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Covariances for the ^{56}Fe radiation damage cross sections

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Objectives of the present work:

- evaluation of covariance matrices for Physical Quantities used for characterization of neutron induced Radiation Damage in Materials
- They include:
  - kinetic energy released by ch.particles *KERMA* - locally deposited Nuclear Heating
  - damage energy *DE* - defines the number of displaced atoms dpa = *0.8*DE/Ed*
  - gas production *(n,xHe), (n,xT), (n,xH)* … - transmuting target nuclei into gases
- Such Uncertainties and Energy-Energy or Reaction-Reaction correlations **were not assessed so far**, whereas the covariances for many cross sections are often presented in modern evaluated data libraries
- Since damage quantities depend on many reactions channels and energy-angular distributions of reaction recoils, the evaluation of uncertainty is not straightforward
- To reach a declared goal, we used an idea of Total Monte Carlo (*TMC*) application to Nuclear Data

This study was stimulated by:

IAEA Coordinated Research Project "Primary Radiation Damage Cross Sections"

(*https://www-nds.iaea.org/CRPdpa/* *or just google "IAEA dpa")*

Method of calculation of Energy-Energy and Reaction-Reaction Covariancies from TENDL random files by TMC

- we used 1 unperturbed (original, < 200 MeV) and 500 random (sampled input parameters of nuclear model, < 20MeV) files for n + ^{56}Fe from TENDL-2013

- all 501 files were processed by NJOY-2012.50+ to get needed physical quantities as ENDF-6 formatted files. Following NJOY modules (additionally to RECONR, BROADR [T = 293K], …) were used:

  HEATR - to calculate KERMA (energy balance designed by MT = 301) and Damage Energy (MT = 444)

  GASPR - to calculate gas production cross sections (n,x^{4}He) = MT207, (n,x^{3}He) = MT206, (n,xt) = MT205, (n,xd) = MT 204 and (n,xp) = MT203

  GROUPR - to produce **desired quantities in grouped-wise format *gendf*** (we selected VITAMIN-J 175gr which covers 10^{-5} eV to 19.64 MeV)

- Fortan-90 code was written to read in ***gendf files*** and to calculate Energy-Energy (E-E) and reaction-reaction (MT-MT) covariance matrices and SPectra Averaged quantities (SPA)

Results: Derived Covariance Matrices, example for Damage Energy (MT=444)

