Bi, Nb.





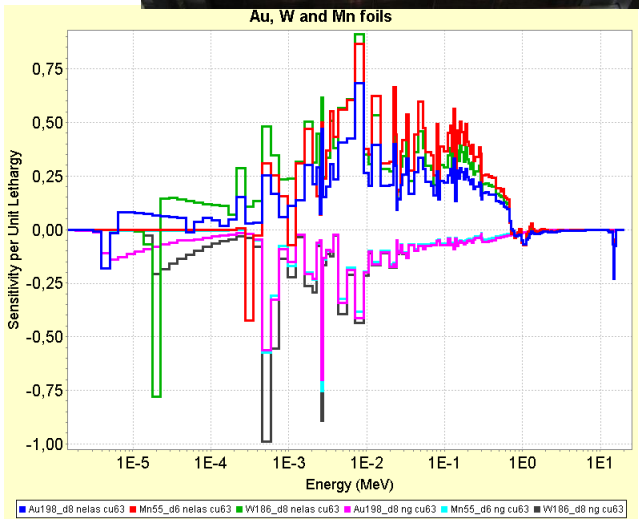
F4E 2016-2018 SINBAD related activities: FNG-Cu & FNG-HCLL

FNG-Copper: ENEA - KIT- JSI collaboration (M. Angelone et al.); pre- and post-analysis in 2014-2015, measurements between Oct. 2014 to March 2015

Block of Oxygen-free **Copper (99.90 wt.%) 60 x 60 x 70 cm^3** placed on Al support was irradiated at 14-MeV d-T Frascati Neutron Generator (FNG). 14 MeV FNG neutron source was located 5.3 cm in front of Cu block of the total weight of 2.2 t.

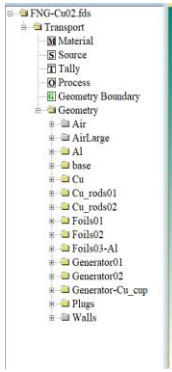
Detectors were placed at **8 locations** up to ~60 cm Cu.

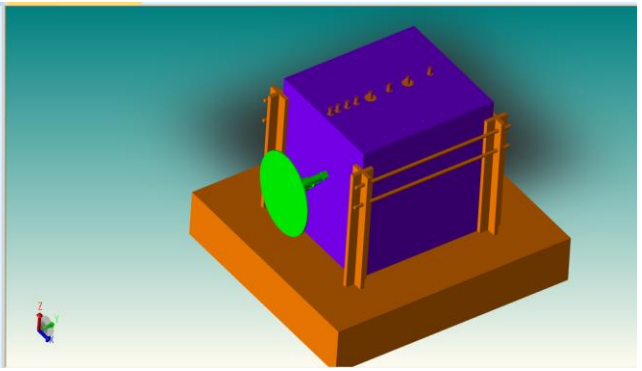
SINBAD evaluation in 2018



SINBAD data include:

- **Main benchmark description** in **PDF including uncertainty evaluations**
- **Computer code inputs**
- **CAD geometry**
- **Sensitivity profiles**
- **Reference documents in PDF**





Computational models:

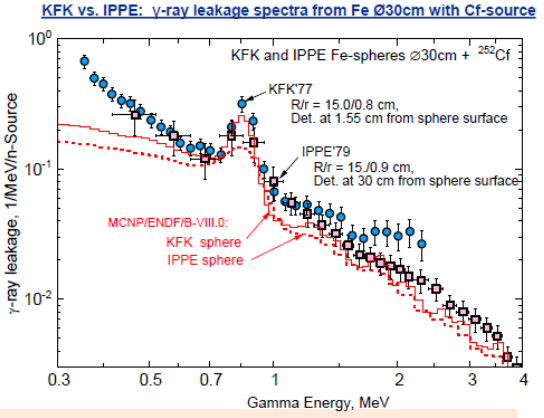
- **MCNP5/6** reference detailed model; n source description:
  - **D-T neutron source subroutine**
  - **MCUNED**;
  - **SDEF cards**
- MCNP & DORT simplified models
- Cross-section sensitivity/uncertainty analysis by **SUSD3D** & **MCSEN**

