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Covariances generation for the cross sections and benchmark responses from the TENDL random files

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INSTITUTE for NEUTRON PHYSICS and REACTOR TECHNOLOGY (INR)

Content = current researches relevant to the topics of this Workshop "TALYS/TENDL development"

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I. Radiation Damage Quantities and their Covariances for Isotopes and Elemental Iron using:

- TENDL-2017 random files for underlaying Nuclear Data
- sampling and propagation of the involved Materials Physics Model parameters

Progress recently:

- ***Isotope ^{56}Fe****: S.Simakov, A. Koning, A.Konobeyev, "Covariances for the ^{56}Fe radiation damage cross sections", EPJ 146(2017)02012 (ND-2016);*
  "Uncertainties and correlations for the ^{56}Fe damage cross sections and spectra averaged quantities based on TENDL-TMC", INDC(NDS)-0719 (2016), p.12 (IAEA TM on dpa-2016)
- ***Elemental Fe:*** *S.Simakov, U.Fischer, A.Koning, A.Konobeyev, D.Rochman ,"Iron NRT- and arc-Displacement Cross Sections and Uncertainties", ICFRM-18 (5-10 Nov 2017 Aomori, Japan)*

II. Propagation of Cross Section Covariancies from TENDL-2017 random files to Spectra of Neutrons and Gammas leakage from thick Iron sphere fed by ^{252}Cf

Progress recently: *first presentation*

III. (n,p) and (n,np) on ^{39}K: existing measurements and evaluations are controversial, but TENDL-2015 seems to be the most reliable

Progress recently:

- *S.P. Simakov, Y. Qiu, U. Fischer, "Status of 39K(n,p)39Ar and 39K(n,np)38Ar cross sections and impact on IFMIF or DONES design", EFFDOC-1318, Apr 2017*
- *Request was submitted to NEA Data Bank HPRL = Request # 45H*

Ia. Radiation Damage Quantities and Covariances for Elemental Iron

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They are computed from Nuclear Data (basic neutron XS) and include:

- kinetic energy released by ch. particles *KERMA* - locally deposited Nuclear Heating
- damage energy *DE and derived NRT-* and *arc*-dpa XS - number of displaced atoms
- gas production *(n,xHe), (n,xT), (n,xH)* … - transmuting target nuclei into gases

NB: *DE* and *dpa* additionally depend on **Materials Physics Models** (see Ib.)

Monte-Carlo method and next procedure were used to quantify Covariances for these aggregate Quantities:

- Damage Quantities were repeatedly computed by NJOY-2012.82 code with 1 + 500 TENDL-2017 random files for every isotope of Fe
- Isotope Covariance Matrices were obtained analysing 228-groups XS from NJOY:

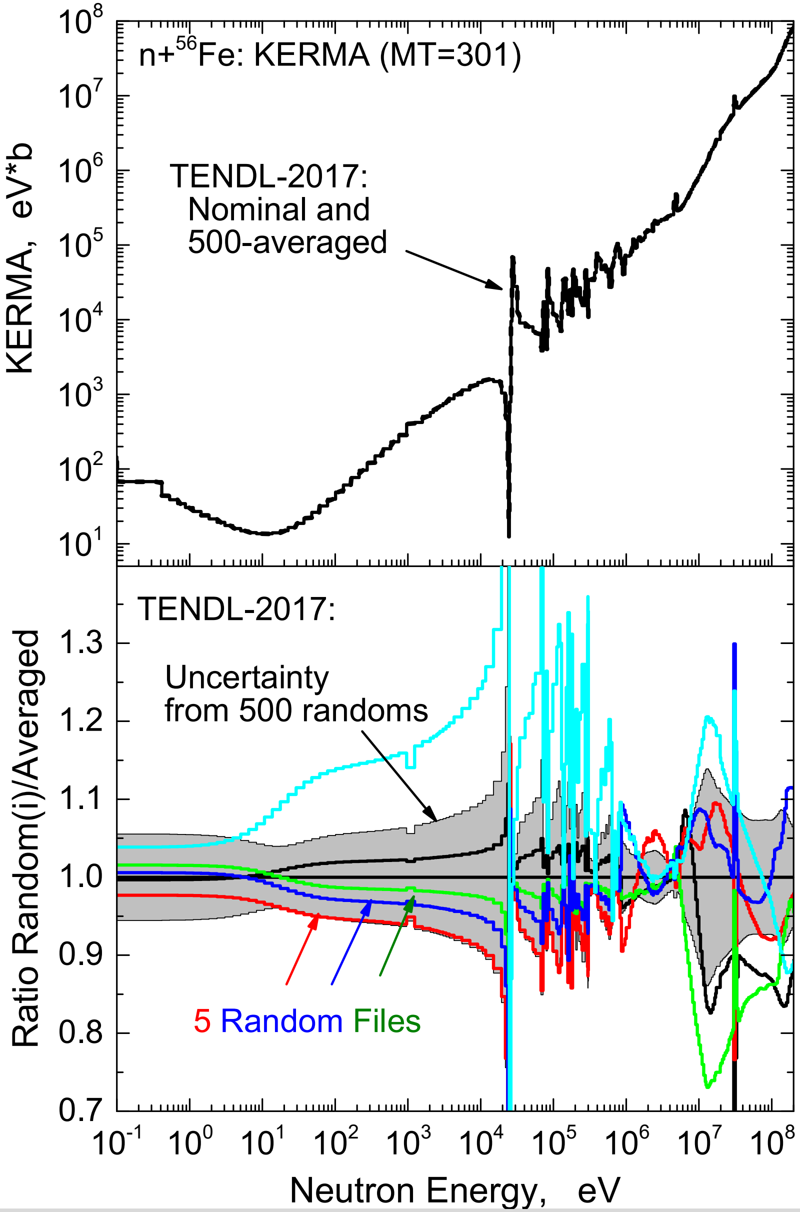
$$\boldsymbol{cov(y_i, y_j)} = \sum_{\boldsymbol{N_{random}}} \frac{(\boldsymbol{y_i} - \boldsymbol{\bar{y}_i})(\boldsymbol{y_j} - \boldsymbol{\bar{y}_j})}{\boldsymbol{N_{random}}},$$

yi – is value at energy bin Ei

- then Elemental Iron XS and Covariances were computed by summing individual isotopes Fe-54(a=5.9%), Fe-56(91.72%), Fe-57(2.1%) and Fe-58(0.28%):

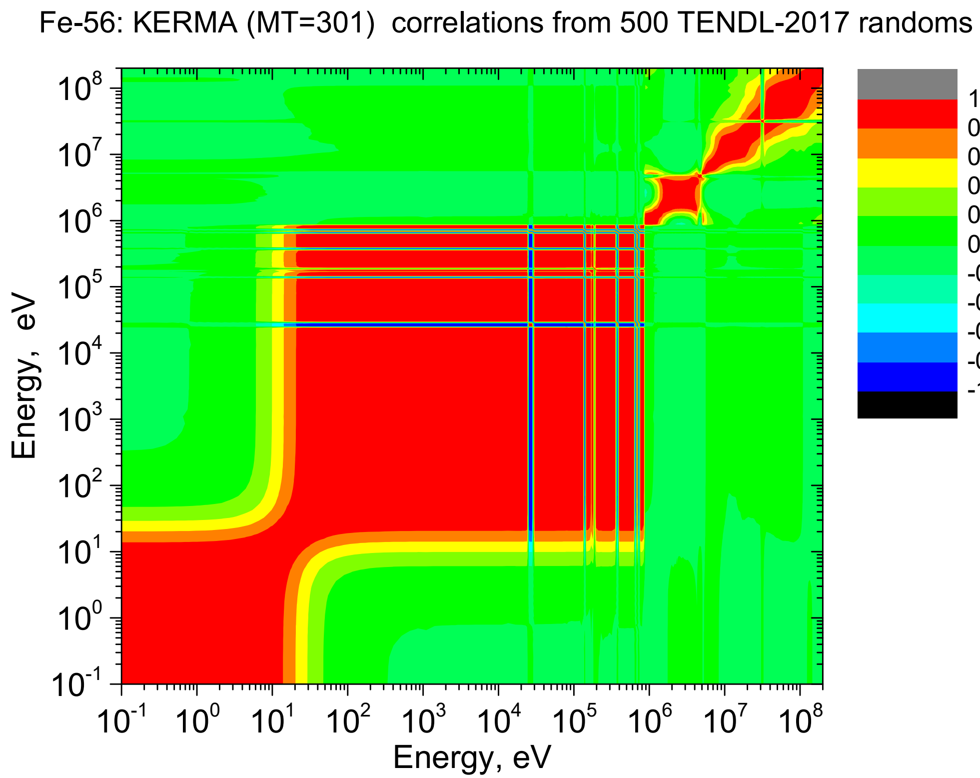
$$\sigma(E_i) = \sum_{n=1}^{4} a_n * \sigma_n(E_i) \quad ; \quad cov(E_i, E_j) = \sum_{n=1}^{4} a^2{}_n * cov_n(E_i, E_j)$$

Results for ^{56}Fe: XS and Correlations for KERMA (MT=301)