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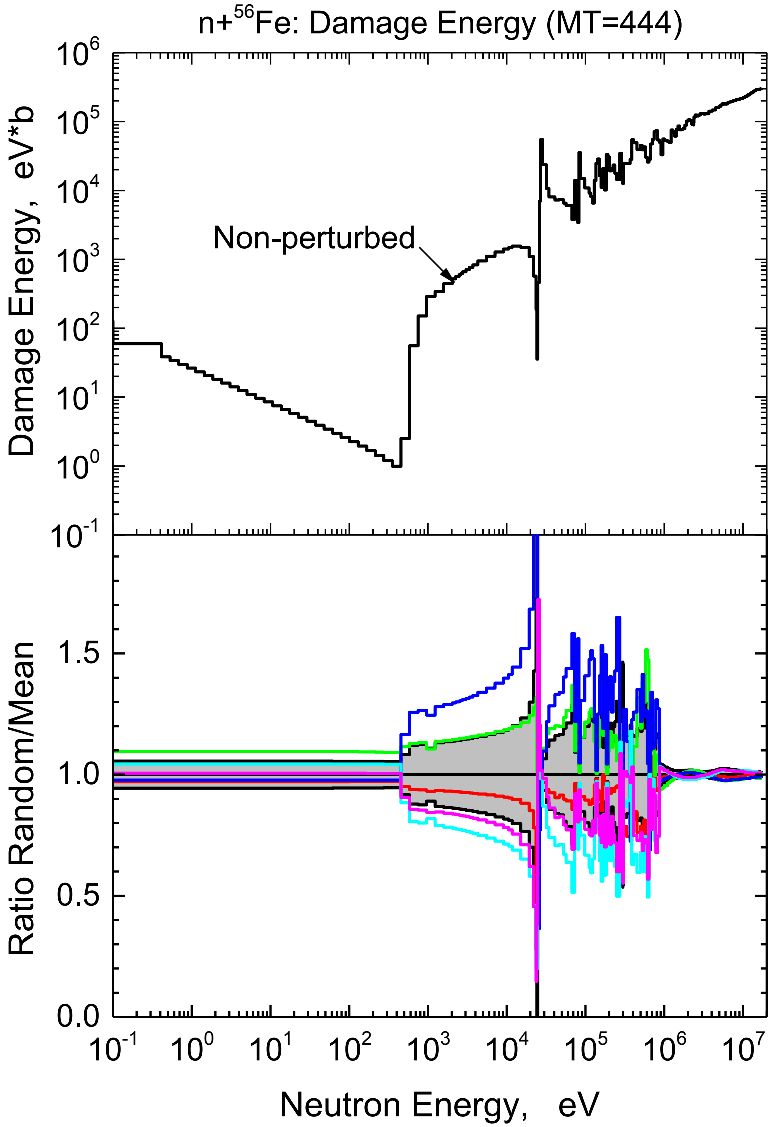
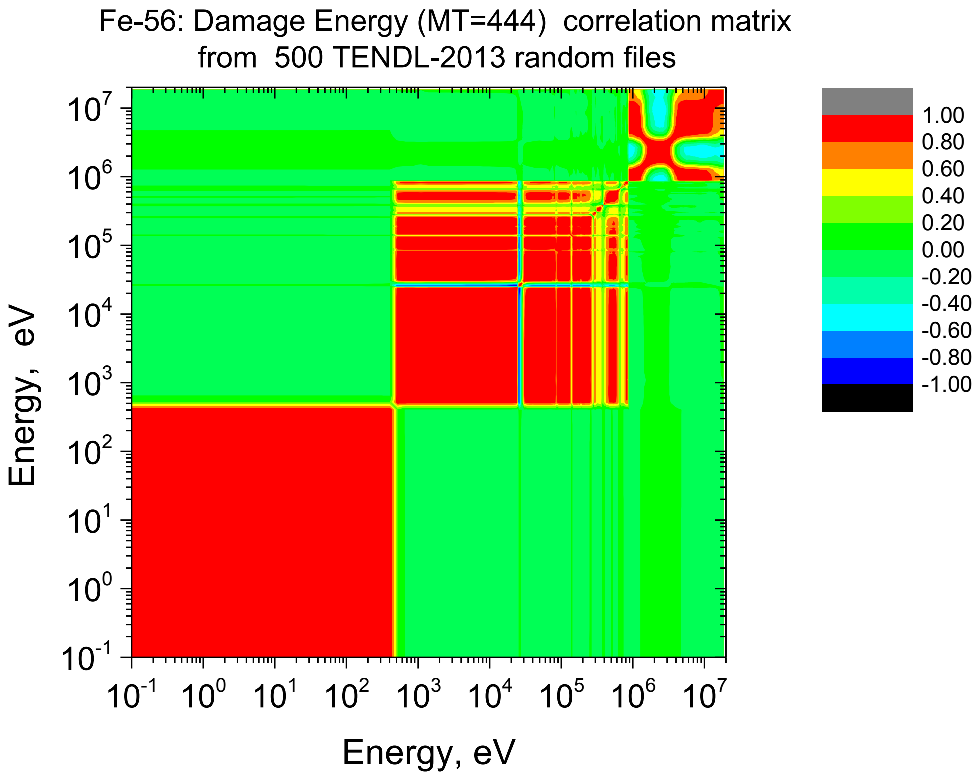
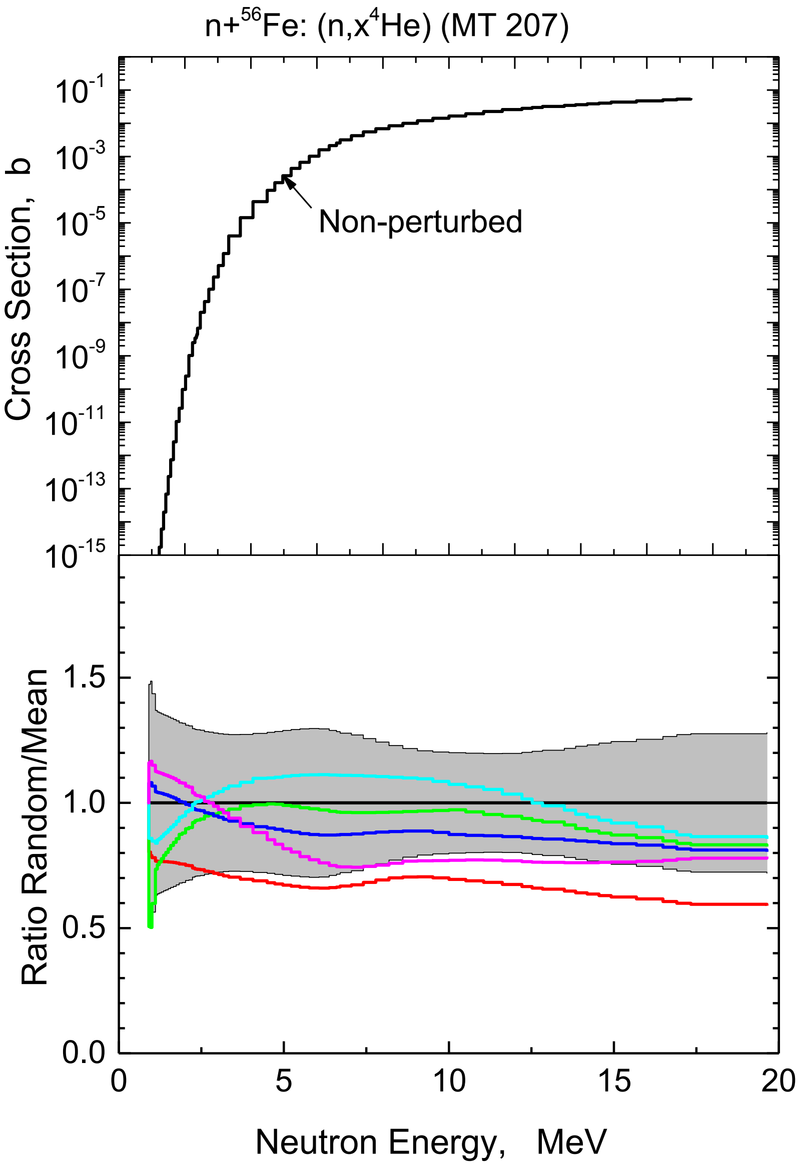


