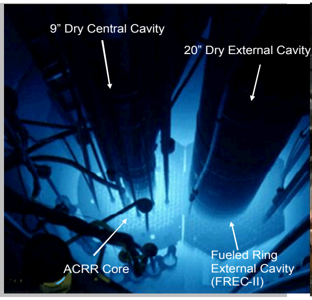
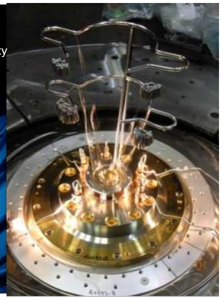
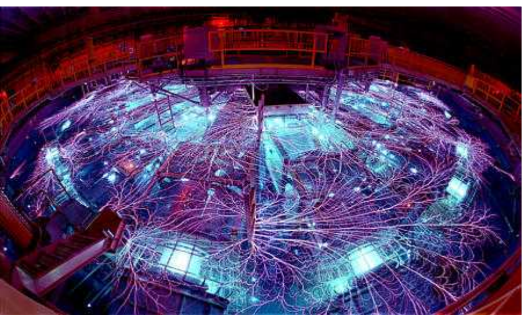
SAND2014-2721C

Covariance Propagation in Spectral Indices







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From: Sandia National Laboratories

Presented at: International Workshop on Nuclear Data Covariances (CW2014)

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

- Definitions
- Background
- Methodology for Treatment of Uncertainties
- Verification of Methodology
- Example Application to Neutron Benchmark Fields
  - ^{252}Cf Spontaneous Fission Standard Benchmark Field
  - ^{235} Thermal Fission Reference Benchmark Field
  - ACRR Central Cavity Reference Benchmark Field

Definitions

- Spectrum-averaged Cross Section, <σ>

$$\bar{\sigma} = \frac{\int_{E_1}^{E_2} \sigma(E)\Phi(E)\,dE}{\int_{E_1}^{E_2} \Phi(E)\,dE}$$

- Spectral Index, $S_{\alpha\beta}$

$$S_{\alpha/\beta} = \bar{\sigma}_{\alpha} / \bar{\sigma}_{\beta}$$

- C/E for Spectral Index, $C_{\alpha\beta}$

$$C_{\alpha/\beta} = [S_{\alpha/\beta}]_{cal.} / [S_{\alpha/\beta}]_{obs.}$$

Background

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- Metrics are needed to report/reproduce radiation environments.
  - Spectrum-averaged cross section is a baseline metric.
- Issue: difficulty in defining a metric that can easily be reproduced.
  - Uncertainty in low-energy spectrum for reactors.
  - Inadequacy of direct measures for integrated reactor power.
- Community moved to the use of a ratio of spectrum-averaged cross sections, a spectral index.
- For validation purpose (spectrum and cross sections), one needs to examine consistency of a calculated-to-experimental (C/E) ratio.
- Any validation activity need a proper treatment of uncertainties.
- Traditionally, analysts treat the cross section uncertainty and the measurement uncertainty but neglect the spectral uncertainty.

Uncertainty Considerations

- Uncertainty in $C_{\alpha,\beta}$ should include contribution from:
  - Calculated SI
    - Cross section for detector reaction – in numerator
    - Cross section for reference reaction – in denominator
    - Neutron spectrum in numerator
    - Neutron spectrum in denominator
    - **Treatment of correlation of spectrum in numerator and denominator – a nonlinear uncertainty propagation.**
  - Experimental SI
    - Measurement for detector reaction
    - Measurement for reference reaction

Uncertainty Formulation

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- Experimental activities uncorrelated, hence add in quadrature.
- Cross section uncertainty contribution in numerator and denominator are assumed to be uncorrelated, hence add in quadrature.
- Best-case spectrum uncertainty: positive correlation of spectrum uncertainty in numerator and denominator, hence cancellation in ratio.

$$\Delta C^{min}{}_{\alpha,\beta} = \sqrt{\Delta\sigma_\alpha{}^2 + \Delta\sigma_\beta{}^2 + \Delta A_\alpha{}^2 + \Delta A_\beta{}^2}$$

- Worst-case spectrum uncertainty: negative correlation of spectrum uncertainty in numerator and denominator, hence add as systematic terms.

$$\Delta C^{max}{}_{\alpha,\beta} = \sqrt{\Delta\sigma_\alpha{}^2 + \Delta\sigma_\beta{}^2 + \Delta A_\alpha{}^2 + \Delta A_\beta{}^2} + \Delta\varphi_{num} + \Delta\varphi_{denom}$$

Methodology

- Spectrum uncertainty is quantified via a covariance matrix.
- Covariance matrix for a spectrum is positive semi-definite and obeys a fluence normalization condition.
  - Symmetric matrix with real entries → Hermitian (self-adjoint)
  - Any real square symmetric matrix with linearly independent columns can be represented as a matrix product of elements based on the eigenvectors and eigenvalues:

$$C = Q\Lambda Q^T$$

- A Hermitian matrix has a Cholesky decomposition:

$$C = LL^T$$

$$C = Q\Lambda^{1/2}(\Lambda^{1/2})^T Q^T = (Q\Lambda^{1/2})(Q\Lambda^{1/2})^T$$

- Sample vector variation of spectrum can be generated as:

$$Z = Lu$$

  - where **u** is a vector of normal/Gaussian distributed random values with mean 0 and standard deviation 1