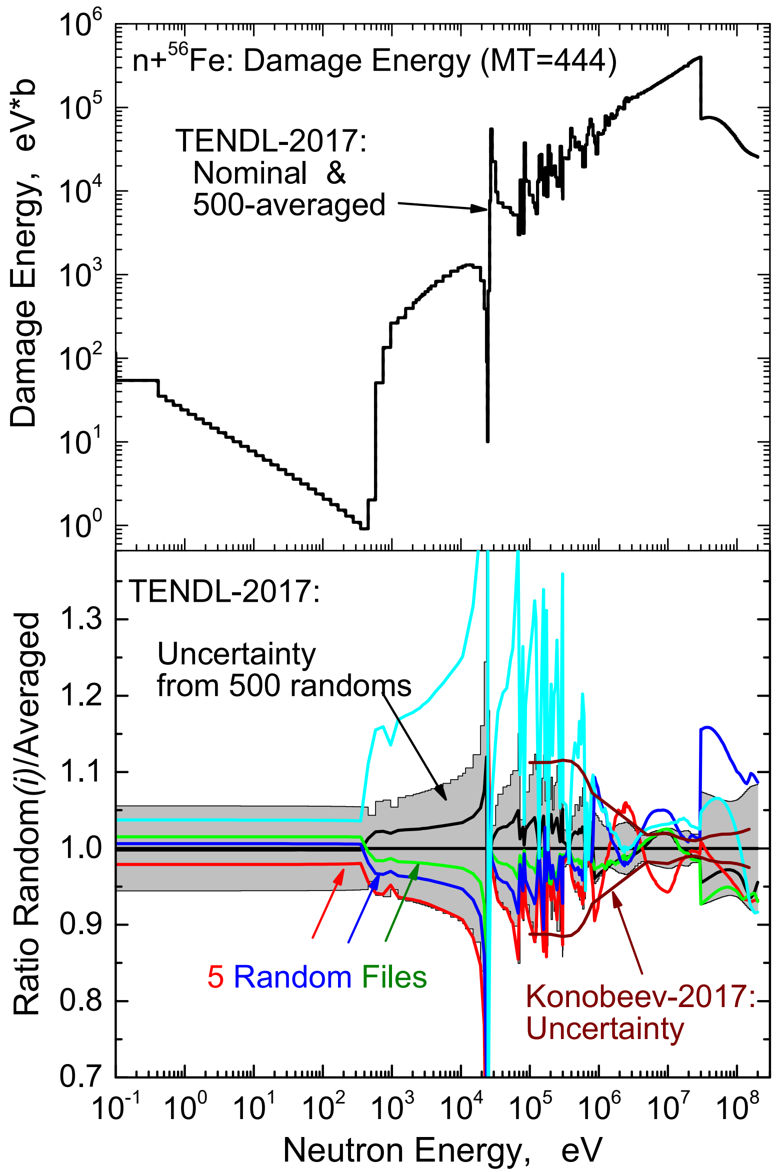


← **XS and Uncertainties < 200 MeV (≈ 5 - 10%)**

↓ **E-E Correlation Matrix (2 regions with ≈ 1)**

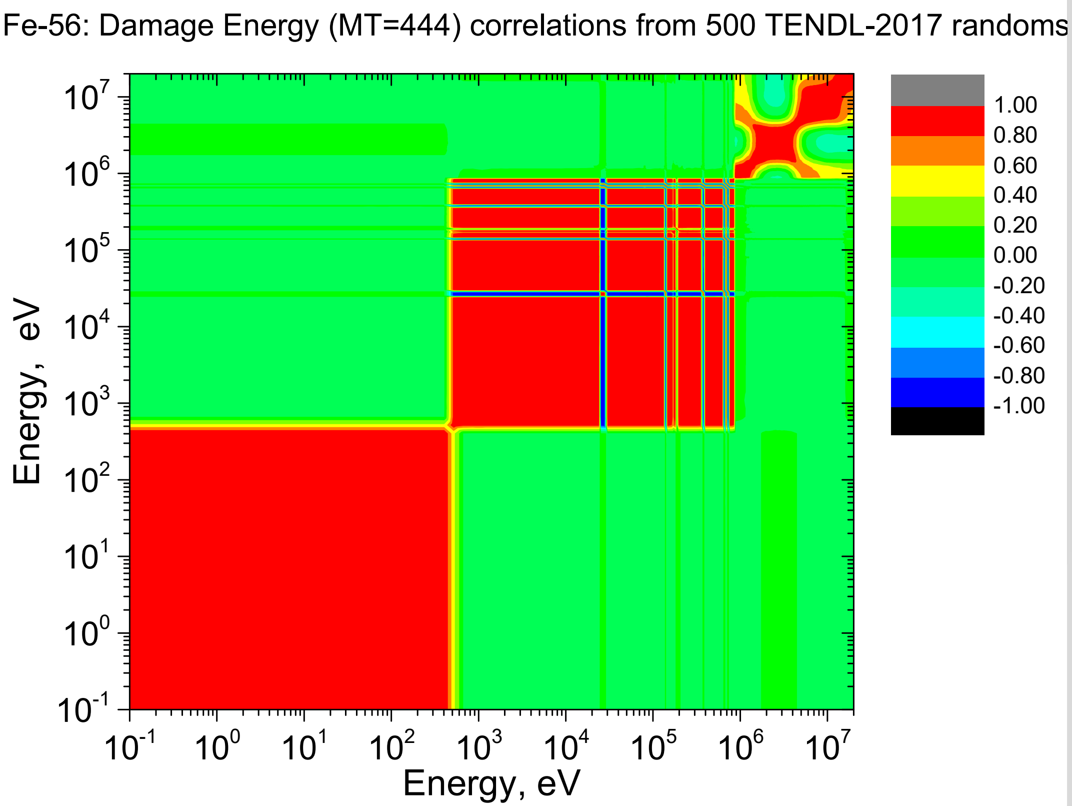


Results for ^{56}Fe: XS & Corr. for Damage Energy (MT=444)

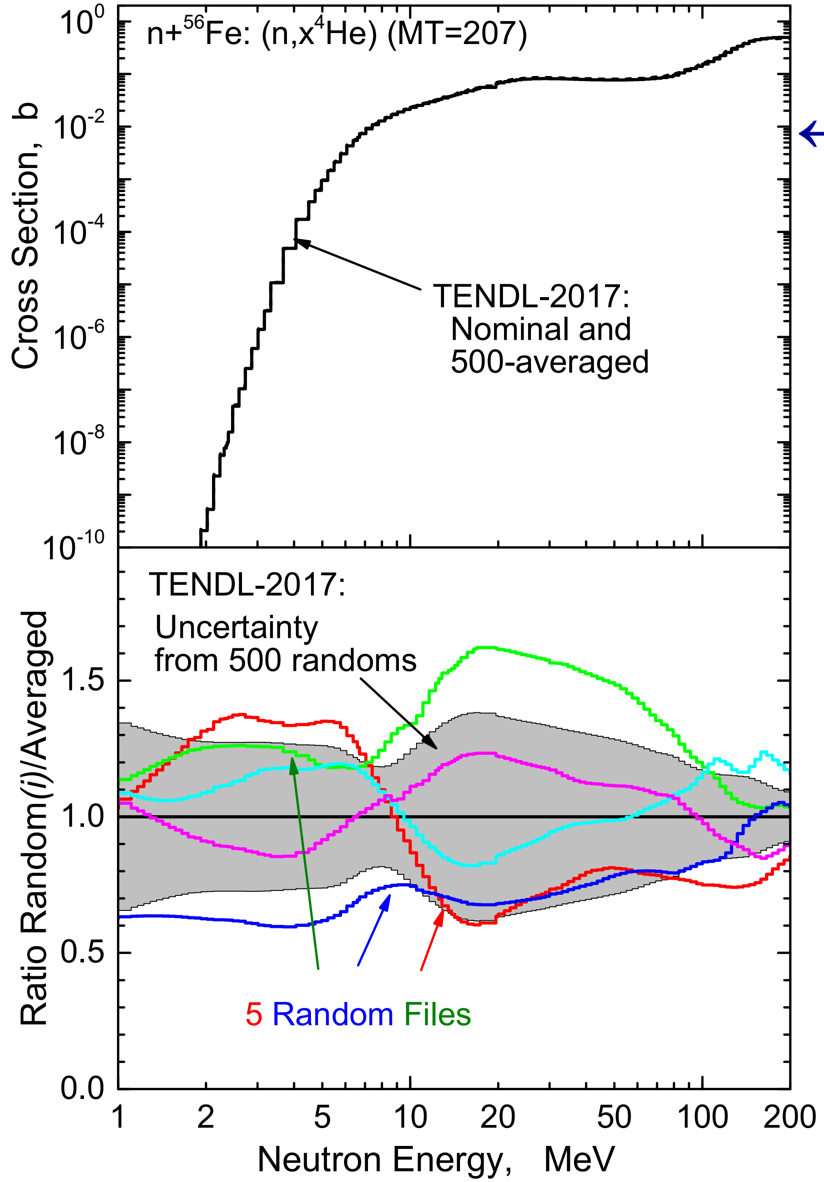


← XS **and Uncertainties (≈ 5 - 15%),**
jump at 30 MeV

↓ E-E **Correlation Matrix (2 regions with ≈ 1)**

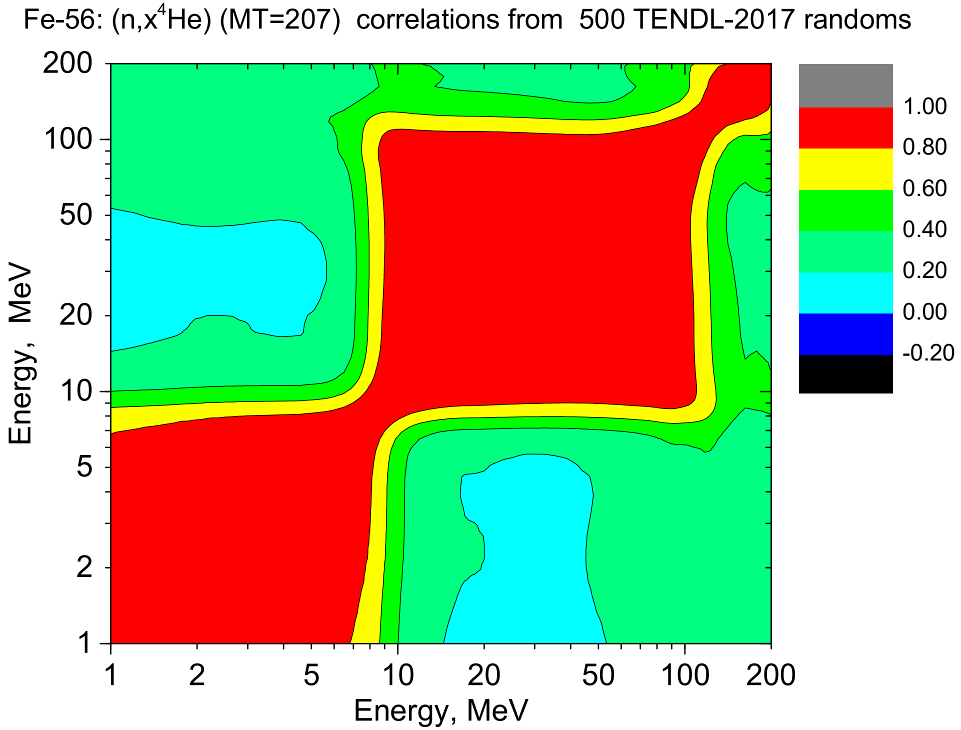


Results for ^{56}Fe: XS and Correlations for (n,x^{4}He) or MT=207



← **XS and Uncertainties <200 MeV (≈ 20-40%)**

↓ E-E **Correlation Matrix**
(≈1 within 50% energy interval)



Results for ^{56}Fe: MT-MT Cross Correlation Matrix for Spectrum Averaged (SPA) Damages in Fission and Fusion Facilities