FNG-WCLL (2021)
FNG tungsten (2022-2023)

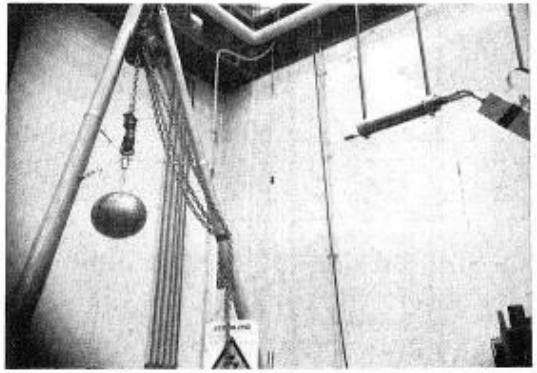
Stanislav Simakov,

- KFK γ-ray leakage (new evaluation)
- ORNL O-broomstick transmission (SINBAD update)

- SINBAD evaluation of KFK-1977 measured gamma from bare ^{252}Cf(s.f.) source and from Ø25, 30 and 35 cm Fe spheres was prepared, including detailed descriptions of facility, methods and final numerical results with uncertainties.
- Update of SINBAD evaluation on ORNL/TSR-II 60”(152.4 cm) Oxygen broomstick with MCNP model input, quality assessment and report on validation analysis and recommendations. Benchmarks are useful for total cross section validation;
- Experimental neutron transmission spectra for 24” (60.96cm), 36”(91.44cm) and probably 72” (182.88 cm) could not be found.
- Importance of evaluating a reference PFGS & DFGS of ^{252}Cf was raised.