Verification Methodology

- Neutron Field: Central Cavity of the Sandia Pulsed Reactor III (SPR-III)
- Least-squares based LSL spectrum adjustment using ;
  - *"a priori"* 640-group SAND-II energy grid for MCNP calculated spectrum
  - 31 measured dosimetry reactions
  - IRDFF v1.02 cross section library
  - Yielded χ^2/dof = 2.193
- Covariance in 89-group using LSL for spectrum adjustment
- Verified: Positive definite covariance; normalization condition
- 3500 Monte Carlo samples for "total Monte Carlo" propagation generated using Cholesky decomposition matrix

Verification Cases

- Spectrum-averaged fluence:
  - 1.000 +/- 0.0047% (correct Monte Carlo propagation)
  - 1.000 +/- 10.11% (uncorrelated result)
- Average Neutron Energy
  - 1.299 MeV +/- 4.387% (correct linear propagation)
    - 1.299 MeV +/- 7.47% (uncorrelated result)
  - 1.298 MeV +/- 4.42% (correct Monte Carlo propagation)
- Spectral Index for Identical reactions
  - Reaction: $^{59}Ni(n,p)^{58}Co$
  - Cross Section: IRDFF v1.02
  - $\langle\sigma\rangle$ result: 55.72 mb +/- 5.82%
  - SI result: 1.00 +/- 0.0%

Example Best-Case: Similar Energy

Methodology	Metric	Value
Covariance Propagation	$^{32}S(n,p)^{32}P$ Xsec	36.14 mb
	Correlated Unc.	5.836 %
	Average Unc.	7.023 %
	$^{58}Ni(n,p)^{58}Co$ Xsec	55.72 mb
	Correlated Unc.	5.82%
	Average Unc.	7.18%
	Spectral Index	0.6485
	Worst-case Unc.	11.66%
	Best-case Unc.	0.0
Monte Carlo Sampling	$^{32}S(n,p)^{32}P$ Xsec	36.17 mb
	Correlated Unc.	5.858%
	$^{58}Ni(n,p)^{58}Co$ Xsex	55.76 mb
	Correlated Unc.	5.835 %
	Spectral Index	0.6485
	Correlated Unc.	0.5377 %

Example Worst-Case: Dis-Similar Energy

Methodology	Metric	Value
Covariance Propagation	$^{197}Au(n,\gamma)^{198}Au$ Xsec	134.7 mb
	Correlated Unc.	5.838 %
	Average Unc.	15.7 %
	$^{58}Ni(n,p)^{58}Co$ Xsec	55.72 mb
	Correlated Unc.	5.82%
	Average Unc.	7.18%
	Spectral Index	2.417
	Worst-case Unc.	11.2%
	Best-case Unc.	0.0
Monte Carlo Sampling	$^{32}S(n,p)^{32}P$ Xsec	134.7 mb
	Correlated Unc.	5.435%
	$^{58}Ni(n,p)^{58}Co$ Xsex	55.76 mb
	Correlated Unc.	5.937 %
	Spectral Index	2.431
	Correlated Unc.	10.62 %

Application: ^{252}Cf(sf)

- Data Source: NBS (NIST) work by J. A. Grundl, NBSIR 85-03151
- 13 spectral indices reported
  - Ratio'd to ^{238}U(n,f) as referencereaction
- Approach:
  - NBS original analysis
    - Used NBS spectrum
  - Updated analysis using IRDFF v1.02 cross sections
    - Used Mannhart ^{252}Cf spontaneous fission spectrum, IAEA-NDS-98
- Results:
  - **0% of the cases (0 of 13) showed the spectral uncertainty to be the dominant uncertainty contributor, 2 of 13 (15%) had spectrum component larger than cross section component.**
  - 8% of cases (1 of 13) deviated by more than 1-sigma: ^{235}U(n,f)

