

IRSN

INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Enhancing nuclear safety

Resonance Parameter Covariance Representation: File32 versus File33

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OUTLINE

- Resonance Region Covariance

- Evaluations for ^{48}Ti ;

- FILE32 to FILE33 conversion;

- Application;

- Concluding Remarks;

Available Covariance Data in ENDF

Contents of File Types (MF)

MF=30: sensitivity data covariance files

MF=31: covariance for average number of neutrons per fissions

MF=32: covariance for resonance parameters

MF=33: covariance for reaction cross sections

MF=34: covariance for angular distributions

MF=35: covariance for energy distributions

MF=36: covariance for angle-energy distributions

MF=37~38: null

MF=39: covariance for radionuclide production yields

MF=40: covariance for radionuclide production cross sections

Conversion from FILE32 to FILE33 Averaged Group Cross Sections

$$\Phi_g \bar{\sigma}_{xg} = \int_{E_g}^{E_{g+1}} \sigma_x(E) \Phi(E) dE$$

$$\Phi_g = \int_{E_g}^{E_{g+1}} \Phi(E) dE$$

Covariance Matrix for Group Cross Sections

If p_1, p_2, \dots, p_n are evaluated resonance parameters such that

$$\sigma_x = \sigma_x(p_1, p_2, \dots, p_n)$$

$$\delta \bar{\sigma}_{xg} = \sum_j \frac{\partial \sigma_{xj}}{\partial p_j} \delta p_j$$

Group Covariance Matrix

$$\langle \delta \bar{\sigma}_{xg} \delta \bar{\sigma}_{xg'} \rangle = \sum_{jk} \frac{\partial \bar{\sigma}_{xg}}{\partial p_j} \langle \delta p_j \delta p_k \rangle \frac{\partial \bar{\sigma}_{xg'}}{\partial p_k}$$

Covariance of the group cross sections depends on the covariance of the resonance parameters p as

$$\langle \delta p_j \delta p_k \rangle$$

These quantities are the resonance parameter covariance stored in the ENDF library (FILE32)

Averaged Group Cross Section

- Alternatively, the group covariance cross section can also be obtained as

$$\langle \delta \bar{\sigma}_{xg} \delta \bar{\sigma}_{xg'} \rangle = \frac{1}{\varphi_g \varphi_{g'}} \int_{E_g}^{E_{g+1}} \int_{E_{g'}}^{E_{g'+1}} \varphi(E) \varphi(E') M(\sigma) dE dE'$$

- $M(\sigma)$ is the covariance representation for the pointwise cross section, that is, the ENDF FILE33 representation.

Question:

Can one find an equivalence ?

$$\begin{aligned}
 \langle \delta \bar{\sigma}_{xg} \delta \bar{\sigma}_{xg'} \rangle &= \sum_{jk} \frac{\partial \bar{\sigma}_{xg}}{\partial p_j} \langle \delta p_j \delta p_k \rangle \frac{\partial \bar{\sigma}_{xg'}}{\partial p_k} \\
 \langle \delta \bar{\sigma}_{xg} \delta \bar{\sigma}_{xg'} \rangle &= \frac{1}{\varphi_g \varphi_{g'}} \int_{E_g}^{E_{g+1}} \int_{E_{g'}}^{E_{g'+1}} \varphi(E) \varphi(E') M(\sigma) dE dE'
 \end{aligned}$$

Diagram illustrating the equivalence between two expressions for the covariance of cross-sections. The top expression shows the covariance as a sum over parameters p_j and p_k , with the term $\langle \delta p_j \delta p_k \rangle$ circled in red. The bottom expression shows the covariance as an integral over energy E and E' , with the term $M(\sigma)$ circled in red. Red double-headed arrows indicate the equivalence between the two expressions.

FILE32 to FILE33 Conversion

Two stages:

Stage 1: Process resonance parameter covariance and generate averaged group cross-section uncertainties and correlation matrices. Either PUFF/AMPX or NJOY/ERRORR can be used;

Note: choice of an appropriate energy group structure and flux weighting spectra.