← **Quantity and Uncertainties (≈ 1- 40%)**

↓ **Correlation Matrix (3 regions with ≈ 1)**

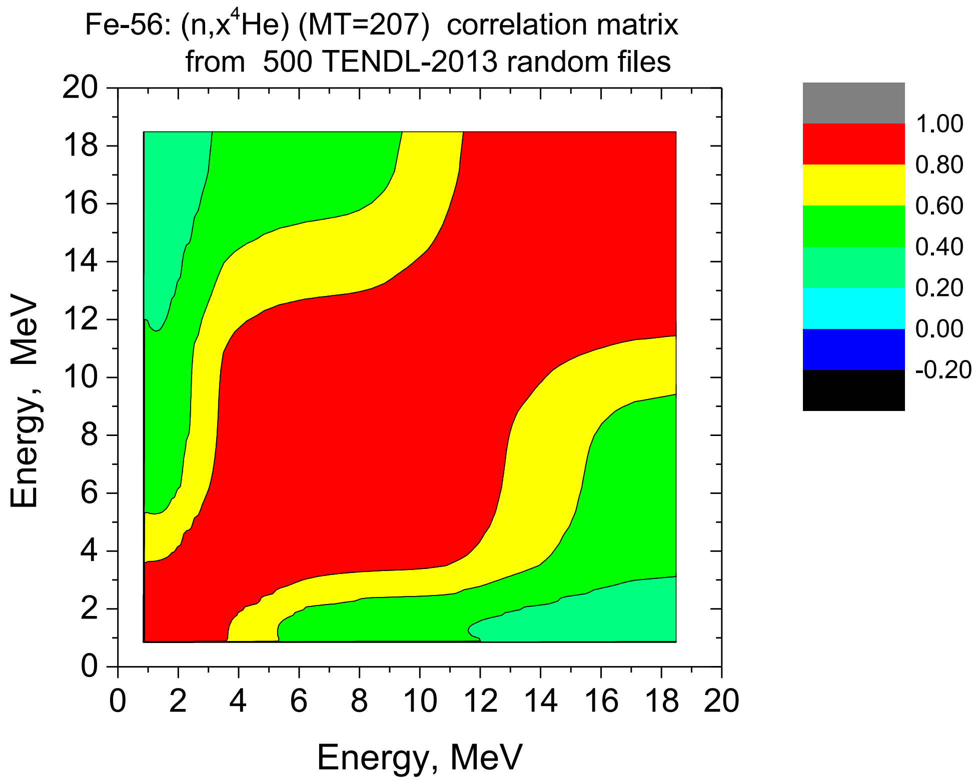


Results: Derived Covariance Matrices, example for gas production (n,x^{4}He) (MT = 207)



← **Quantity and Uncertainties (≈ 30%)**

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



Results: Statistical Significance (Convergence) of 175gr Uncertainty and 175 x 175gr E-E Correlation Matrix, example:

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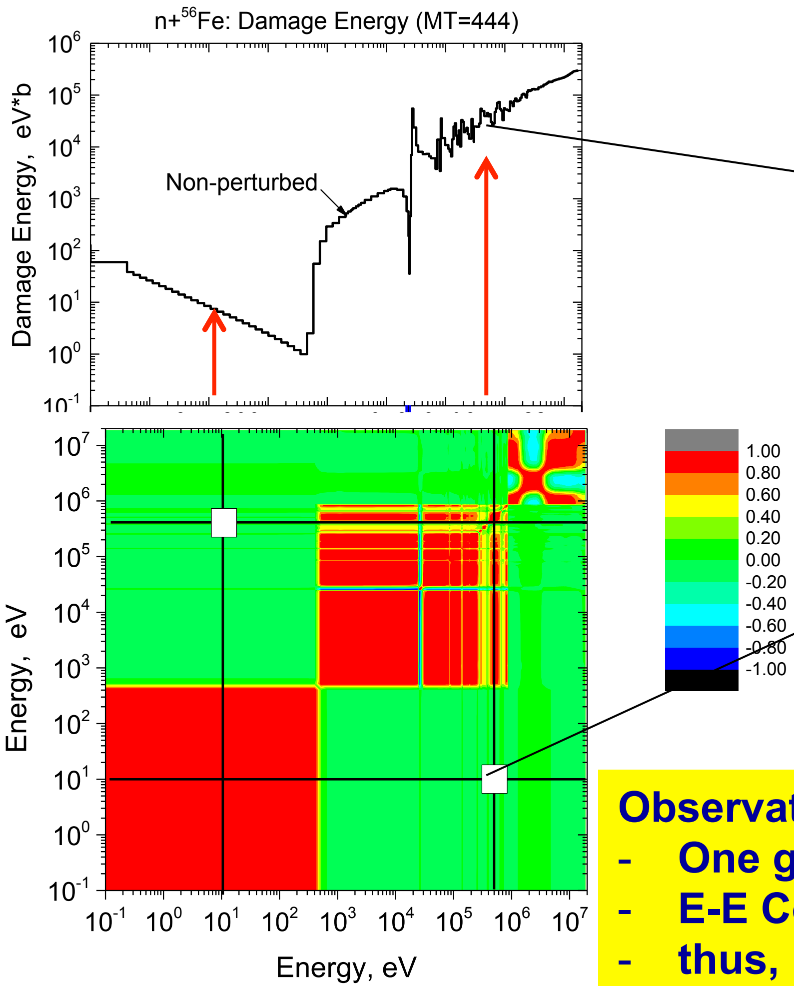
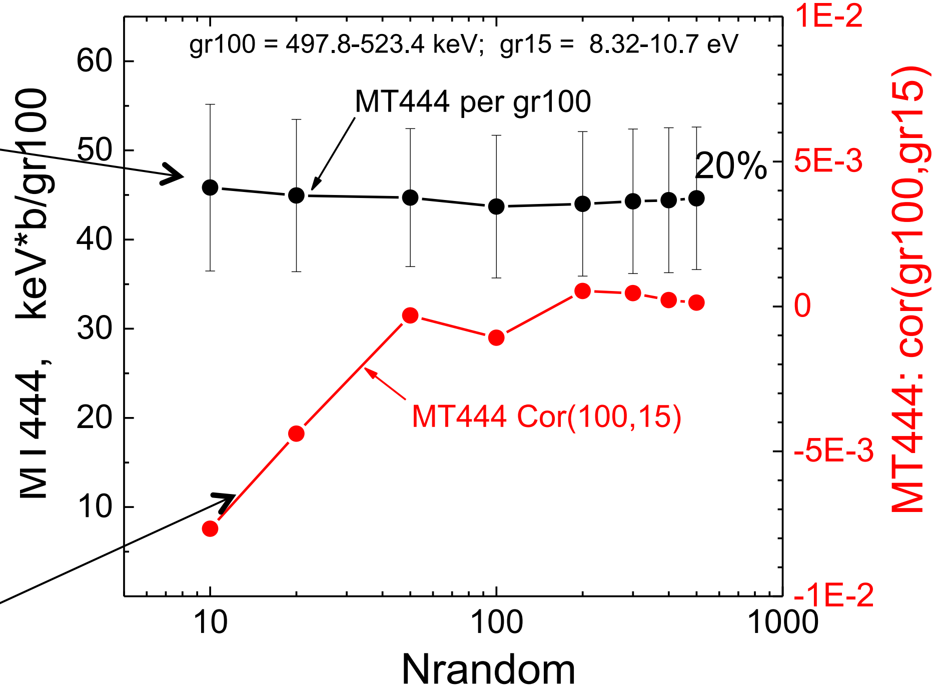
MT444: σ(E) and Cor(E,E)