Our Results: $C_{\alpha,\beta}$ for $^{252}Cf(sf)$

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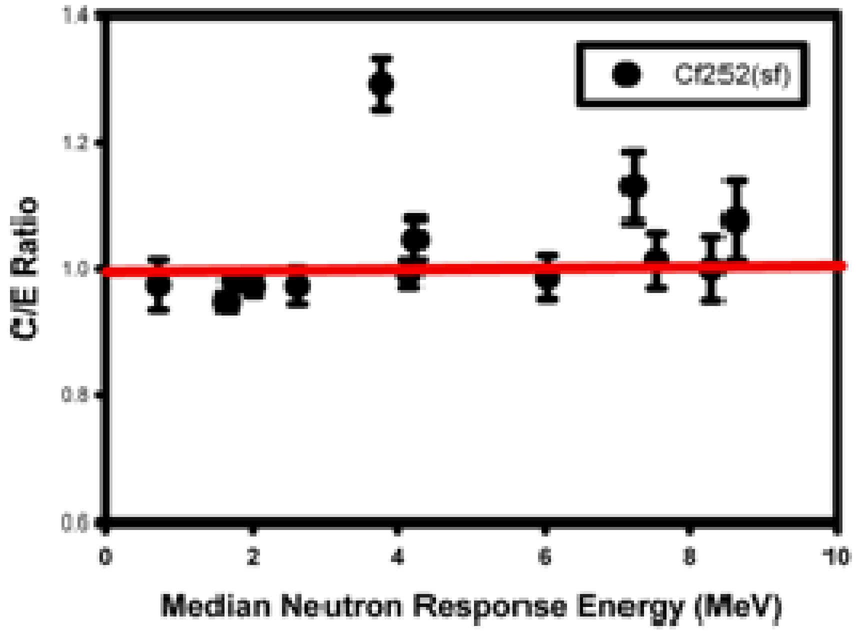
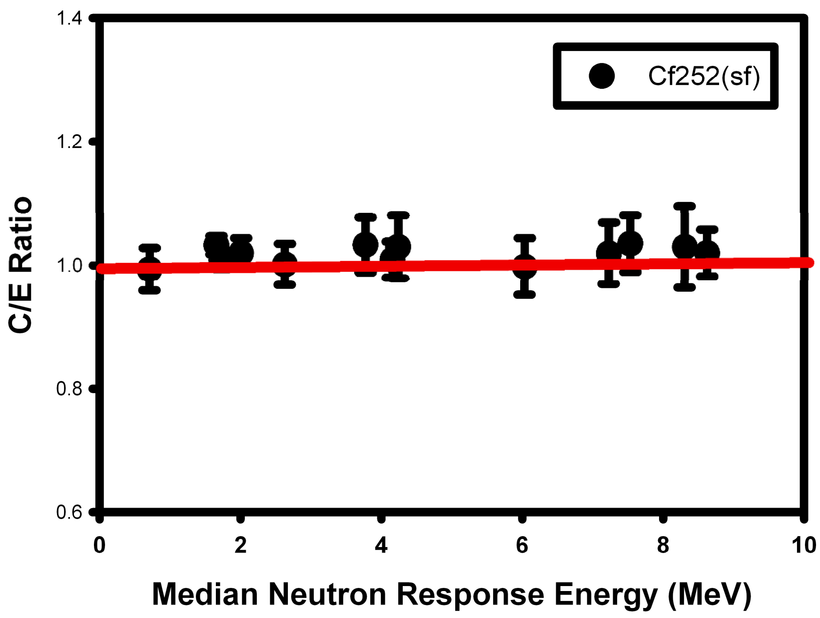
Reaction	Expt. SI Unc.	Xsec. Unc.	Spct. Unc.	$C_{\alpha\beta}$	$C_{\alpha\beta}$ Unc.
$^{237}Np(n,f)$	1.50%	1.69%	0.24%	1.020069	2.37%
$^{115}In(n,n')$	2.80%	1.66%	0.40%	1.001451	3.34%
$^{47}Ti(n,p)$	3.20%	2.73%	0.64%	1.033157	4.31%
$^{58}Ni(n,p)$	2.10%	1.74%	0.76%	1.009256	2.91%
$^{54}Fe(n,p)$	3.00%	3.62%	1.41%	1.030588	4.95%
$^{46}Ti(n,p)$	3.20%	3.05%	1.19%	0.998062	4.63%
$^{63}Cu(n, \alpha)$	3.60%	2.97%	1.38%	1.01935	4.91%
$^{56}Fe(n,p)$	3.20%	2.62%	1.45%	1.035295	4.43%
$^{48}Ti(n,p)$	3.20%	5.31%	1.55%	1.029717	6.42%
$^{27}Al(n,\alpha)$	3.20%	**0.72%**	**1.61%**	1.02009	3.71%
$^{239}Pu(n,f)$	1.20%	0.46%	0.086%	1.008722	1.45%
$^{235}U(n,f)$	1.20%	0.42%	0.091%	**1.032812**	**1.44%**
$^{197}Au(n,\gamma)$	3.20%	**0.57%**	**1.04%**	0.993622	3.48%

Application: $^{252}Cf(sf)$

NBS Reported Results



Updated Results with IRDFF



Interpretation of ^{252}Cf(sf) Results

- How do we explain the difference in NBS and updated IRDFF analysis:
  - Discrepant NBS activity is for **^{47}Ti(n,p) reaction**. Old cross section used in NBS analysis. Mannhart previously uncovered and fixed the cross section issue.
  - Changes in other cross sections improved the agreement
    - ^{63}Cu(n,α) near 7.22 MeV
    - ^{27}Al(n, α) near 8.6 MeV
  - No SIs are reported where the low energy portion of the spectrum in this field dominated the response, e.g. no ^{6}LI or ^{10}B reactions.
    - ^{197}Au(n,γ) reaction present but median response was at 0.71 MeV