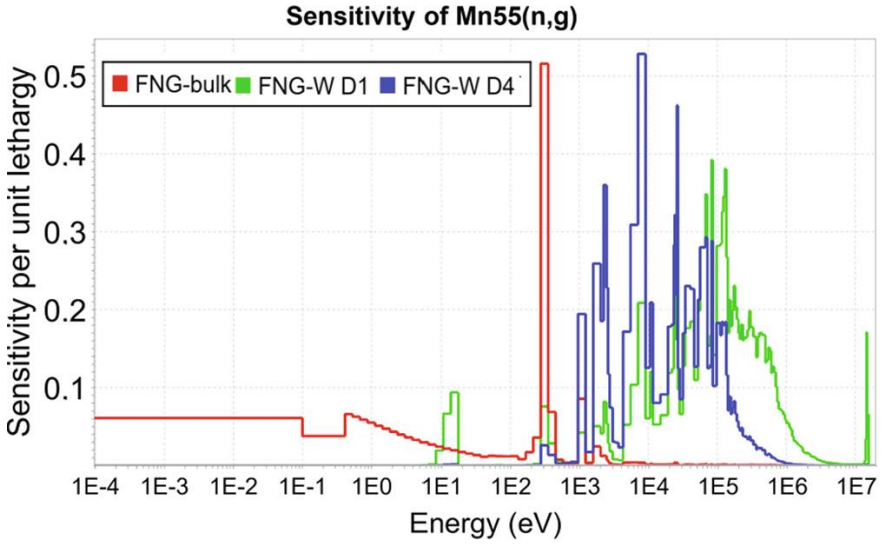


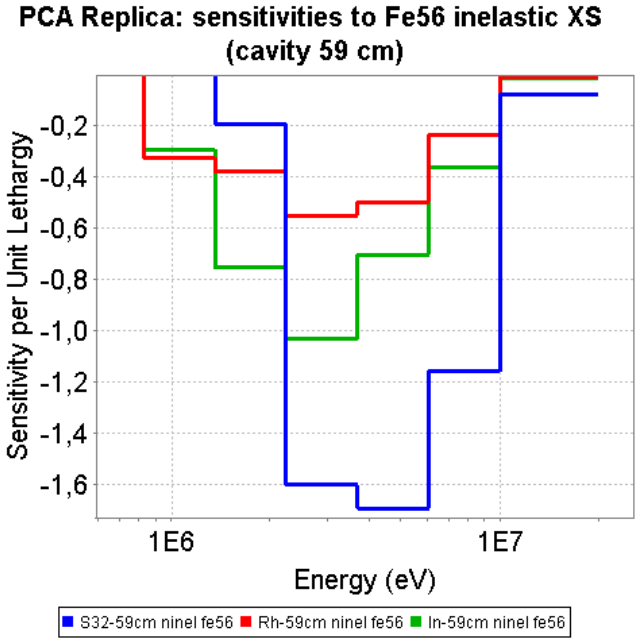
KFK set-up:

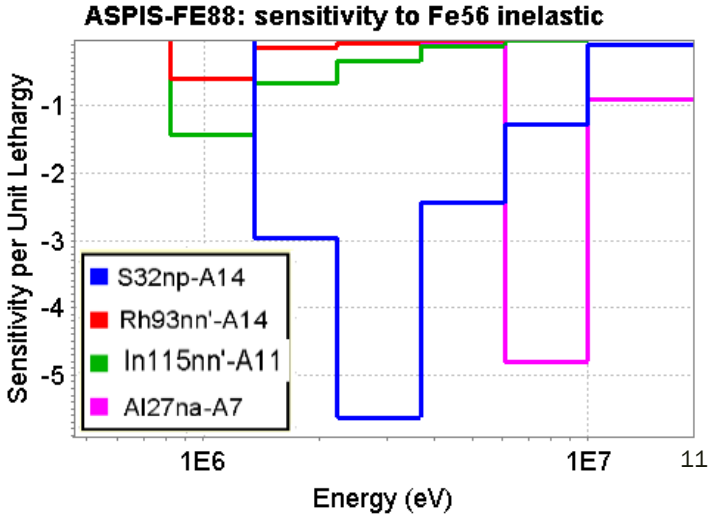


Sensitivity profiles

S/U performed for several benchmark experiments: ASPIS Fe88, PCA Replica, FNG (Cu, W, HCPB, HCLL, …), VENUS-3, LLNL. Format: SensitivitiesViewer (Nicola Soppera)