MT444: σ(gr100) and Cor(100,15)



Observations:

- **One group σ and Δσ converge at Nrandom = 50-100**
- **E-E Correlation Elements converge at Nrandom ≈ 200**
- **thus, 175 gr presentation of Cov Matrix (< 20 MeV) from 500 random files is statistically correctc**

Results: ENDF-6 formatted E-E and MT-MT Damage Covariances to store in evaluation file

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175 gr E-E relative covariance matrices for **MT=203-444** were converted in ENDF-6 **MF33 file** (NB = 5, symmetric), *thanks to A.Konobeyev*

MF33/MT203-444 file was processed by COVEIGE code (*thanks* to *A.Trkov*):
small negative eigenvalues ≥ (1-6)E^{-8} were found
(however they always give positive variances in facility spectra considered)

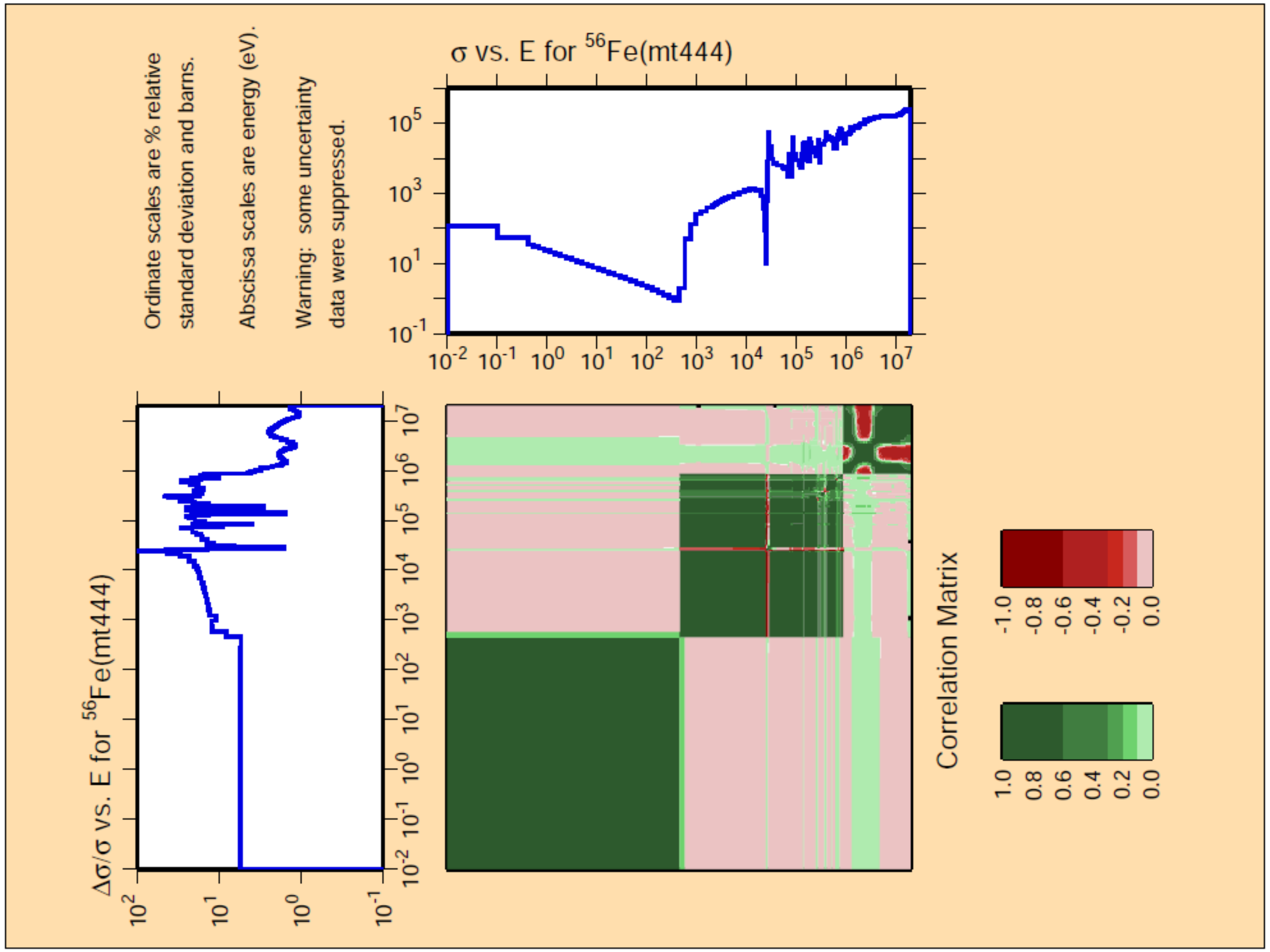
MF33MT203-444 was then added to **TENDL-2013 ^{56}Fe** file for purpose of checking on myENDF (*https://www-nds.iaea.org/exfor/myendf.htm* *thanks to V. Zerkin*) by:

- CHECKR (WARNINGS: IN MF=33 MT= 203 ALLOWED IN DERIVED FILES
  ERROR FOUND: SECTION 33/203 NOT IN DIRECTORY, …)
- FIZCON (ERROR FOUND: SECTION 33/203 NOT IN INDEX, ….)
- STANEF (OK!)