Enlargement of C/E for SI's in $^{252}Cf(sf)$

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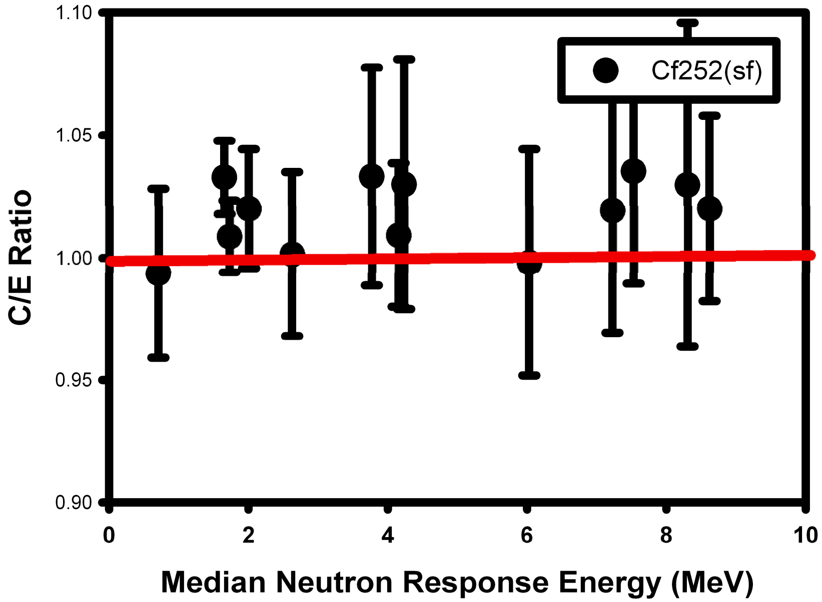
- Enlarged view of $C_{\alpha\beta}$ ratios shows excellent agreement in standard $^{252}Cf(sf)$field

Updated Results with IRDFF



Application: ^{235}U(th)

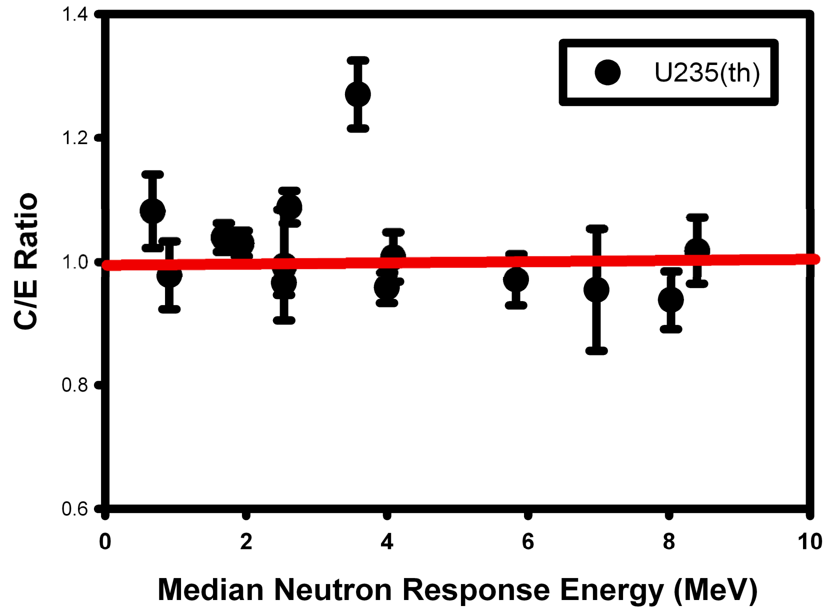
- Data Source: NBS (NIST) work by J. A. Grundl, NBSIR 85-03151
- 14 spectral indices reported
  - Ratio'd to ^{238}U(n,f) reference reaction
- Approach:
  - NBS original analysis
    - Used NBS spectrum
  - Updated analysis using IRDFF cross sections
    - Used JENDL-4 ^{235}U thermal fission spectrum
      - Selected over ENDF/B-VII due to positive definite covariance attribute
- Results:
  - **71% of the cases (10 of 14) showed the spectral uncertainty to be the dominant uncertainty contributor**
  - 21% of cases (3 of 14) deviated by more than 1-sigma
    - consistent with expectations for definition of the 1-sigma level