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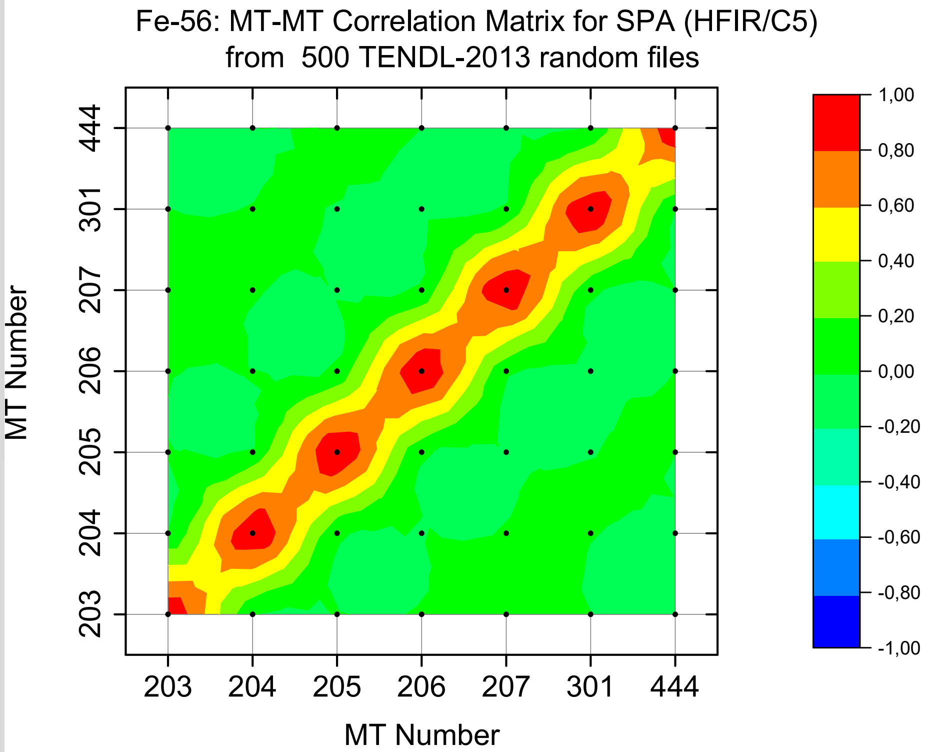
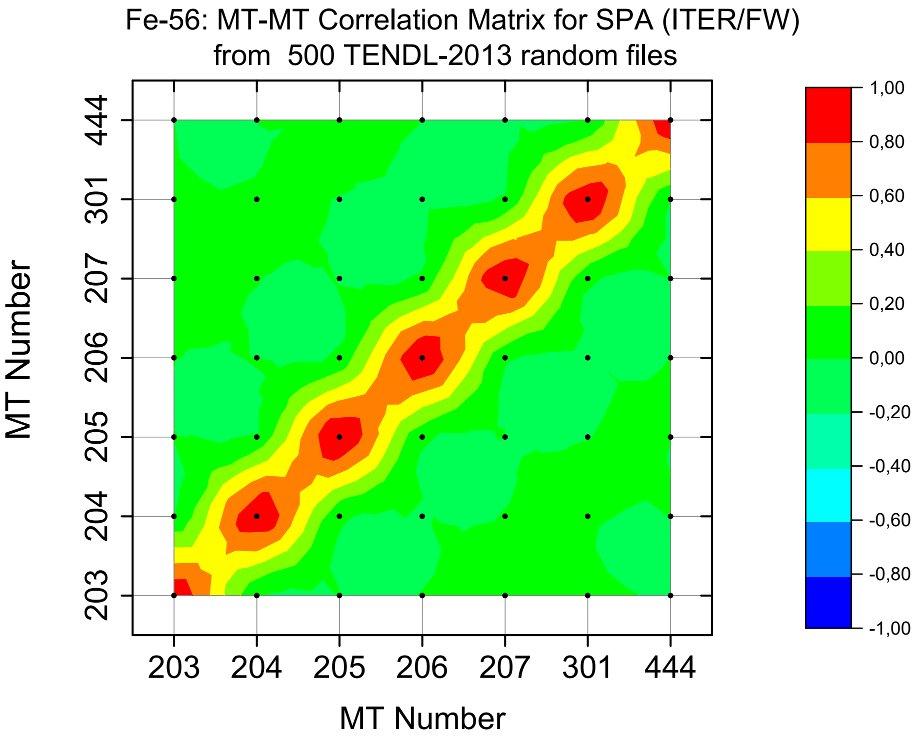
↓ MT-MT for Fission (HFIR/C5)



↓ MT-MT for Fusion (ITER/FW)



Findings: NO practically significant MT- MT correlations, i.e. Correlation ≤ 1%

Results for ^{00}Fe: XS and Correlations for KERMA (MT=301)

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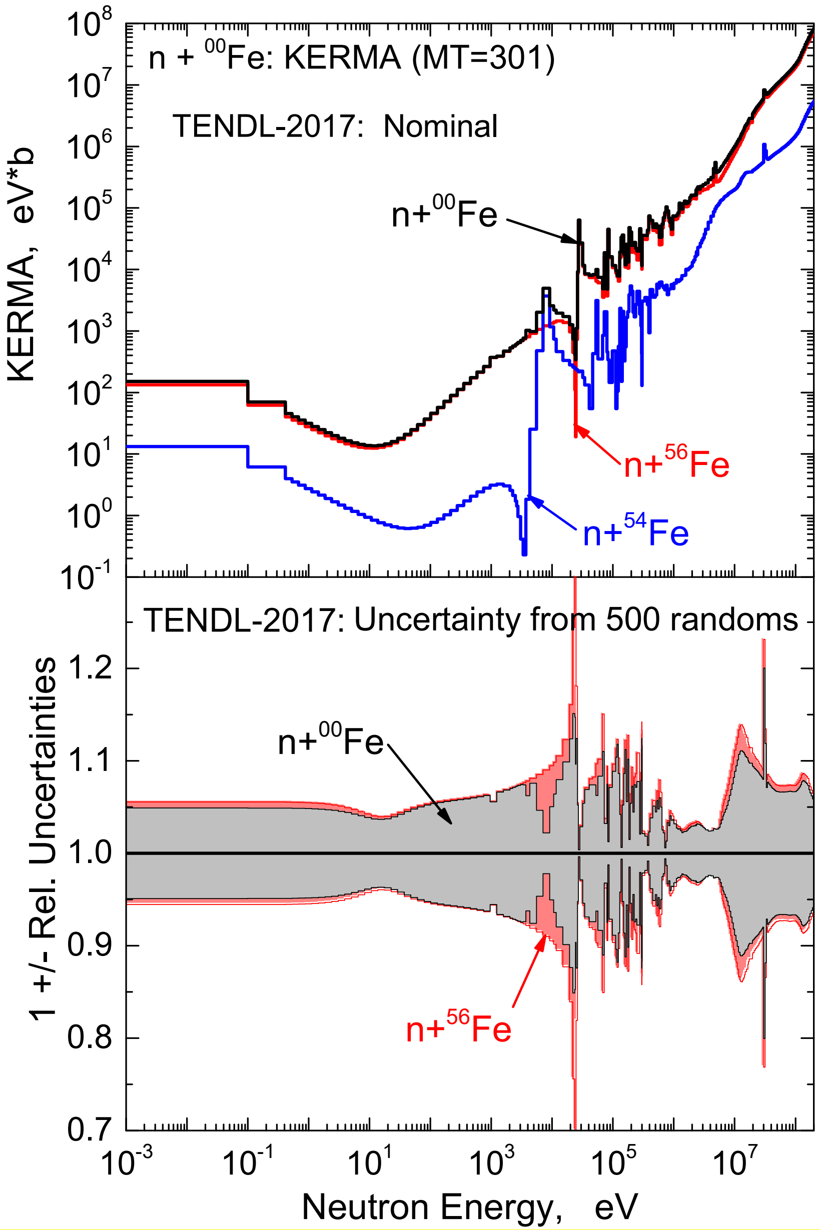
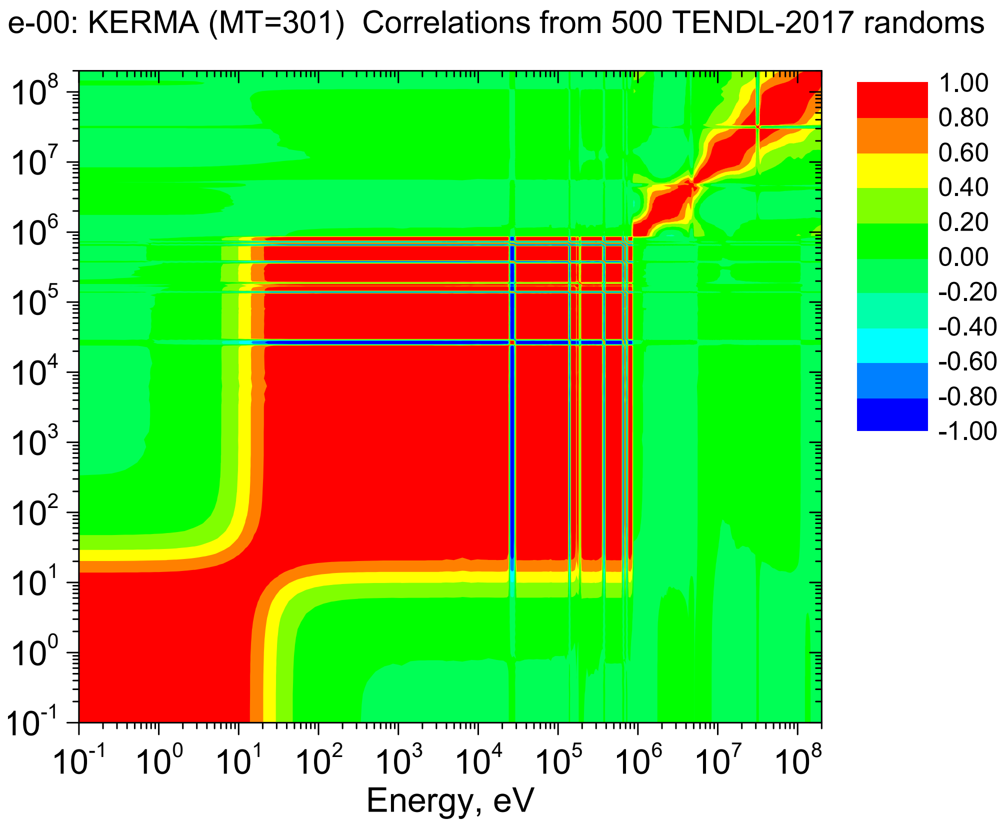


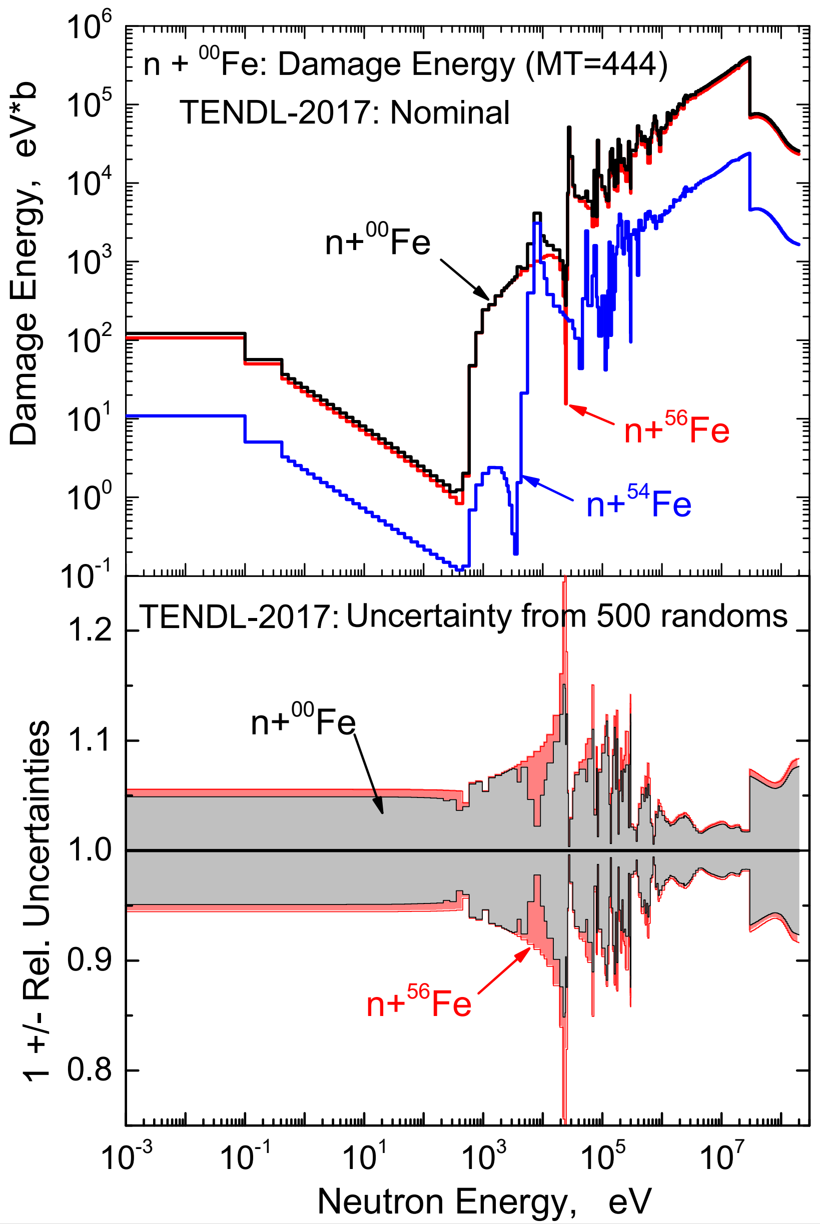
– XS **and Uncertainties < 200 MeV (≈ 5 - 10%)**