Stage 2: Conversion of cross section uncertainty and covariance generated in stage 1 into the ENDF FILE33 format;

Note: Simple way that this can be achieved is by using the COVCON module of the AMPX code system.

Application

- Process the ^{48}Ti resonance parameter evaluation;
- Choice of two energy group structures:
 - Coarse: 44 groups
 - Finer : 380 groups
- Use AMPX/PUFF to process the covariance data;

^{48}Ti Resonance Evaluation

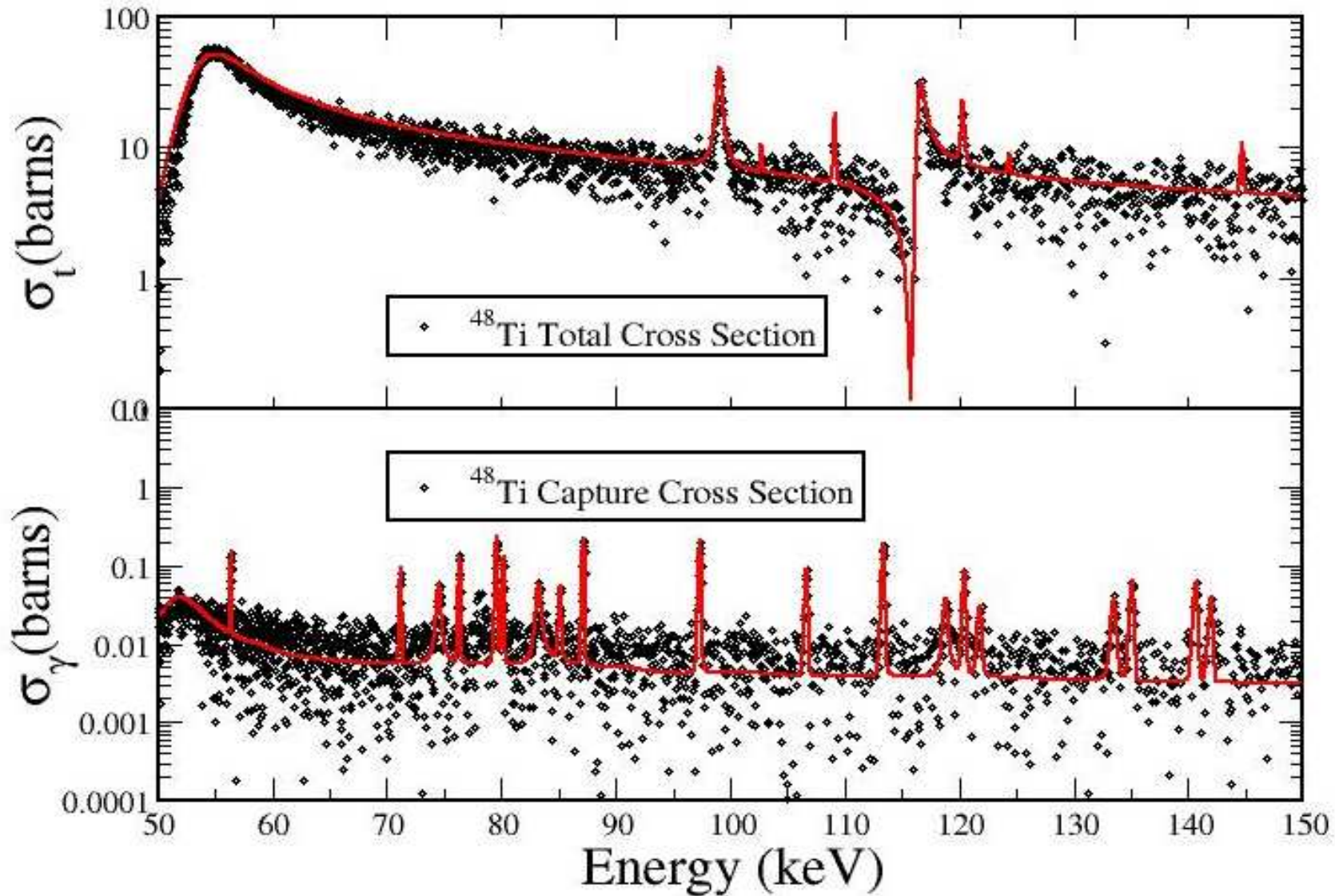
- Evaluation tool: SAMMY
- Energy range: Thermal to 400 KeV
- Experimental Data Base: transmission, capture
- Resonance Formalism: R-Matrix (Reich-Moore)
- Final Results: Resonance Parameters (RP) and Resonance Parameter Covariance (RPCM)