Results: $C_{\alpha,\beta}$ for $^{235}U(th)$

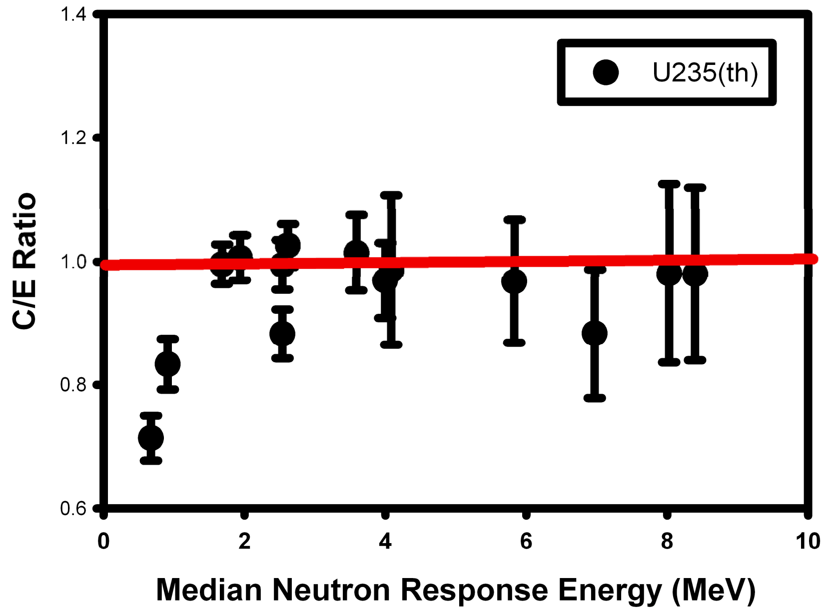
Reaction	Expt. SI Unc.	Xsec. Unc.	Spct. Unc.	$C_{\alpha\beta}$	$C_{\alpha\beta}$ Unc.
$^{237}Np(n,f)$	1.7%	1.689%	1.099%	1.006216	3.6286%
$^{93}Nb(n,n')$	9.0%	2.659%	2.22%	0.882392	4.4849%
$^{115}In(n,n')$	2.0%	1.681%	2.31%	0.994655	4.04557%
$^{47}Ti(n,p)$	4.2%	2.784%	4.43%	1.014135	6.03340%
$^{58}Ni(n,p)$	2.0%	1.749%	5.06%	0.96926	6.29753%
$^{54}Fe(n,p)$	3.5%	2.126%	2.09%	0.985939	12.2782%
$^{46}Ti(n,p)$	3.0%	3.191%	2.753%	0.967744	10.2960%
$^{63}Cu(n,\alpha)$	10.0%	3.090%	10.70%	0.883243	11.8241%
$^{48}Ti(n,p)$	4.2%	5.606%	13.02%	0.980577	14.7317%
$^{27}Al(n, \alpha)$	4.2%	0.750%	13.02%	0.979511	14.2724%
$^{239}Pu(n,f)$	1.7%	0.461%	0.462%	0.995686	3.23907%
$^{235}U(n,f)$	1.7%	0.417%	0.456%	1.026186	3.37307%
$^{10}B(n, \alpha)$	4.5%	0.069%	2.09%	0.833304	4.90081%
$^{6}Li(n,\alpha)$	4.5%	0.0647%	2.753%	0.713872	5.07067%

Application: $^{235}U(th)$

NBS Reported Results



Updated Results with IRDFF

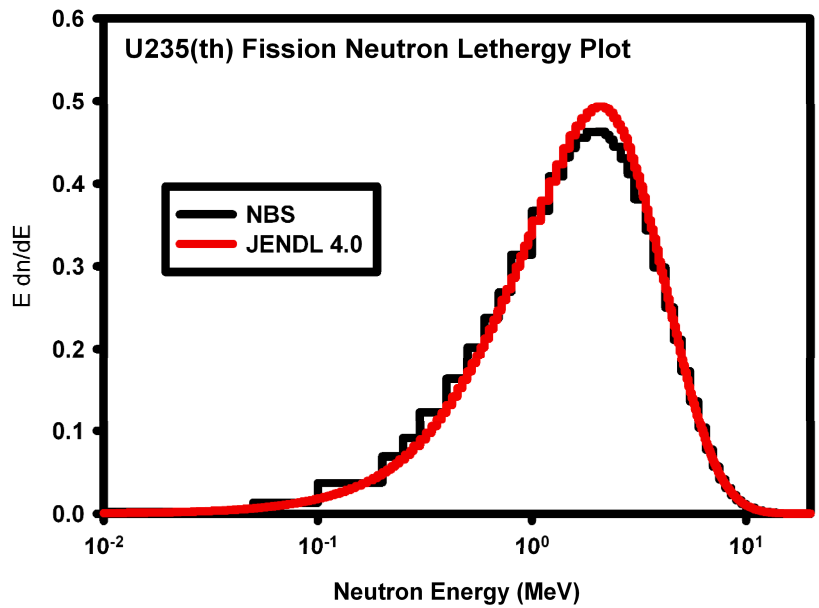


Interpretation of ^{235}U(th) Results

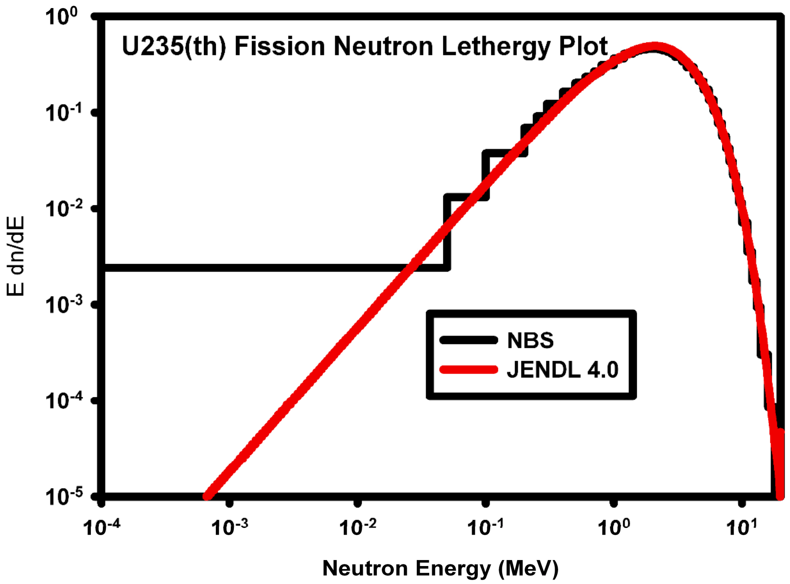
- How do we explain the difference in NBS and updated IRDFF analysis:
  - Discrepant NBS activity is for **^{47}Ti(n,p) reaction**. Old cross section used in NBS analysis. Mannhart previously uncovered and fixed the cross section issue.
  - NBS spectrum reported a much **smaller energy-dependent cross section uncertainty** than the JENDL-4 or ENDF/B-VII.1 evaluations.
    - E.g. at 8 MeV: JENDL-4 uncertainty = 13%, NBS uncertainty = 5.3%
  - NBS used a 45-group representation that was not adequate for low energy portion of spectrum critical for **$^{6}Li(n,\alpha)$ and $^{10}B(n, \alpha)$** ratios.
    - NBS report cautioned about use of low energy detectors in this field "because of uncertainties in the graphite return field". Rather, the 1-meter cavity at SCK/CEN is recommended.