Finally **the whole file (TENDL-2013 ^{56}Fe + MF33 with MT 203-444)** was successfully processed by NJOY-2012.50 (ERROR, COVARR)

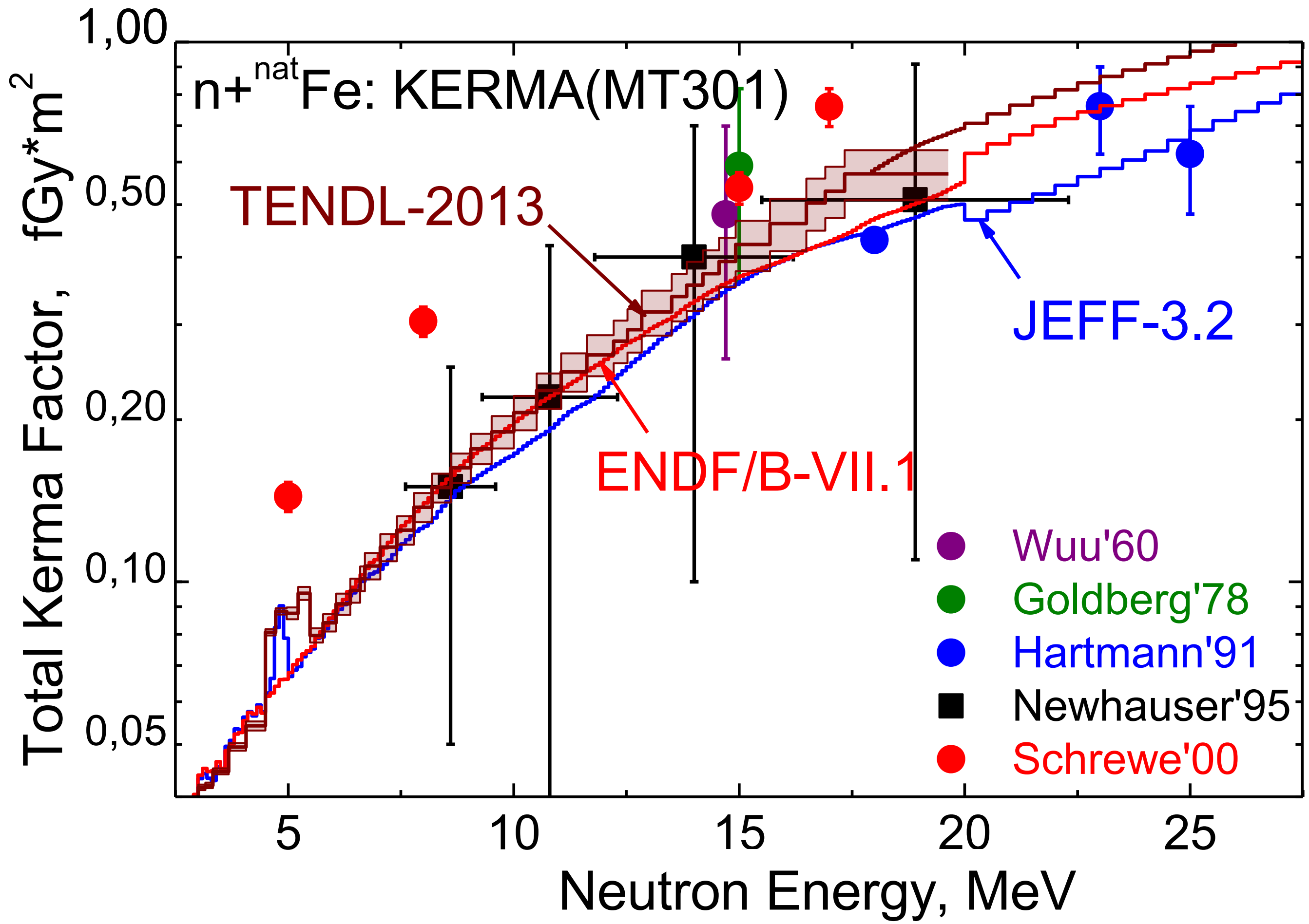
- illustrative plots on the next slide =>

Results: Damage Uncertainty and E-E Correlation in ENDF-6: plots from NJOY-2012, example for MT 444