↓ E-E **Correlation Matrix (2 regions with ≈ 1)**



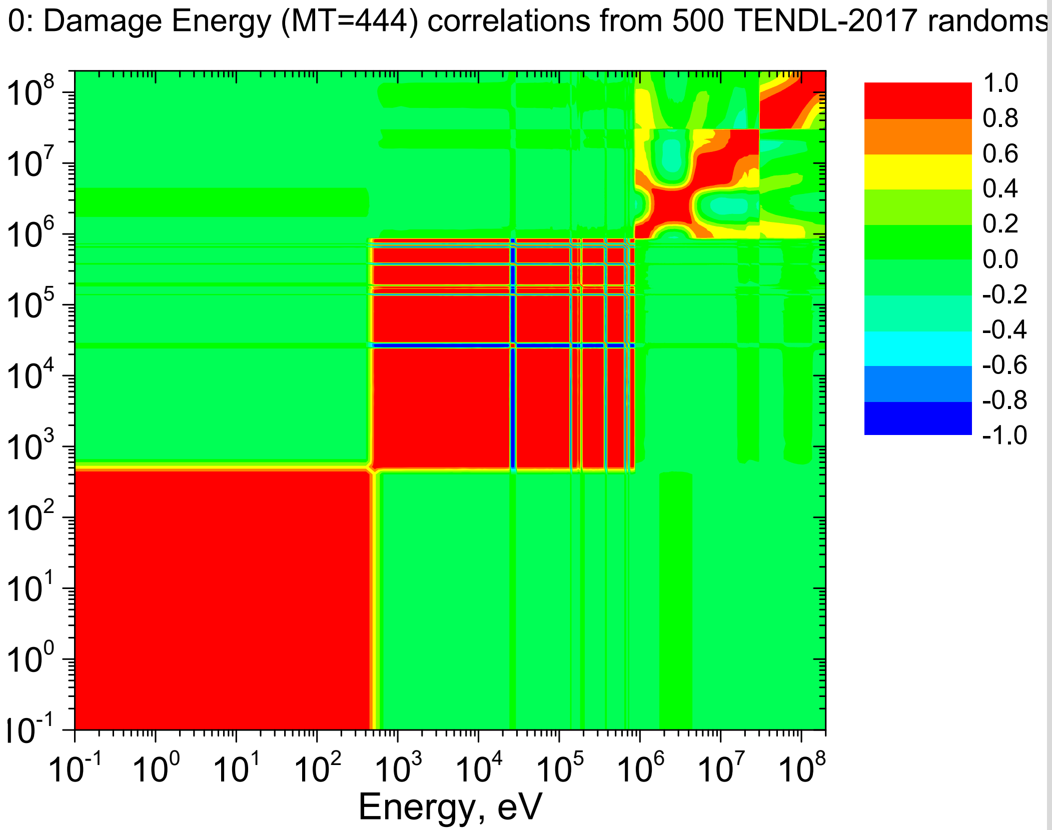
Observation: Elemental Iron is defined predominantly by Fe-56, but near 10 keV – by Fe-54

Results for ^{00}Fe: XS and Correl. for Damage Energy (MT=444)



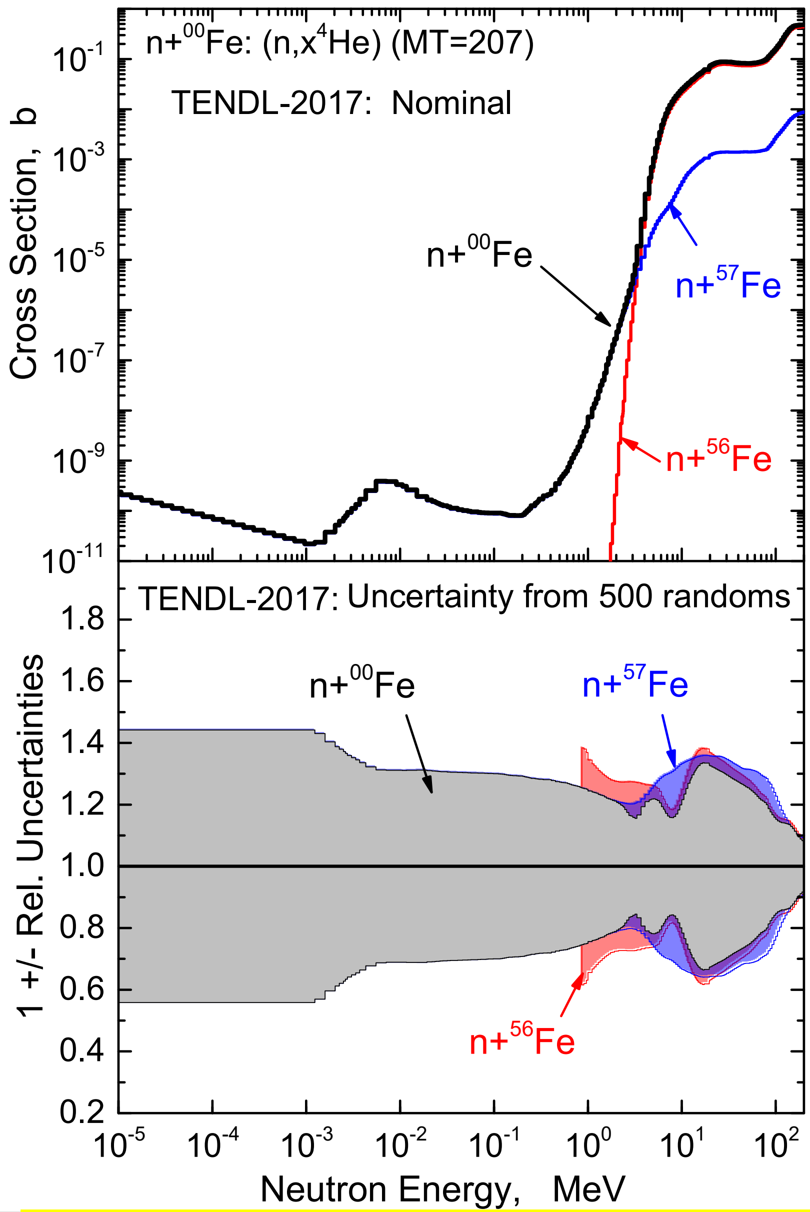
← XS **and Uncertainties (≈ 5 - 15%),** jump at 30 MeV

↓ E-E **Correlation Matrix (2 regions with ≈ 1)**



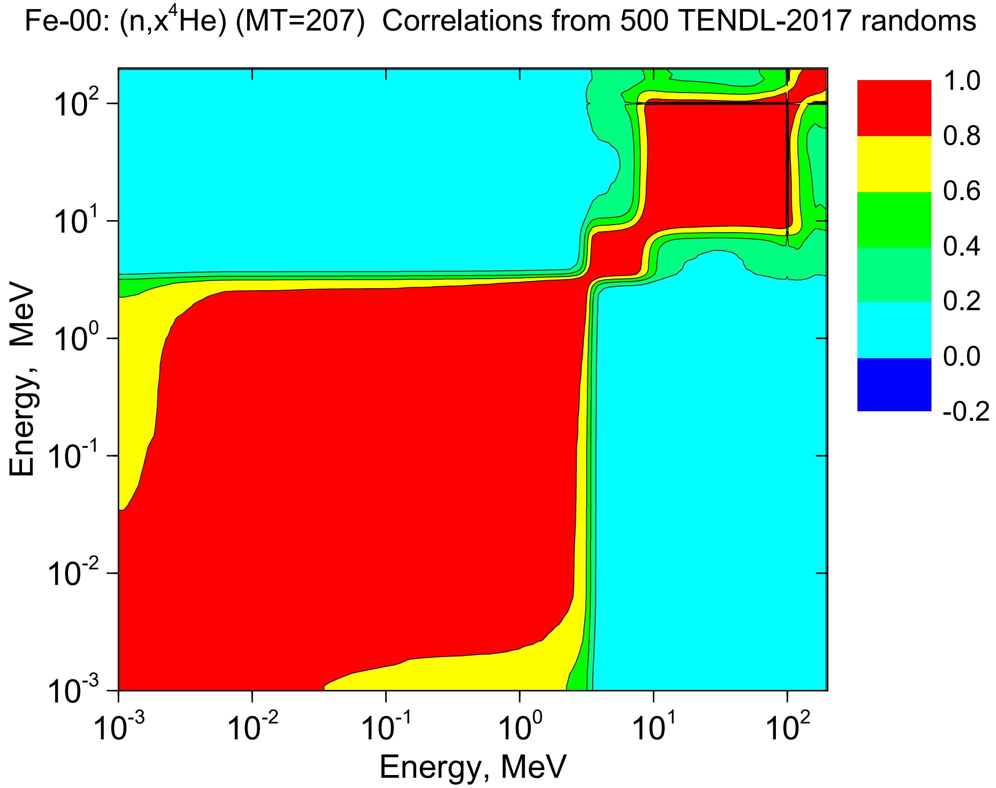
Observation: Elemental Iron is defined predominantly by Fe-56, but near 10 keV – by Fe-54

Results for ^{00}Fe: XS and Correlations for (n,x^{4}He) i.e. MT=207



← XS & Uncertainties <200 MeV ≈ 20-40%

E-E Correlation Matrix: full correlation (≈ 1) within 2 energy intervals



Observation: Elemental Iron is defined by Fe-57 below 3 MeV but by Fe-56 above 3 MeV

Ib. Materials Data Uncertainties for Natural Iron due to ***Partition of Recoil Energy***

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Physical Phenomena = Partitioning of Recoil Energy between Damage Energy and Ion Energy Losses due to Electrons Excitation

It affects only Damage Energy (no impact on KERMA or gas production)

Partitioning Function used by NJOY was represented by M.Robinson who fitted J.Lindhard' theory of energy partition between atomic and electronic motion