Comparison of NBS and JENDL-4 ^{235}U(th) Fission Spectrum

Linear-Log lethergy Plot

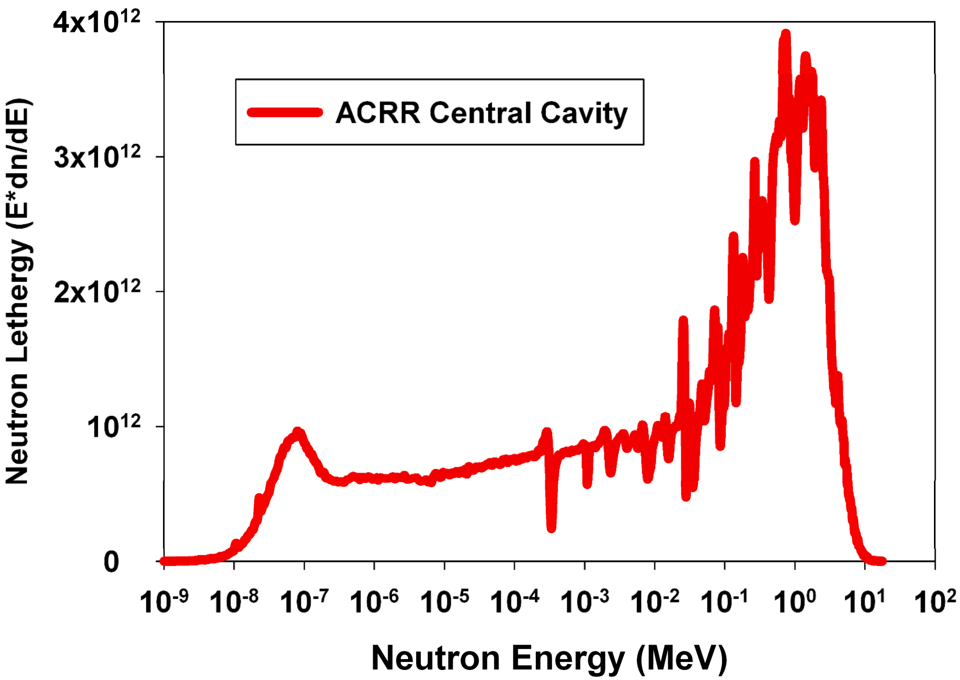


Log-Log Lethergy Plot



Application: ACRR Central Cavity

- "pool-type" reactor
- "*a priori*" neutron spectrum used in LSL spectrum adjustment
  - Produced with MCNP6
  - ENDF/B-VII.1 cross sections
  - 640-group SAND-II output representations
  - Structure represents resonances in cross sections for reactor materials, e.g. oxygen
- 40 measured activities
- χ^2/dof = 2.06