Details noticed: NJOY automatically added ≈ 20 groups to 175gr in our MF33

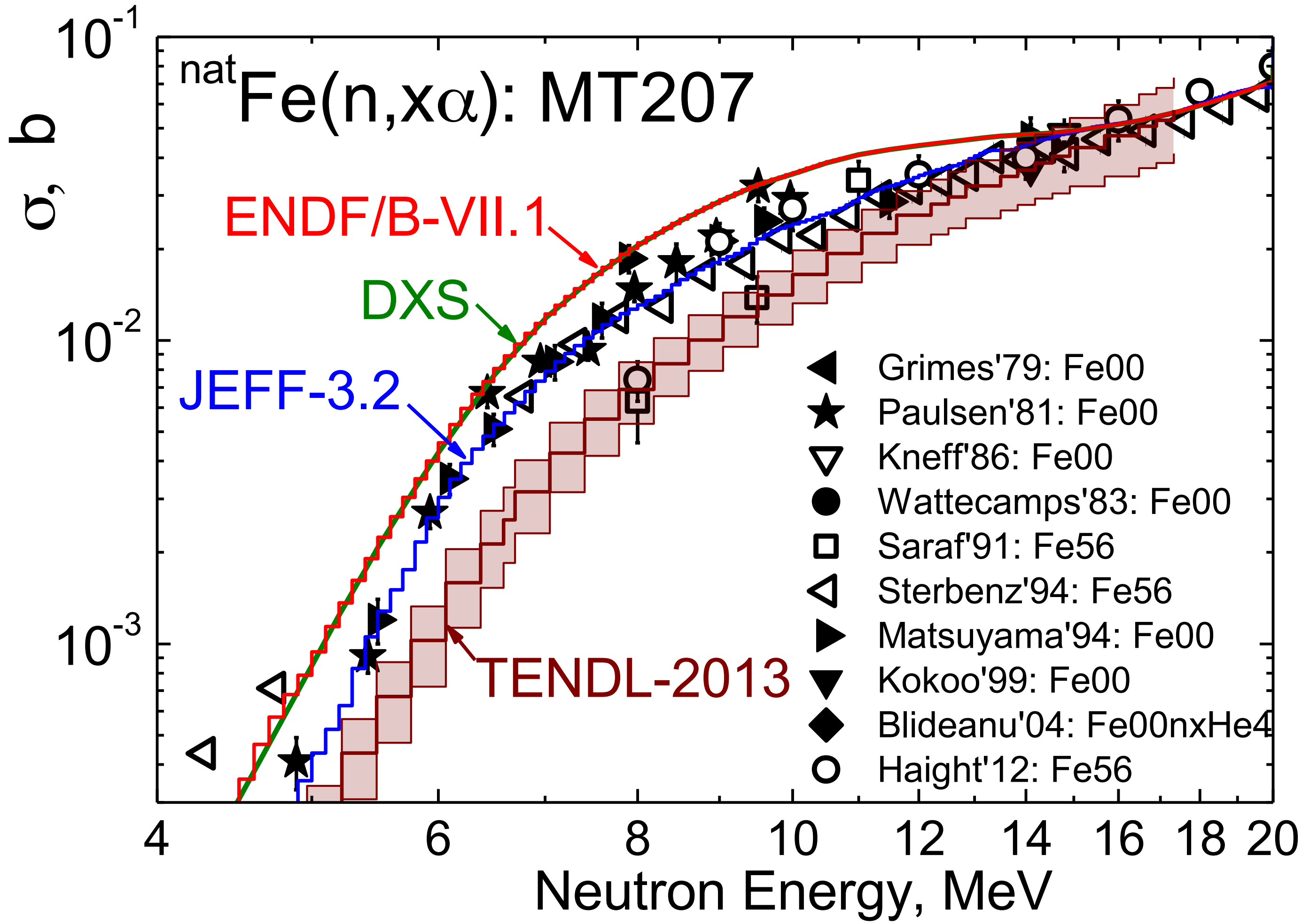
Results: Experimental Validation of Uncertainties - it is possible to do for (1): KERMA



Observations:

- **Uncertainties from TENDL random files (^{56}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 …**
- **Mixing of isotopes data by MIXR/NJOY-2012 was tricky … (*solved by O.Cabellos, A.Kahler*)**

Results: Experimental Validation of Uncertainties - it is possible to do for (2): (n,xα)