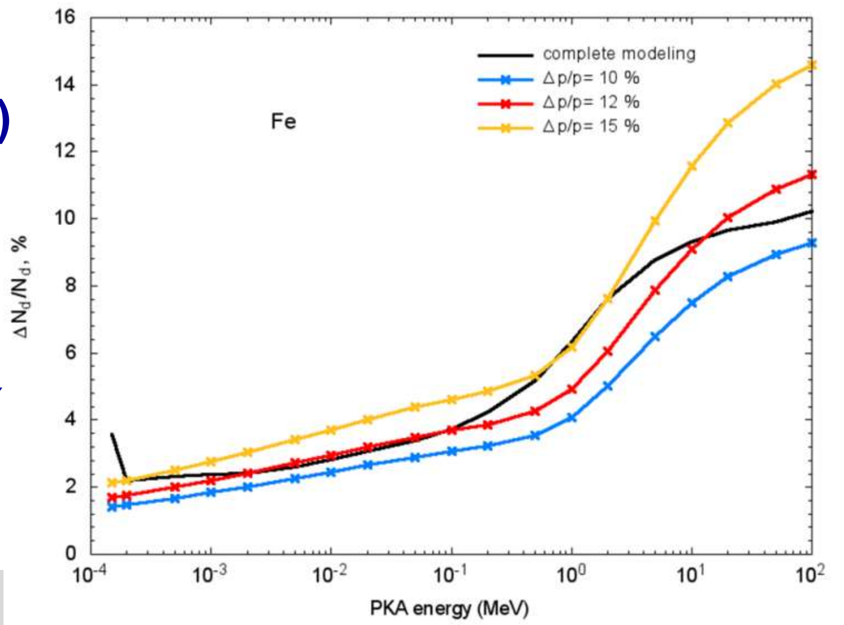
$$E_{dam}(T_{PKA}) = T_{PKA}/(1 + k(Z,A)\, g(T_{PKA}/E_L))$$

$$g(\epsilon) = (\alpha = 1)\,\epsilon + (\beta = 0.40244)\,\epsilon^{3/4} + (\gamma = 3.4008)\,\epsilon^{1/6}$$

$$\epsilon = T_{PKA}/E_L = \frac{A_2\, T_{PKA}}{(A_1 + A_2)} * \frac{a}{(Z_1\, Z_2\, e^2)}$$

Method we used for Materials Data (Partition) Covariance estimation:

- 12% variation of *α, β,* γ (to reproduce Nuclear and Electronic Losses spread modelled by IOTA code, *A.Konobeyev*)
- generation 500 random MT=444 files by NJOY
- calculation of Covariance for each Isotopes
- mixing them for Elemental composition



Ib. Materials Data Uncertainties for Natural Iron due to *Lattice Threshold Energy and Primary Defects surviving*

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Damage Energy **transferred to lattice Atoms (*DE* = MT444):**

***NRT-DE XS [eV*b]*:** $DE_{NRT}(E) = \sum_i \int_{E_d}^{T} \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\ dT_i$

arc-DE XS [eV*b]: $DE_{arc}(E) = \sum_i \int_{E_d}^{T} \nu(T_i) \frac{d\sigma(E,T_i)}{dT_i} P(T_i)\ dT_i$

$$\begin{cases} 0, & 0 < T_{d,i} < E_d \\ 2\,E_d/0.8, & E_d < T_{d,i} < 2\,E_d/0.8 \\ T_{d,i}, & 2\,E_d/0.8 < T_{d,i} < \infty \end{cases}$$

then Cross section for Number of *Displacement per Atom (dpa)*:

***NRT-dpa XS [b]*:** $\sigma_{NRT-dpa}(E) = \frac{0.8}{2\,E_d} DE_{NRT}(E)$

***arc-dpa XS [b]*:** $\sigma_{arc-dpa}(E) = \frac{0.8}{2\,E_d} DE_{arc}(E)$

Following these definitions Additional Uncertainties are associated with:

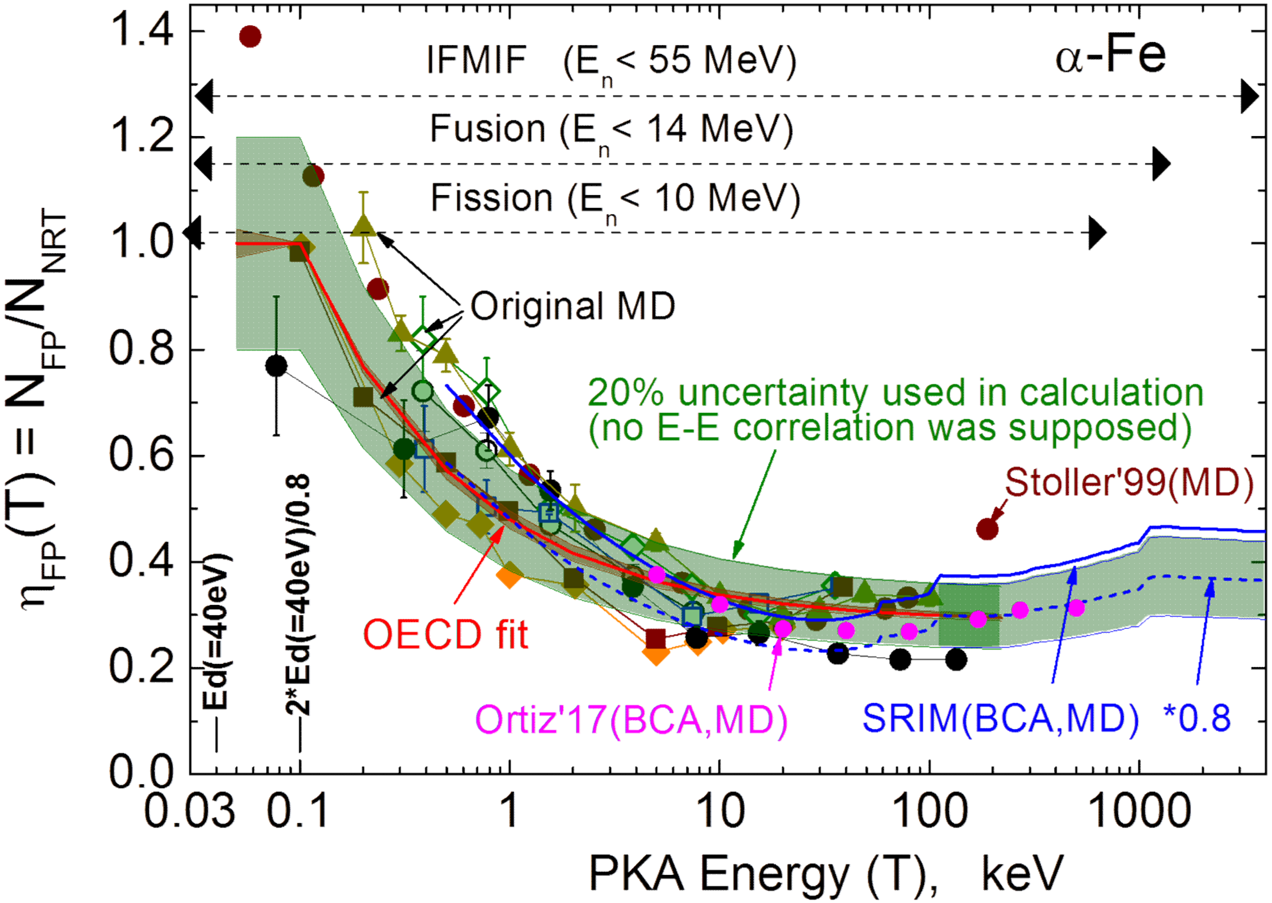
- **Lattice Threshold Energy *E_d***=(41 ± 2)*eV => Rel. Cov: diag.= 5%, off-diag = 1.0 => Fluctuation of low Integration limit

  *Ref: *) K. Nordlund et al., NIM B246(2005)32: " … The average of all the many-body potential average thresholds is 41 ± 2 …"*

- **Primary Defects (FP) surviving function *v(T)*** – its uncertaity was implemented by ***v(T)*** random sampling within the MD spread, next slide ➔

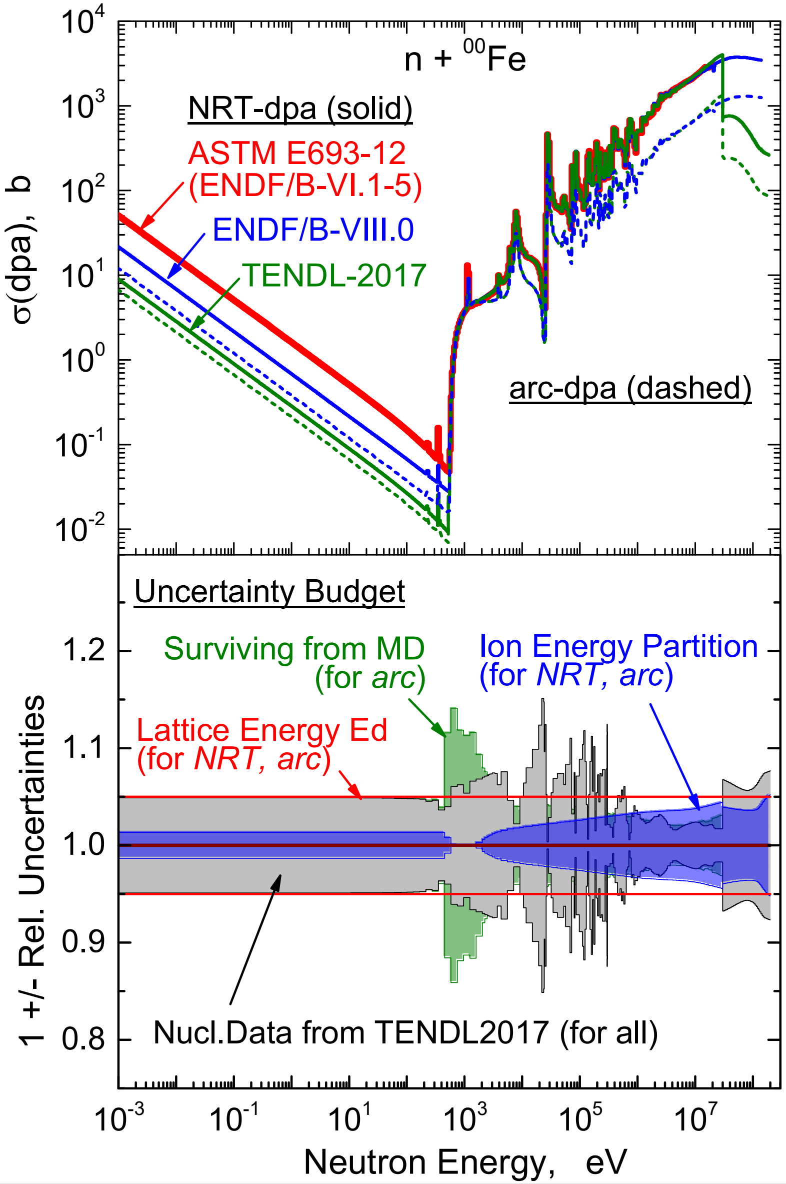
Ib. Materials Data Uncertainties for Natural Iron:
Primary Defect surviving function (efficiency)

available MD and BCA simulations results, OECD fit 2015 and what we used:

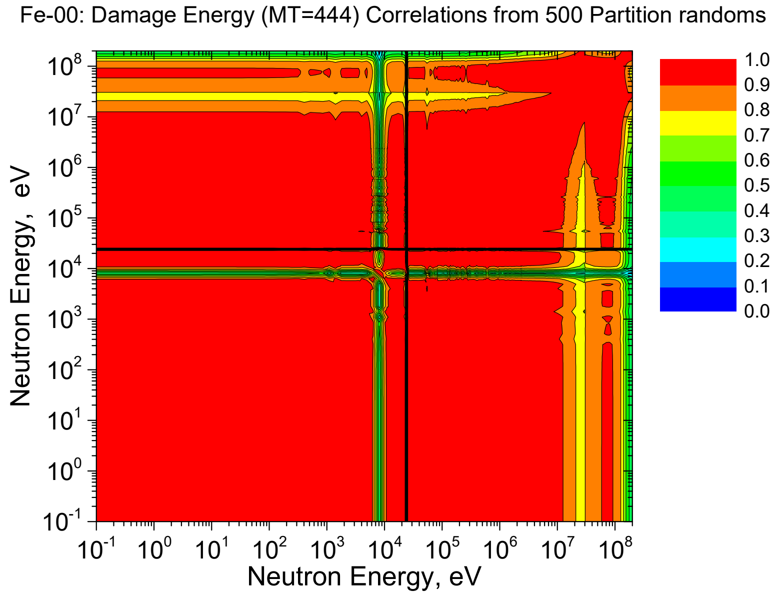


still open issue: quantification of Energy-Energy correlations

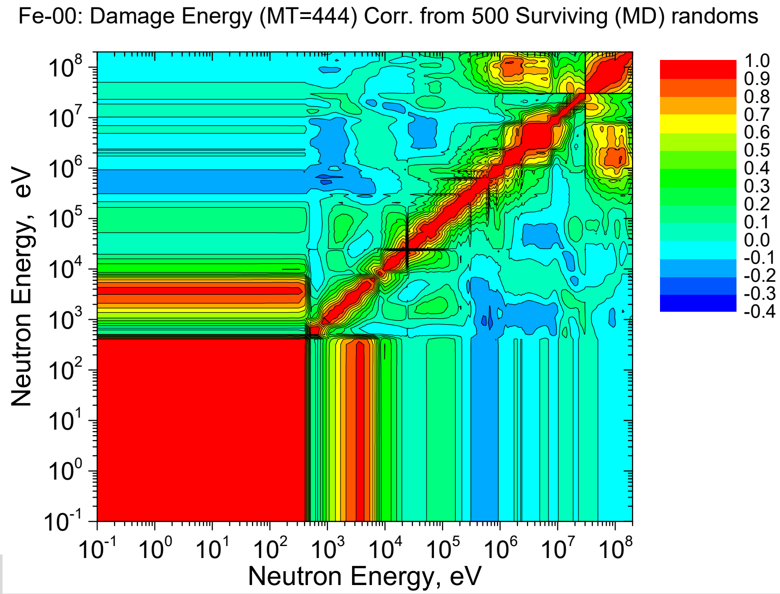
Ia+b. Summary Nuclear + Materials Data XS and Covariancies for Natural Iron



PKA Energy Partition



MD Surviving



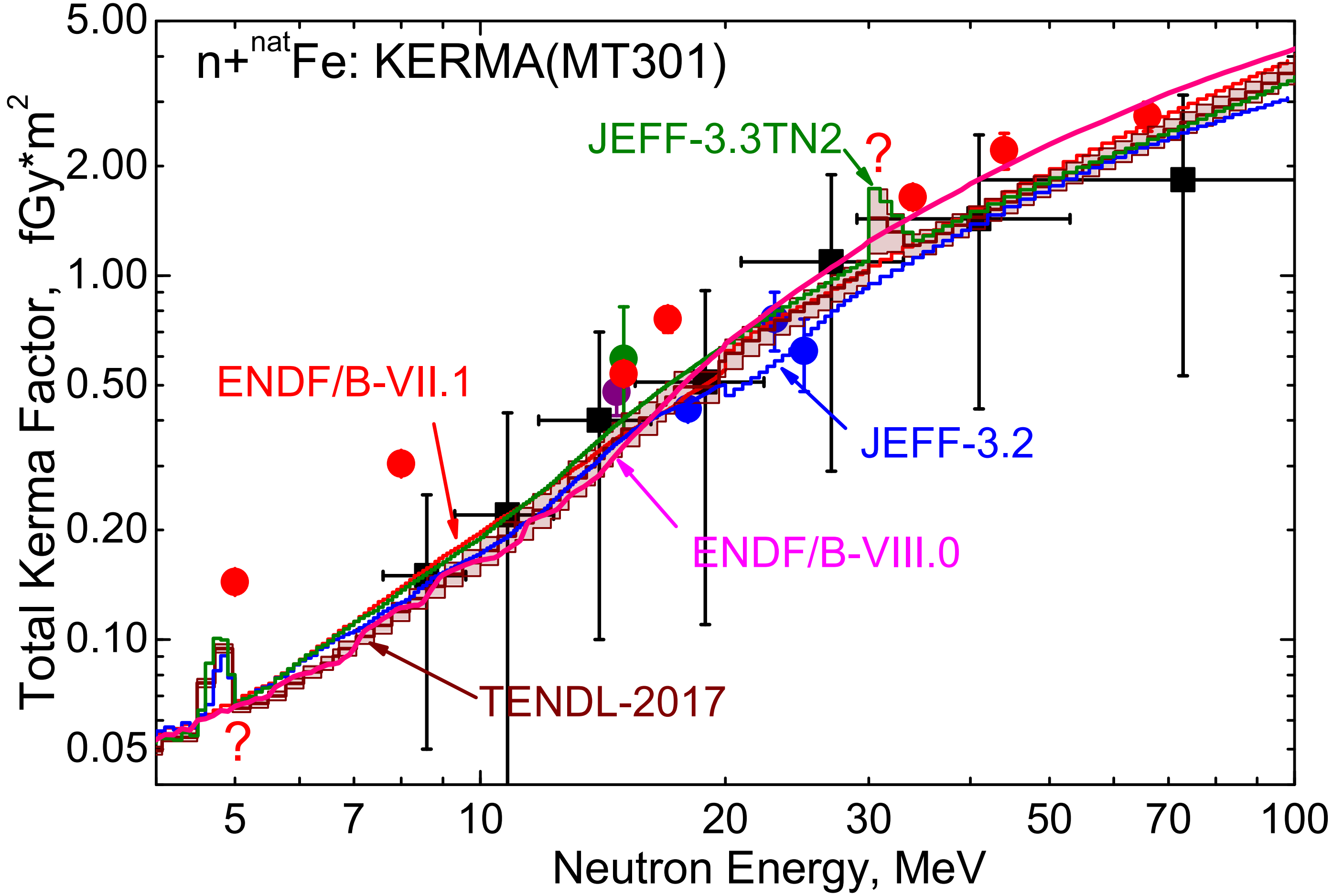
Ic. Experimental Validation of Damage XS and Uncertainties

It is possible to do (since measurements exist) for:

- **KERMA**
- **gas production: practically only *(n,x^{4}He)***
- **dpa: only *arc* but not *NRT* (since non measurable)**

N.B. Such Experimental data exist only for Elemental Iron, with several exceptions - for ^{56}Fe(n,xα)

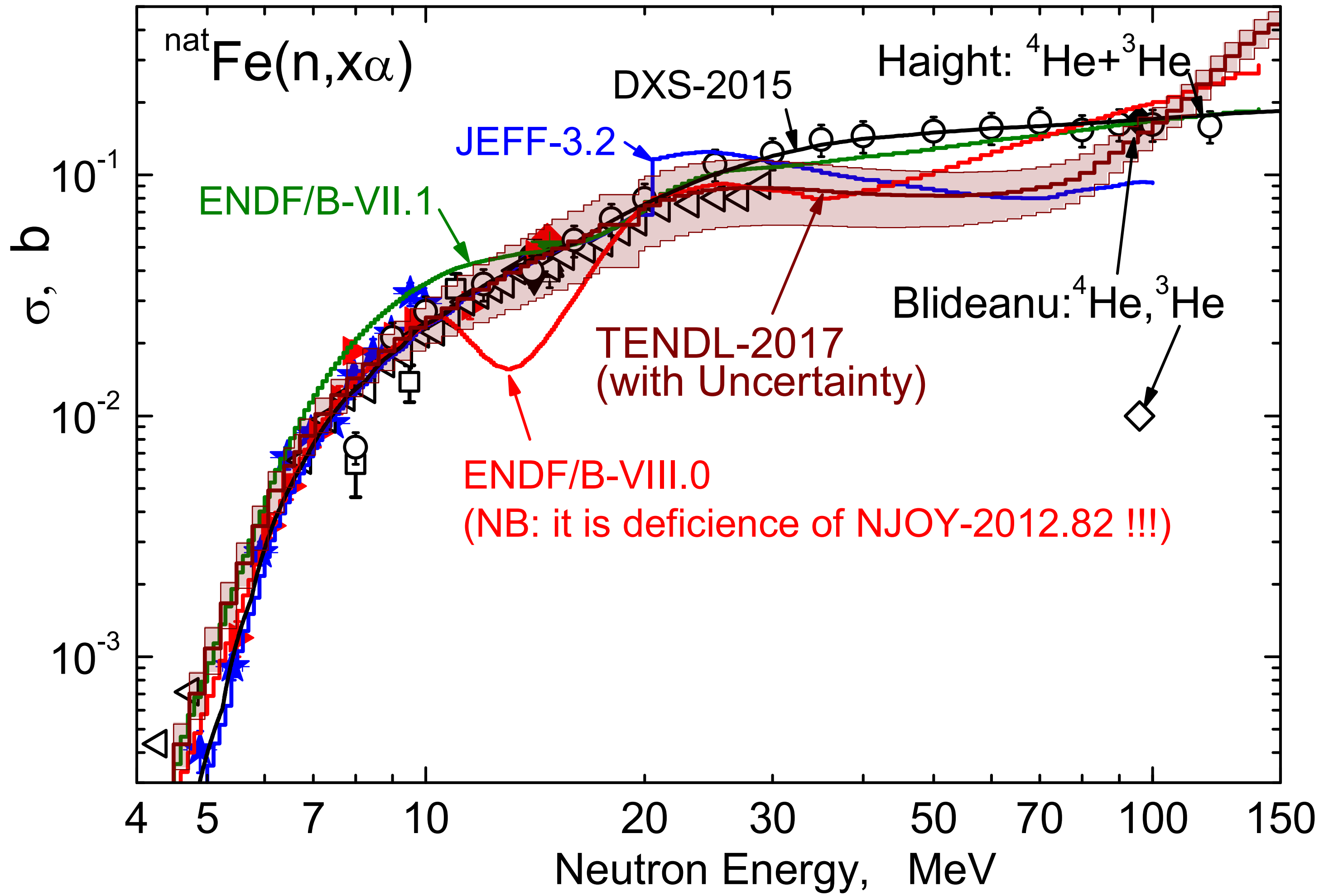
Experimental Validation of XS and ND Uncertainties: KERMA