C/E for SI's for ACRR Central Cavity

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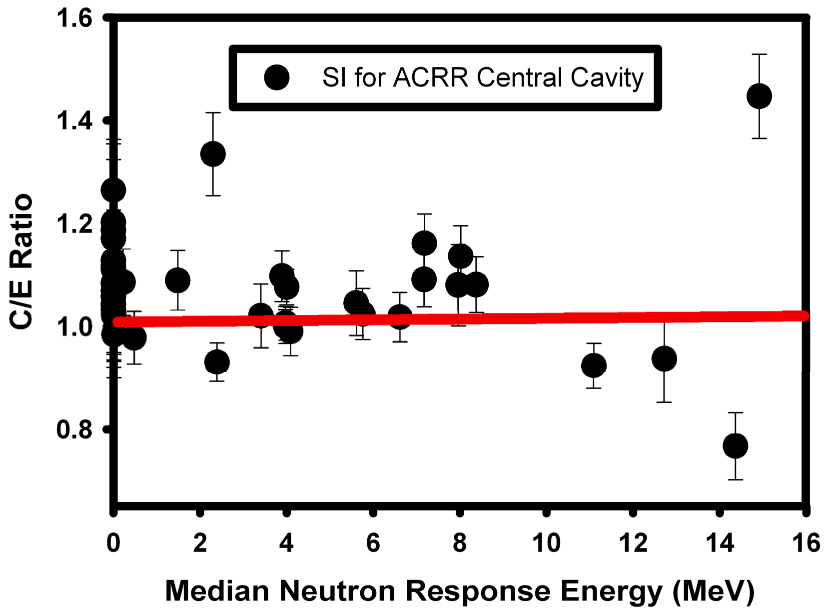
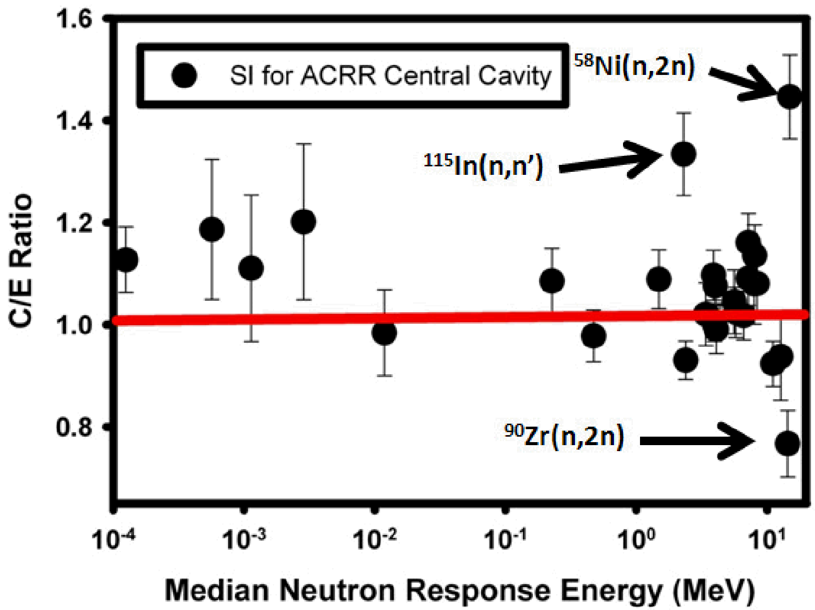
Linear Energy Axis



Logarithmic Energy Axis

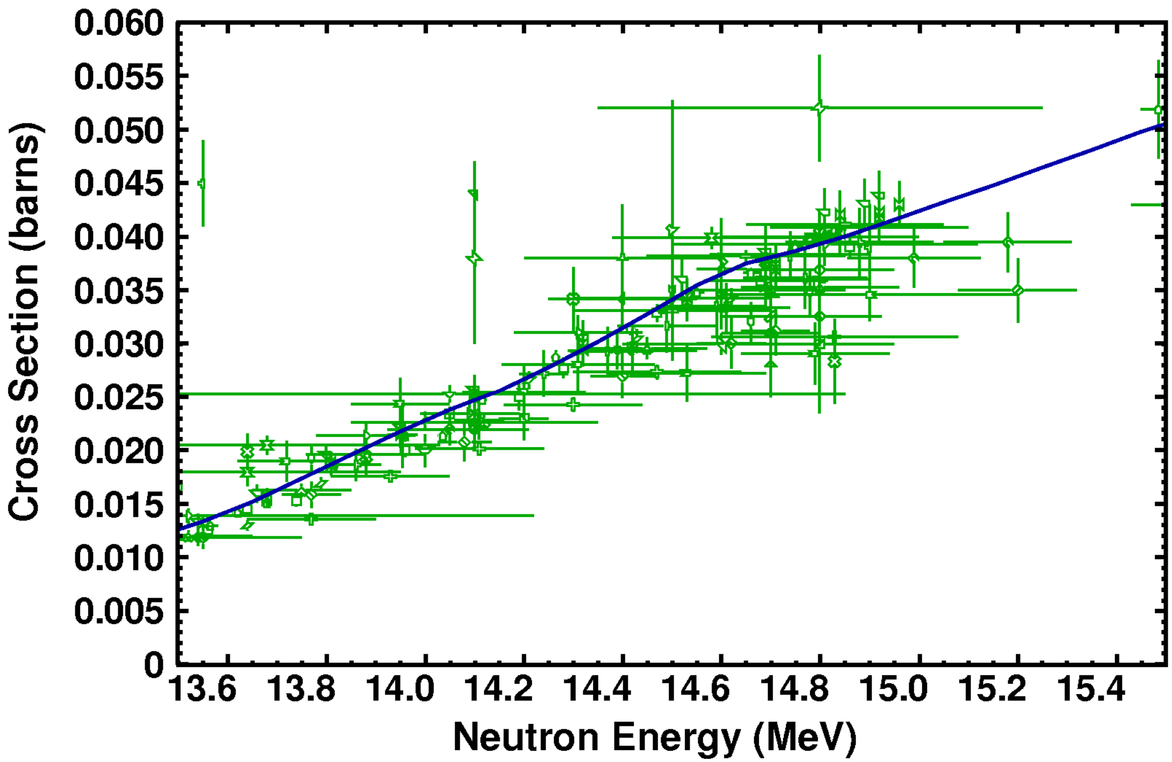


Results of ACRR Central Cavity Analysis

- In 62% of sensors (25 of 40) the spectrum is the dominant uncertainty contributor
- 4 of the 39 $C_{\alpha,\beta}$ ratios deviate from 1 by more than 3-sigma
  - ^{55}Mn(n,γ) with Cd cover
    - SNL analysis often shows difficulties with this reaction
  - ^{56}Fe(n,p) with B_4C cover
    - Cover correction suspect since reaction without cover shows good agreement
  - ^{58}Ni(n,2n)
    - In conflict with 3 other reactions in the high energy ~14-MeV response region: ^{90}Zr(n,2n); ^{93}Nb(n,2n); ^{59}Co(n,2n)
    - Measurement needs to be replicated
    - Cross section updated in IRDFF v1.03
  - ^{115}In(n,n')
    - Questions are being pursued about measurement