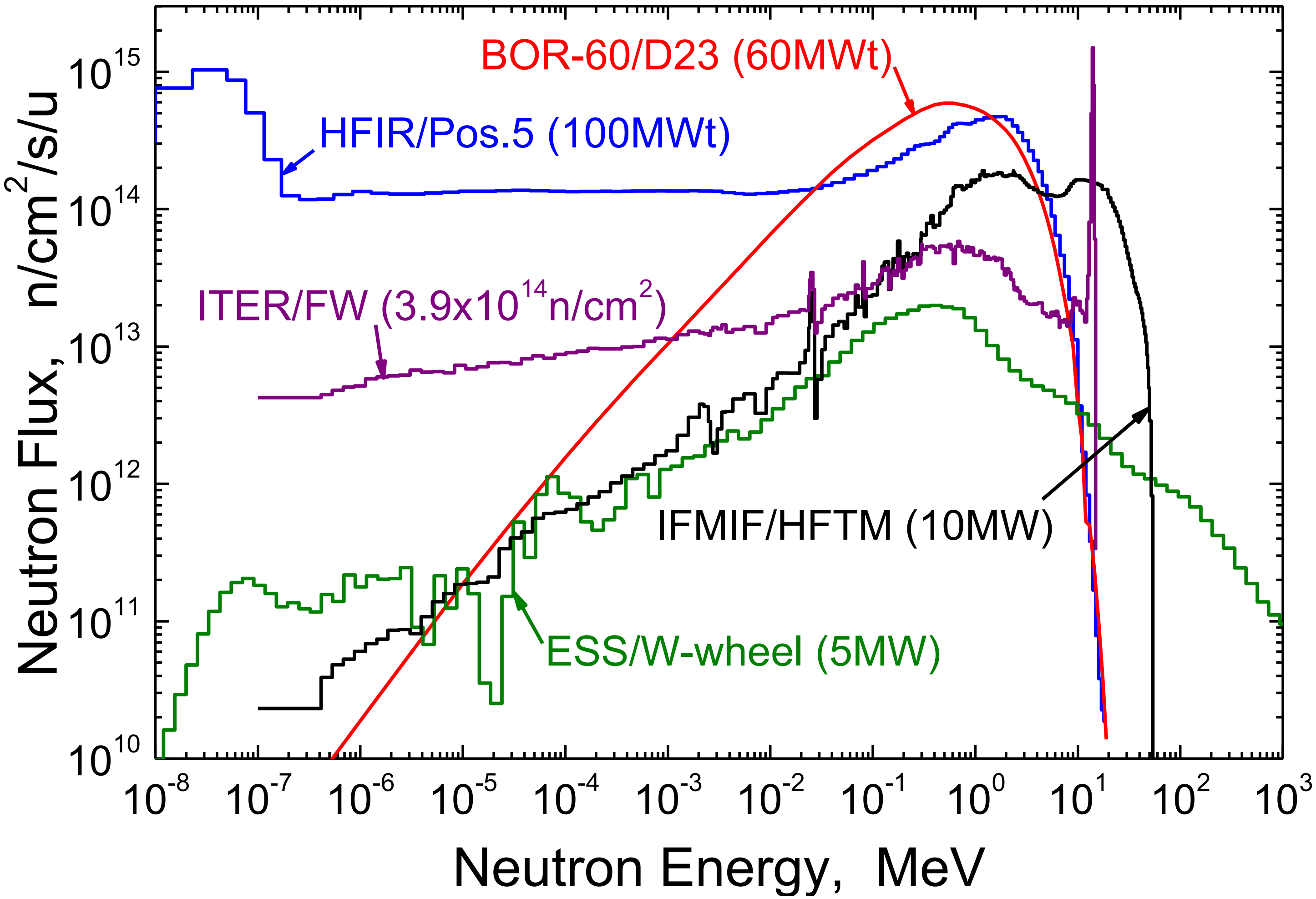


Observations:

-Uncertainties from TENDL-2013 random files (^{56}Fe, 20%) ≈ bulk Experimental Unc. (10-20%)

-however TENDL-2013 underestimates the mean values of cross section

Practical Applications: Spectrum Averaged (SPA) Damage and Uncertainties in Nuclear Facilities - Spectra



For representative calculation of SPA we selected:
HFIR/C5 (Fission), ITER/FW (Fusion) & IFMIF/HFTM (Spallation)

Practical Applications: Spectrum Averaged (SPA) Damage Uncertainties and MT-MT Corr. for HFIR, ITER & IFMIF

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Bold - full E-E correlation matrix, *Italic – ignoring off-diagonal elements*

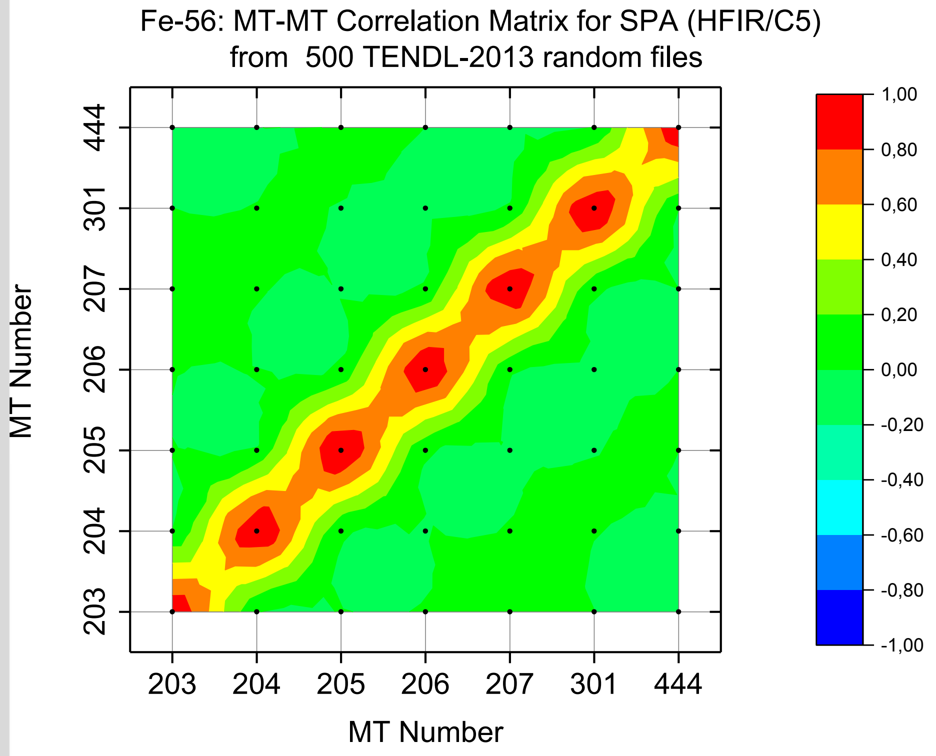
Facility/Location	HFIR/C5	ITER/FW	IFMIF/HFTM
Neutron Flux [n/cm^2/s]	5.10E+15	3.90E+14	7.32E+14
Averaged Energy [MeV]	0.41	3.47	7.00
NRT Displacements [dpa/fpy]	**30.5 ± 0.95 (3.1%)** *30.5 ± 0.24 (0.8%)*	**10.4 ± 0.16 (1.5%)** *10.4 ± 0.05 (0.5%)*	**25.1 ± 0.36 (1.4%)** *25.1 ± 0.09 (0.4%)*
KERMA [W/Kg]	**277 ± 7 (2.7%)** *277 ± 2 (0.7%)*	**246 ± 21 (8.7%)** *246 ± 12 (4.9%)*	**469 ± 31 (6.7%)** *469 ± 10 (2.2%)*
(n,x^{4}He) [appm/fpy]	**5.7 ± 1.3 (23%)** *5.7 ± 0.3 (6%)*	**92 ± 21 (23%)** *92 ± 12 (13%)*	**136 ± 31 (23%)** *136 ± 11 (7.8%)*
(n,x^{1}H) [appm/fpy]	**37 ± 6.3 (16.9%)** *37 ± 1.6 (4.4%)*	**410 ± 72 (17%)** *410 ± 41 (10%)*	**642 ± 102 (16%)** *642 ± 31 (4.9%)*
MT-MT correlation: max. between (n,x^{4}He) & (dpa)	204-206 = + 1.05% **207-444 = - 5.9E-5**	205-206 = + 1.07% **207-444 = + 1.8E-4**	204-206 = + 0.66% **207-444 = + 1.4E-4**