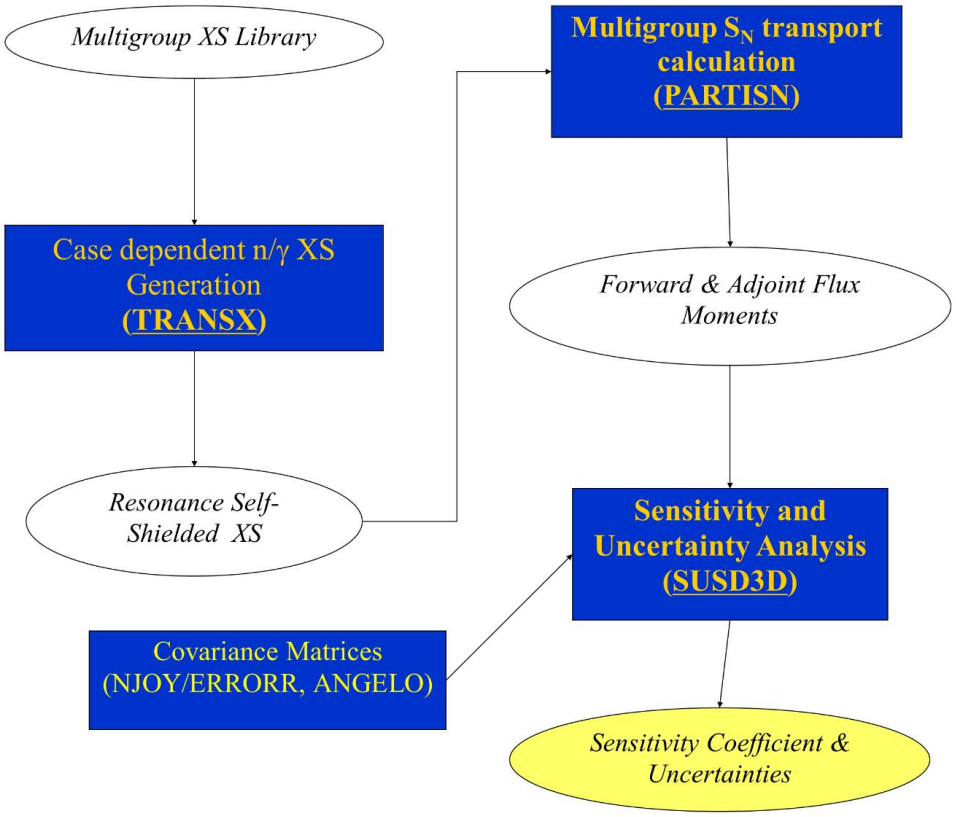






SUSD3D/XSUN-2023

S/U of k_{eff}, β_{eff}, shielding (fixed source problems); suitable for fission, fusion, …



Extension to S/U analysis of gamma related quantities (gamma flux, heating, etc.):

- **MF16** (capture/inelastic/…γ production),
- **MF23, MF26:** sensitivity to photon interaction (total, (in)coherent scattering, pair production, photoelectric,...)
- Sensitivity to n&γ source

• **Covariances in Covfils, Coverx & Boxr formats**

• **FENDL-3.2 211/42 neutron/gamma library**

XSUN2023 Nuclear Data

- up to 440 nuclides

- **Transport cross sections** in Vitamin-J 175- and ECCO 33- energy groups from **JEFF-3.3**, **ENDF/B-VIII.0, FENDL-3.2 (211n/42g)**
- **Covariance matrices** processed by NJOY or ANGELO from:
  - **JEFF-3.3** in ECCO 33n & VITAMIN-J 175n structures
  - **ENDF/B-VIII.0** (ECCO 33 & VITAMIN-J 175n)
  - **FENDL-3.2 / 3.1d** (211n/42g)
  - Older nuclear data from ENDF/B-VII.1, JENDL-4.0u, COMMARA-2, SCALE-6.0 and IRDFF for limited number of isotopes
  - **COVFILS, COVERX** or **BOXR** formats
  - **Processing:** NJOY (-99, 2016, -21), PUFF-4, ANGELO-LAMBDA
- **Ongoing:**
  - Release of XSUN-2023 package through NEA DB

FENDL-3.2 /-3.1d Covariance Data in XSUN-2023

- Covariance data only available for neutrons for some isotopes. No information for gammas! Not necessarily consistent with the cross sections in the distribution data.

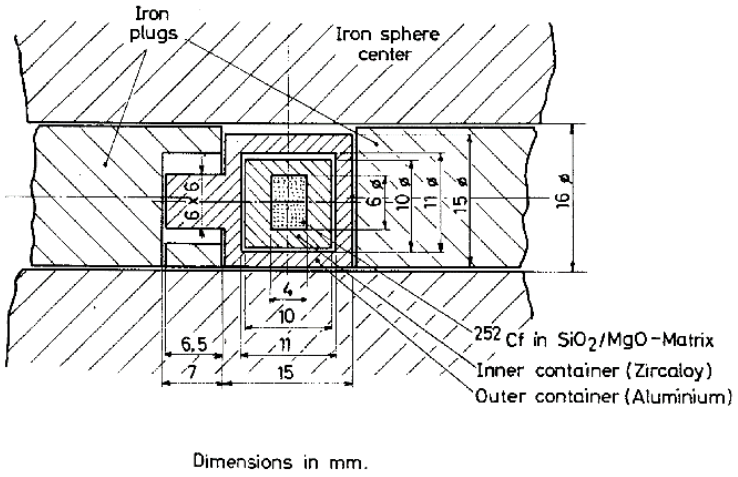
- Covariance matrices processed by NJOY or ANGELO, mathematical verification by LAMBDA code:

- **Number of nuclides with negative eigenvalues: 2**
  - **Ni58, Ti50**
- **Number of |corr(I,j)| > 1.0: 69 matrices**
  - $100 > |C_{ij}| > 10$: ^{46}Ti
  - $10^3 > |C_{ij}| > 100$: ^{182}W
  - $10^4 > |C_{ij}| > 10^3$: ^{16}O
  - $10^5 > |C_{ij}| > 10^4$: ^{33}S
  - $10^7 > |C_{ij}| > 10^6$: ^{32}S
  - $10^8 > |C_{ij}| > 10^7$: ^{13}C
  - $10^9 > |Cij| > 10^8$: ^{34}S

FENDL-3.2d (211 neutron/42 gamma energy groups)	Neutron	Gamma
MATXS files	192	192
GROUPR	193 (^{252}Cf)	62
Covariance (Covfils)	54	0

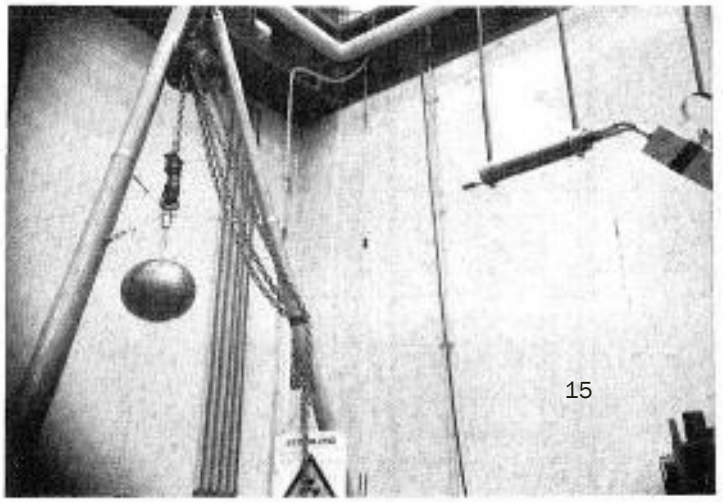
KFK γ-ray leakage benchmark (1975 – 1977)
new SINBAD evaluation by S. Simakov

- SINBAD evaluation of KFK-1977 measured gamma from bare **^{252}Cf(s.f.) source** and from **Ø25, 30 and 35 cm Fe spheres** was prepared within WPEC SG47, including detailed descriptions of facility, methods and final numerical results with uncertainties (under review within SINBAD TF).
- Neutron spectra measured using proton recoil and ^{3}He spectrometers
- **Gamma spectra** between 300 keV and 3 MeV were measured with Si(Li) Compton spectrometer. Measurement **uncertainties ~10 - 20%.** Due to the neutron background effects the authors of the experiment recommended to restrict the use of experimental data to the **0.5 – 2 MeV** range.



Dimensions in mm.