Observations:

- **Uncertainties from TENDL-17 random files (Fe, 5-10%) ≤ Experimental Uncert. (6 - 100%)**
- **Scattering of scarce Measurements is large: Schrewe'00 data seem have systematic error**
- **New KERMA measurements for Fe are needed …**
- **ENDF/B-VII or -VIII looks to be the best since others show artificial peaks – reason ?**

Experimental Validation of XS & ND Uncertainties: (n,xα)

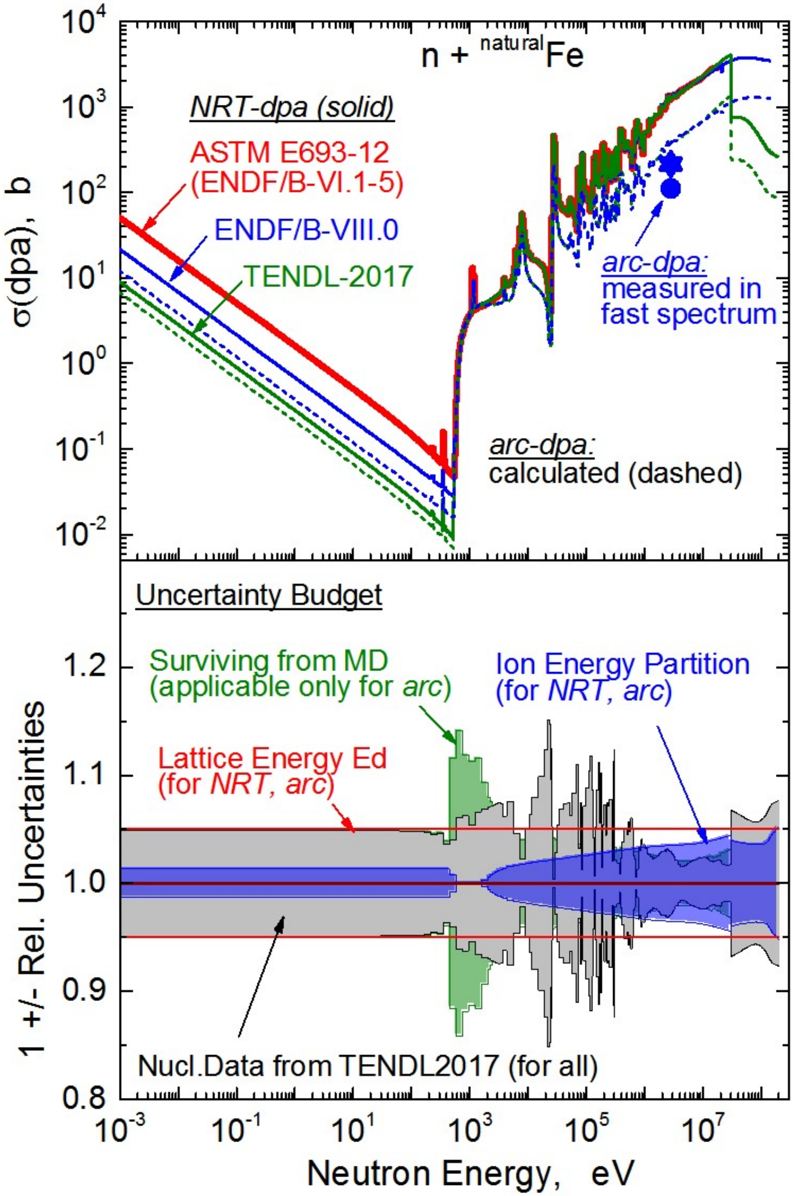


Observations for natFe:

-Uncertainties from TENDL-2017 random files (20%) ≈ bulk Experimental Unc. (10-20%)

- Evaluations best agreeing with Measurements: DXS-2015 (and supposely ENDF/B-VIII.0)

Comparison of *NRT-dpa* with ASTM E693-12 and Exp. Validation of *arc-dpa* XS & Uncertainties



Findings

1. *NRT-dpa (solid curves)*:

- **ASTM E693-12 = ENDF/B-VI.1-5**
- **ENDF/B-VIII.0 results to different values below 600 eV due to lower (n,γ)**
- **TENDL-2017: jump at 30 MeV and even lower (n,γ)**

2. *arc-dpa (dashed curves)*:

Existing measurements in Reactors at 4ºK	Computed *dpa* averaged in $^{235}U(n_{th},f)$ PFNS
Horak'76 = 111 ± 19 b Takamura'86 = 217 b Wallner'88 = 213 b	*arc-dpa* = 261 ± 26 b *NRT-dpa* = 841 ± 67 b

NB: NPI/Rez performes measurement of dpa !

3. Full Uncertainty budget for *NRT* - *arc*-dpa(E):

Component (Source)	SPA (only Diag)
Nucl. Data (TENDL-2017)	≈ 2 % (≈ 0.5 %)
PKA Partition (Stopping)	≈ 7 % (≈ 0.1 %)
FP Surviving (MD)	> 2 % (≈ 0.7 %)
Ed (MD)	≈ 5 %

II. Propagation of TENDL-2017 Uncertainties to Spectra of Neutrons and Gammas leaking from Iron Shells with Cf source

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- ***How it was done:***

- MCNP-6 simulation of neutron-gamma transport was re-run
1 + 500 times with TENDL-2017 random files for every Fe isotopes

- each run (1.E+9 events) takes ≈ 3 min on 300 CPUs of KIT server;
total Wall time ≈ 16 hours (i.e., it is a feasible task !)

- f95 code was written to read in the neutron and gamma leakage spectra
from 501 MCNP output files and to compute Covariancies Matrices

- ***Experiment which was simulated:***

- Iron sphere (R/r = 30/1cm, dia = 60 cm) with ^{252}Cf(s.f.) source
carried out in IPPE by L.Trykov et al.

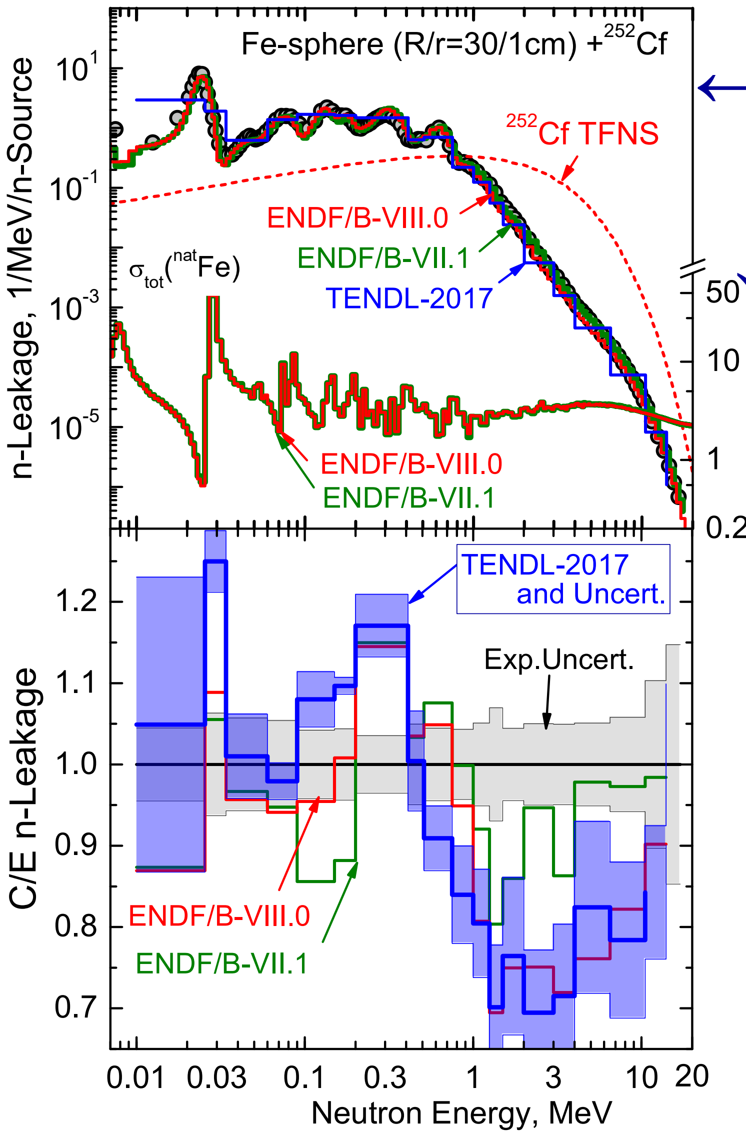
- Neutron and Gamma spectra were measured by Stilben Detector
(PM Pulse Height Distribution were de-convoluted in Energies)

- Details, Numerical Data and Documentation - in ICSBEP (ALARM-FeCf-001)

NB: Benchmarking of neutron transport data by spheres measured in IPPE and Řež is currently a collaboration topic between Research Centre Řež (Bohumil Jansky) and (KIT)

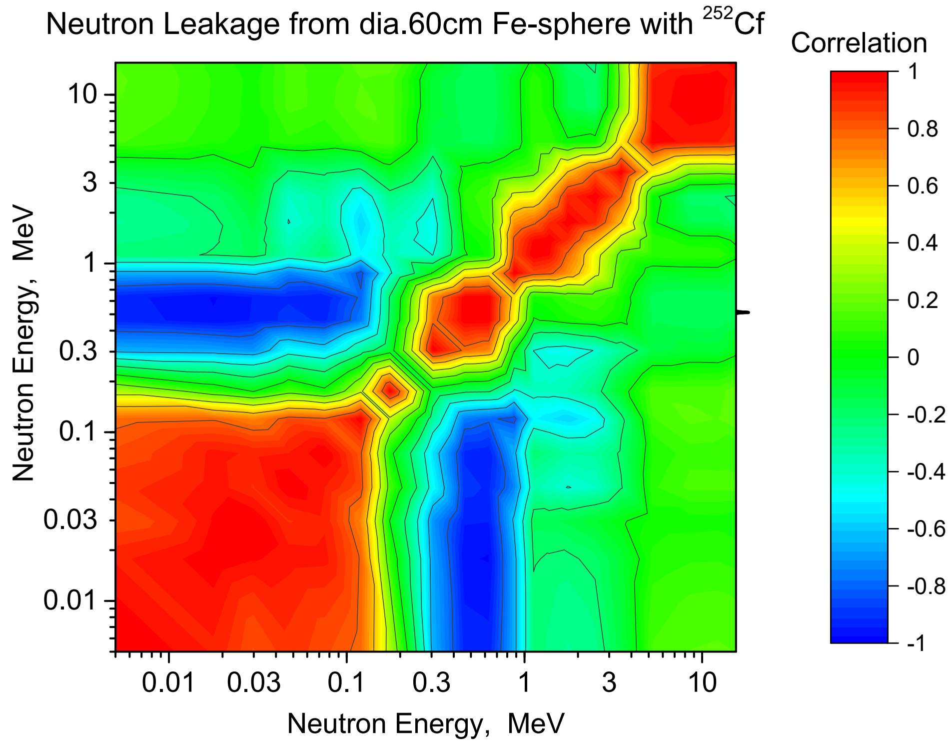
Results: Covariancies obtained from TENDL-2017 for Fe sphere:

1. Neutron Leakage Energy Spectrum



← **n Leakage** and **Uncertainties ≈ 2 - 18%**

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



Findings for n-Leakage: - Uncertainties (≈ 2-18%) from TENDL-2017 are comparable with Experimental
- E-E correlations will play role only below 100 keV

Results: Covariancies obtained from TENDL-2017 for Fe sphere
2. Gamma Leakage Energy Spectrum

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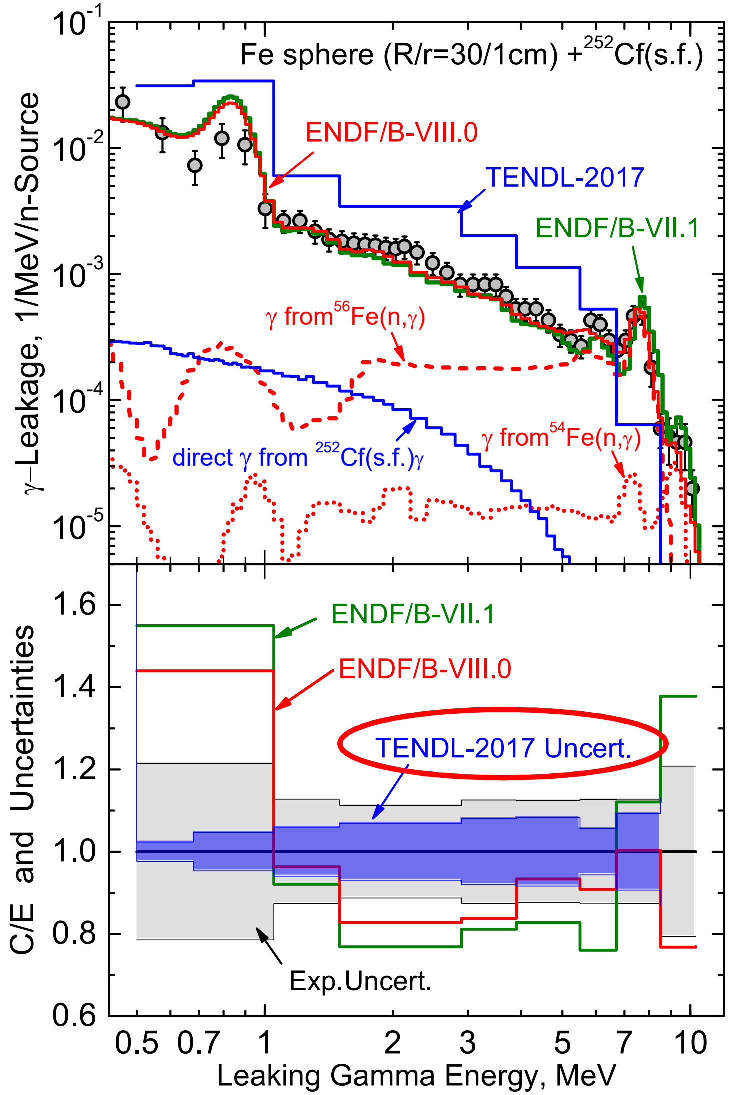
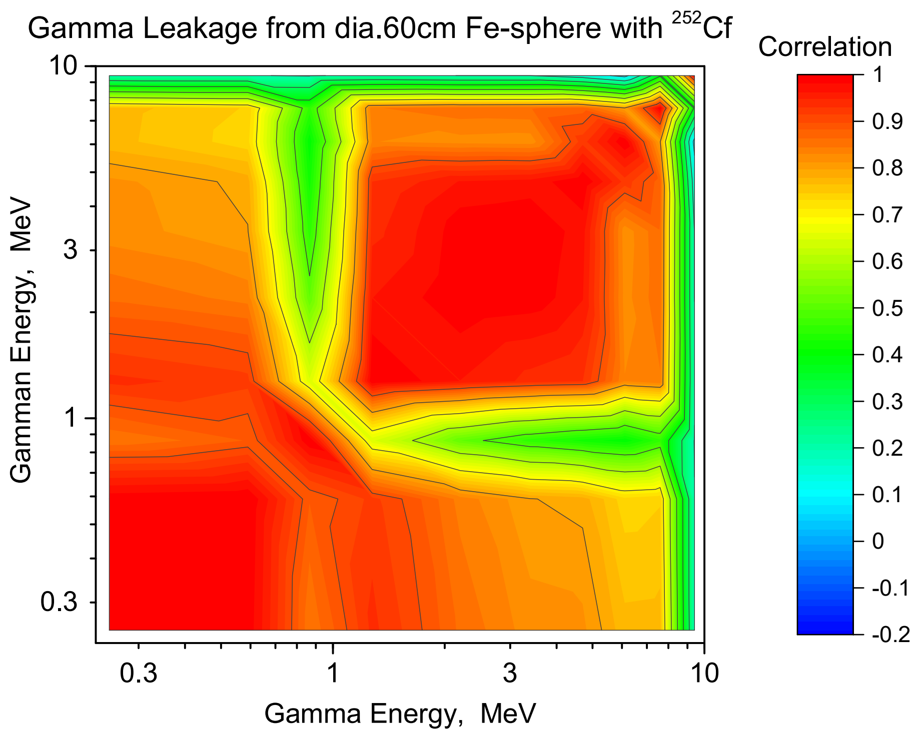


← **γ Leakage and Uncertainties ≈ 2 - 12%**

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



Findings for γ-Leakage: - Uncertainties (≈ 2-12%) from TENDL-2017 are lesser than Experimental
- TENDL-2017 overestimates measurements
- E-E correlations will play role in whole energy range 100 keV - 10 MeV

III. Status of Experimental and Evaluated Data for $^{39}K(n,p)\,^{39}Ar$ ($T_{1/2}$ = 269 y) and $^{39}K(n,np)^{38}Ar$ (*stable*)

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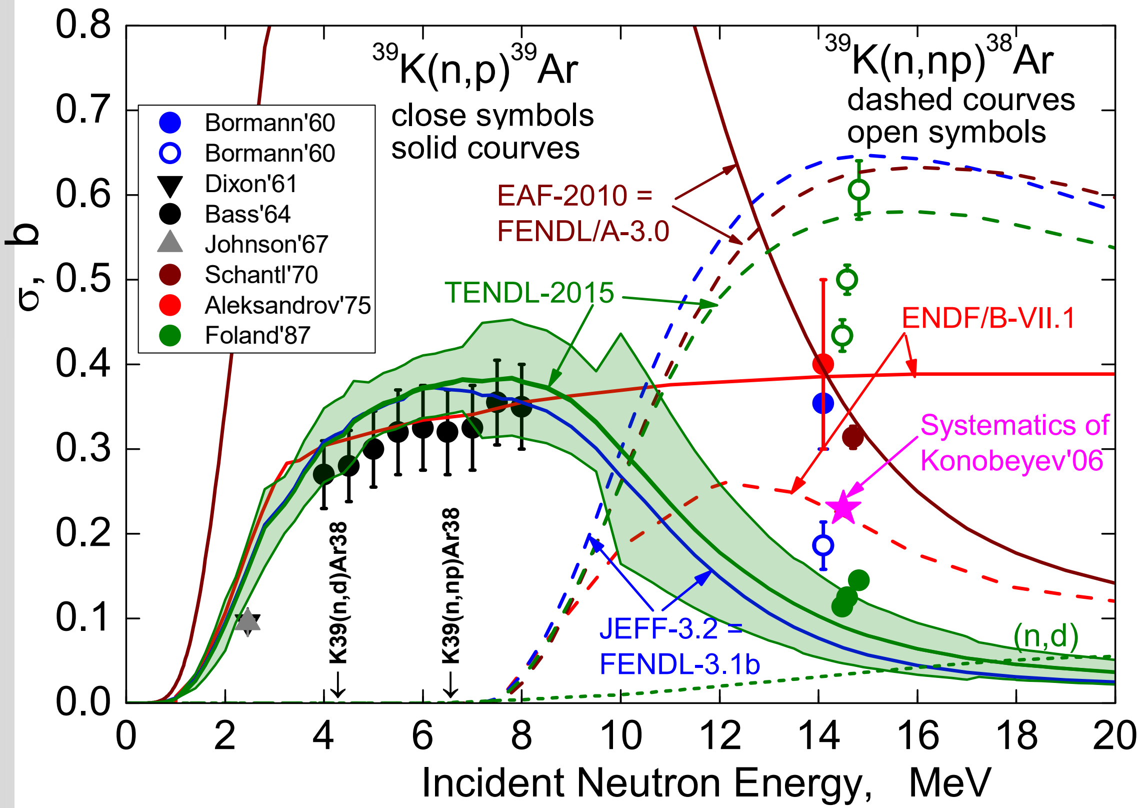
IFMIF neutronics: - ^{39}Ar is main contributor to long-lived radioactive inventories in NaK
- it is crucial to know the total amount of Ar gas transmuted from K

Fusion Plant neutronics: - ***long-term*** activation of bulk cement/concrete due to $^{39}K(n,p)^{39}Ar$



Observations for Measured Data

Three Experiments at 14 MeV

1. **Bormann'60 – p-spectroscopy**
2. **Aleksandrov'75 - p-spectroscopy**
3. **Schantl'70 – Activation**

delivers 3 times higher for $^{39}K(n,p)$
but 3 times lower for $^{39}K(n,np)$
than this one

4. **Foland'87 - AMS**

Observations for Evaluations

1. $^{39}K(n,p)^{39}Ar$ reaction:

- **ENDF/B-VII.1, FENDL/A-3.0=EAF-2010 seem to be wrong**
- **JEFF-3.2 and FENDL-3.1b are physically more reasonable**
- **TENDL-2015 is likely the best**

2. $^{39}K(n,p)+^{39}K(n,np)$ total Ar production:

all, except FENDL/A-3.0=EAF-2010, predict comparable XS

Summary

I. Uncertainty of (1) basic cross section (Fe isotopes TENDL-2017 randoms) and (2) Covariancies of Partition, Primary defect surviving functions and Lattice Threshold Energy were propagated to Covariancies (full Budget) of aggregate cross sections, i.e. Fe damage quantities computed by NJOY processing code

II. The same random TENDL-2017 files were used to estimate Covariancies for Benchmark Responses, i.e. energy spectra of neutron and gamma leaking from Iron sphere with ^{252}Cf computed by MCNP transport code

III. since TENDL evaluation base on nuclear reaction models/parameters (=TALYS) which are fitted to the wide range of targets, energies and reactions, then TENDL could be even more predictive than individual target evaluations if the later are fitted to specific reaction and/or to wrong experimental data, as it seems happened for $^{39}K(n,p)$ and $^{39}K(n,np)$

Recalling a history of collaboration between LC&FNG of NPI/Řež and INR of KIT:

- *2001/2002 (initiated by Pavel Bém) – (EASY Workshops, 2014 ...) - 2010: measurement (NPI) & analysis/modelling (KIT) of n-sources spectra, validation of n- and d-activation reactions, high energy dosimetry reactions …*
- *2011 - 2016 (IAEA CRP on IRDFF validation and extension): (n,xn) dosimetry reactions (NPI) and SPA in ^{252}Cf spectrum (Research Center) (see actual requests in HPRL under Special Quantities)*