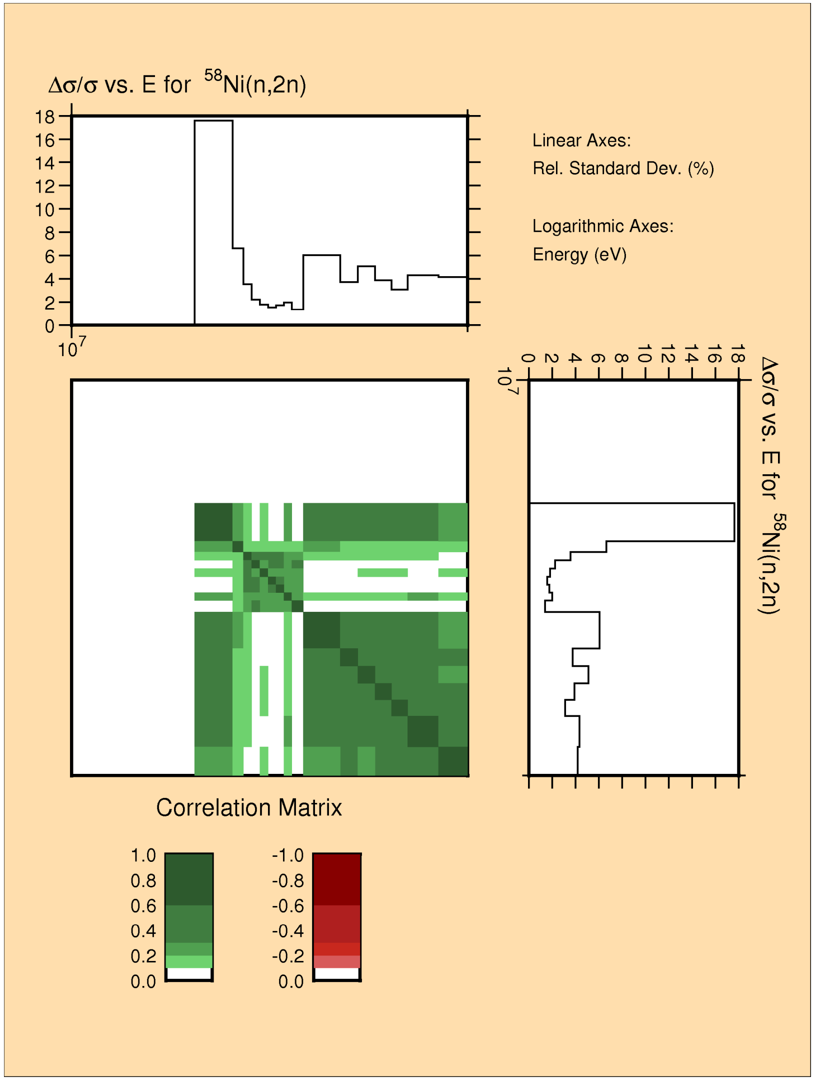
EXFOR Data Comparison for ^{58}Ni(n,2n) IRDFF Cross Section

- This cross section is in adequate agreement with 14-MeV EXFOR data – but there is a large variation in the experimental measurements



IRDFF Covariance ^{58}Ni(n,2n) Cross Section

- This cross section shows a small but highly correlated uncertainty
- This uncertainty is in conflict with observed variation in the raw EXFOR raw data, but the evaluator would have performed a much more rigorous investigation of the available experimental data when he set the uncertainty as captured in the nuclear data evaluation.



^{58}Ni(n,2n) Cross Section Agreement in Other Neutron Benchmark Fields

- Cross section shows good C/E agreement in ^{252}Cf(sf) and ^{235}U(th) benchmark neutron fields

Radiation Field Bench-mark Field	Metric		C/E
	Spectrum-Averaged Cross Section (mb)		
	Experimental	Calculated [Unc. (φ | σ)][1] [E_{05}, E_{50}, E_{95}][2]	
^{252}Cf spontaneous fission	0.008952 +/- 3.57%	0.00915 [6.043% | 1.63%] [13.063, 14.891, 18.214]	1.0221 +/- 7.21%
^{235}U thermal fission	0.0036 +/- 7%	0.00378 [11.5% | 1.799%] [12.986, 14.67, 17.789]	1.04 +/- 13.58%

Conclusions

- The contribution from the spectrum uncertainty typically dominates the overall uncertainty for spectral indices and must be addressed in analyses.
  - An exception is the very well characterized ^{252}Cf standard neutron field
- A methodology is presented for determining this spectral uncertainty component in the calculated SI and C/E ratio.
  - When a spectrum covariance matrix is available, i.e. when its uncertainty is characterized, a Cholesky decomposition can be applied to generate a random draw and a "total Monte Carlo" approach can be applied to accurately capture the uncertainty in a non-linear quantity like the spectral index.
- Example applications of this methodology are presented.

Questions?