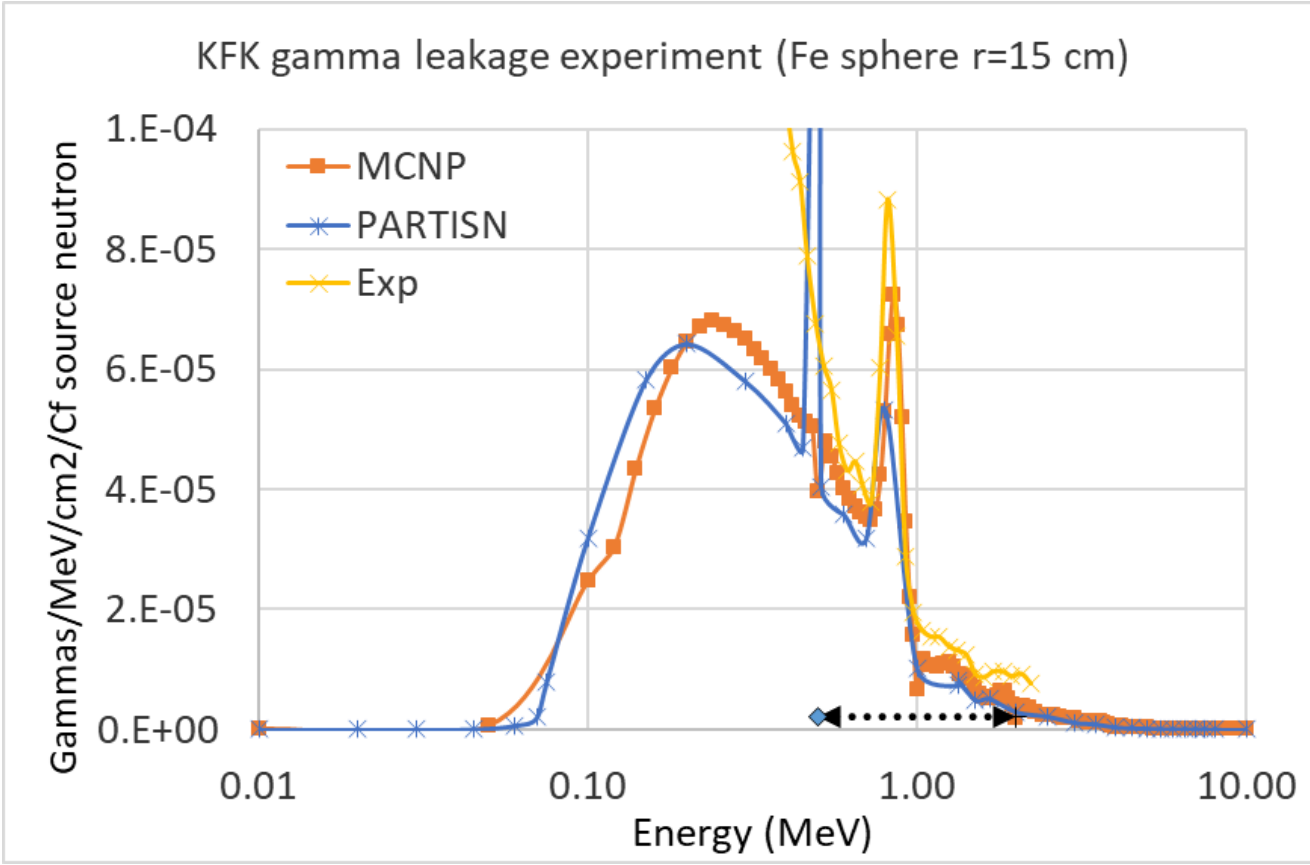
KFK set-up:



KFK γ-ray leakage benchmark – Gamma flux sensitivity/uncertainty

Computational models

- MCNP5 (prepared by S.Simakov)
- PARTISN, 1D, S_{48}/P_5
- Nuclear data: FENDL3.2, pointwise / 211n/42γ

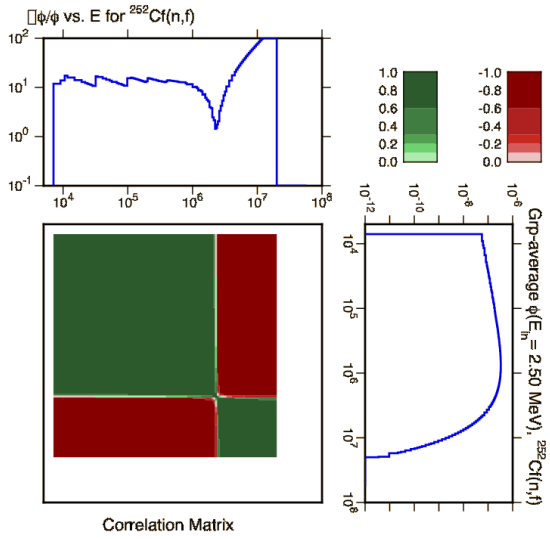


Computational uncertainty

- ^{252}Cf neutron and gamma source
- Neutron cross sections
- Gamma cross sections
- Geometry and modelling approximations