Findings:

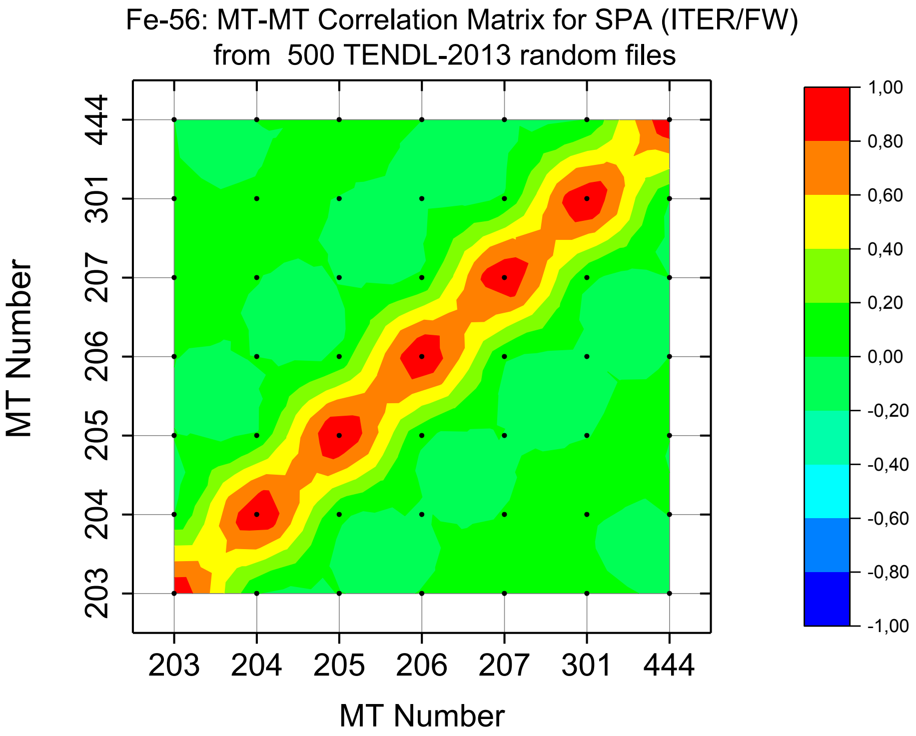
- **Nuclear Data Covariances result to 1.5 - 23% for SPA in Fission, Fusion and Spallation**
- **Neglecting E-E correlations reduces SPA Uncertainties by 2-3 times**
- **MT-MT correlations are small: for most practically important Cor (207,444) < 2 E-4**

Practical Application: MT-MT Correlation Matrix for SPA Damage - results for MT=203-444

↓ MT-MT for HFIR/C5



↓ MT-MT for ITER/FW



Findings: NO practically significant MT- MT correlations (Correlation ≤ 1%)

Practical Applications: Damage Uncertainties from Nuclear Data vs. Material Physics in representative Facilities

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SPA Damage Uncertainties for ^{56}Fe in IFMIF/HFTM, ITER/FW and HFIR/C5

Source of Uncertainty:	Nuclear Data	Material Physics
Damage Energy DE	± (1.4 - 3.1)%	
Lattice Thresh. Ed = 40 ± 2 eV*		± 5.0%
Sum Uncertainty for NRT-dpa = 0.8*DE/2Ed	**± (5.2 - 5.9)%**	
Defect Surviving Efficiency		OECD fit ± 2%** **Spread MD ~ ± 20%****
Sum Uncertainty for arc-dpa ~ 0.8*DE/2Ed*Efficiency	**± (5.2 - 5.9)% + ± (≈ 20)%**	
KERMA ≡ local Nuclear Heating	± (2.7 - 8.7)%	do not contribute
(n,xα) or (n,xH)	± 23% or ± 17%	do not contribute

*) *K. Nordlund et al., NIM B246(2005)32*

**) *"Primary Radiation Damage in Materials", Report NEA/NSC/DOC(2015)9, OECD 2015*

Findings: Material Physics parameters add 5% to *NRT*-dpa and 20% to *arc*-dpa

Summary

- E-E & MT-MT Covariance Matrices for Damage Quantities (Damage Energy, KERMA, Gas production) in ^{56}Fe were derived from TENDL-2013 random files
- E-E Covariance Matrices were written in ENDF-6 format as MF33 file, added to unperturbed evaluation and tested on positive definiteness and format compliance by standard checkers and NJOY
- for practical application (i.e. energy weighted quantities in representative fission, fusion or spallation facilities) the Uncertainty were (*first time ?*) estimated as:
  1.3-3.0% for NRT-dpa, 3-9 % for KERMA and 17-23% for Gas-production
- uncertainty for NRT/arc-dpa has to be additionally increased by 5/20% which stem from Material Physics
- Reaction-Reaction correlations found to be small: He-dpa < 2E-4, gas-gas < 1E-2