S/U: ^{252}Cf neutron and gamma source - uncertainty

γ (0.5 - 2 MeV)	^{252}Cf neutron			^{252}Cf gammas		
Sphere radius (cm)	Total	Prompt	Delayed	Total	Prompt	Delayed
12.5	50.94%	50.93%	0.01%	49.06%	23.44%	25.63%
15	63.54%	63.53%	0.01%	36.46%	17.56%	18.12%
17.5	82.72%	82.70%	0.02%	17.28%	10.10%	7.18%

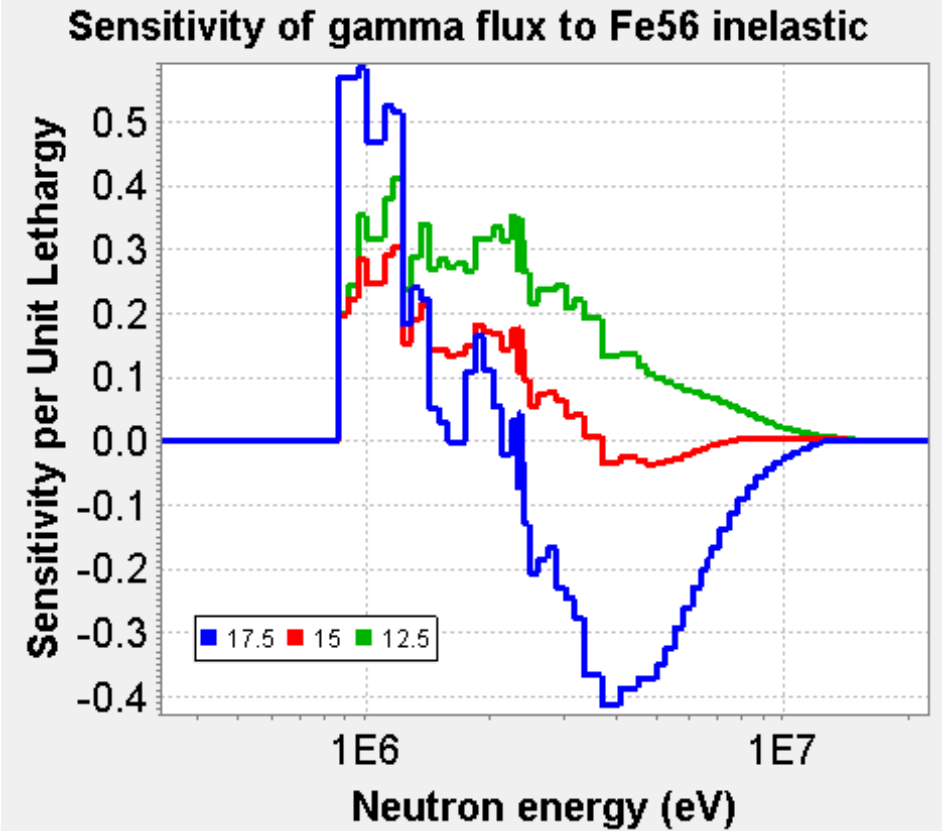


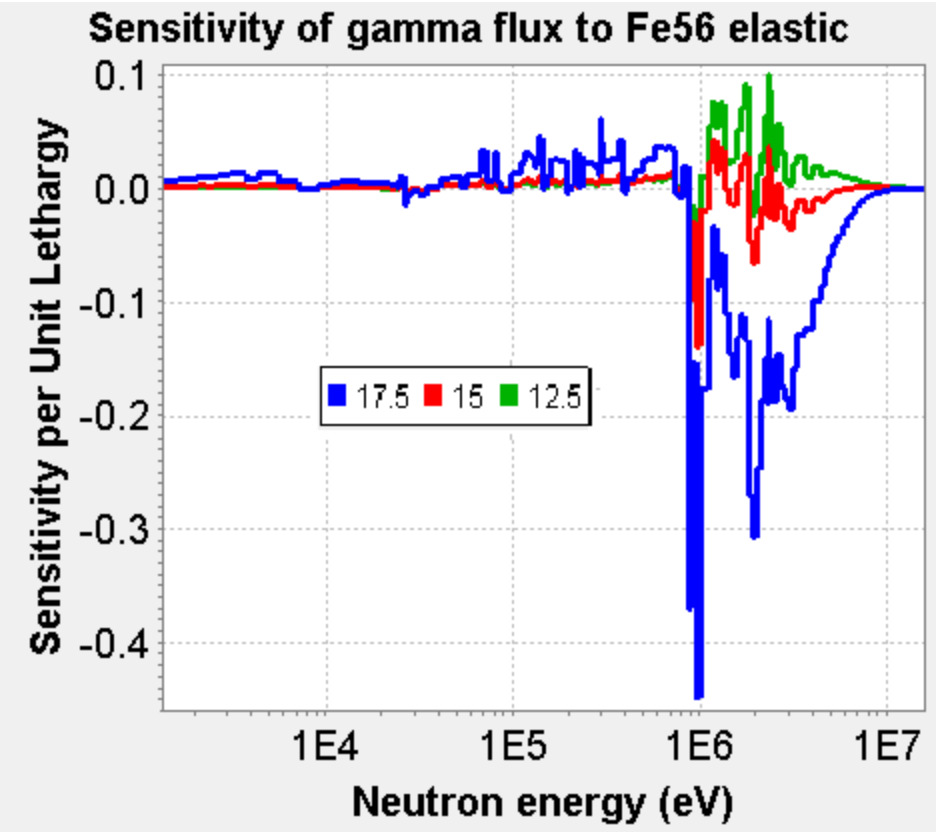
Uncertainty in 0.5-2MeV γ flux due to uncertainty in prompt/delayed fission neutron and gamma spectra. **Flat 20% uncertainty was assumed for fission gamma spectra**. PFNS uncertainties from JENDL-4.0 (=JENDL-5 = ENDF/B-VIII.0)

γ (0.5 - 2 MeV)	^{252}Cf neutron	^{252}Cf gammas	
Sphere radius (cm)	Prompt	Prompt	Delayed
12.5	6.6%	6.1%	4.5%
15	8.0%	5.0%	3.3%
17.5	9.5%	2.7%	1.4%

Nuclear data S/U: KFK-1977 (Ø 25, 30, 35 cm spheres)

Sensitivity of gamma flux E= 0.51-2 MeV at R= 16.3-16.8cm to neutron and gamma cross sections





Conclusions

- UKAEA is involved in several fusion projects, interest in FENDL project;
- Shielding benchmarks provide a powerful means for V&V of FENDL nuclear data. Feedback on future evolution of SINBAD is needed to continue its development as a framework for storing standard, verified and validated sets of experiments, available to international community;
- IAEA with its wide membership may be interest in more intensive cooperation, and encourage active involvement of fission, fusion & accelerator users in shielding benchmark database activities; shielding experts needed;
- New version SUSD3D/XSUN-2023 to be available from NEA DB with FENDL-3.2 multigroup nuclear data (and covariances), new: gamma-ray S/U analysis
- Gamma spectra S/U analysis of different KFK Fe spheres reveal interesting dependencies of γ flux sensitivity to the inelastic and elastic XS (sign inversion);
- Improvements needed in covariance matrix data: consistency with XS, mathematical verification, processing issues, gamma-ray covariances, gamma emission spectra, ^{252}Cf prompt/delayed gamma source, SAD/SED, …

SINBAD (Radiation Shielding Experiments Data Base)

Shielding Materials

- Fe/SS (27 benchmarks)
- H_2O (11)
- Air (9)
- Na (6)
- Concrete (5)
- Pb, W, Si/SiC (4)
- Graphite, Al (3)
- O, V, Cu (2)
- Li, Mn, Ni, N, Nb, Be, Th, Bi, $(CH_2)_{2n}$ (1)
- Multiple materials (18)