Experimental Data Base

(measurements done at ORELA)

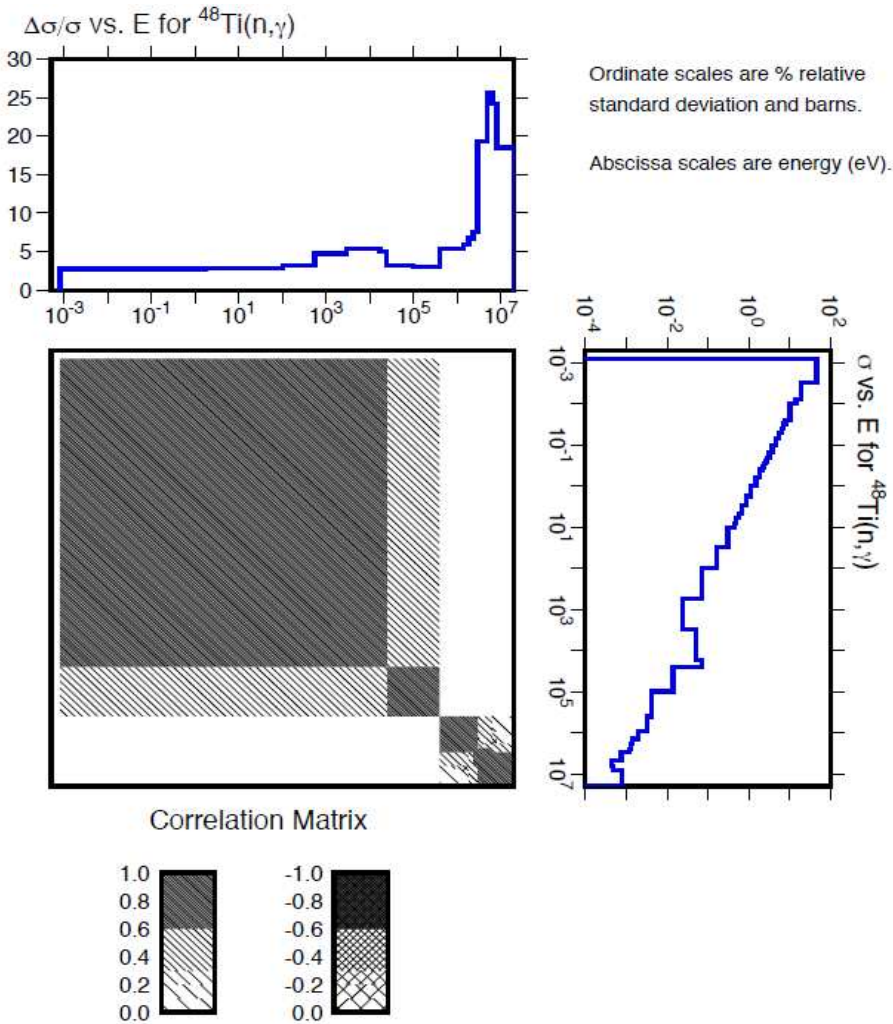
Data Set	Energy Range (keV)	Flight Path (meters)	Density (at/b)
Natural Titanium			
Transmission	0.01 - 500.0	79.827	0.052966
Transmission	0.01 - 500.0	79.827	0.008785
Capture	0.01 - 500.0	40.116	0.035158
Enriched 48 (99.32 %)			
Transmission	0.01 - 500.0	79.827	0.028185
Transmission	0.01 - 500.0	79.827	0.0011821
Capture	0.01 - 500.0	40.116	0.0091386

Fitting of the total and capture cross sections



Uncertainty and the correlation for the capture cross section

Uncertainty and the correlation for the capture cross section



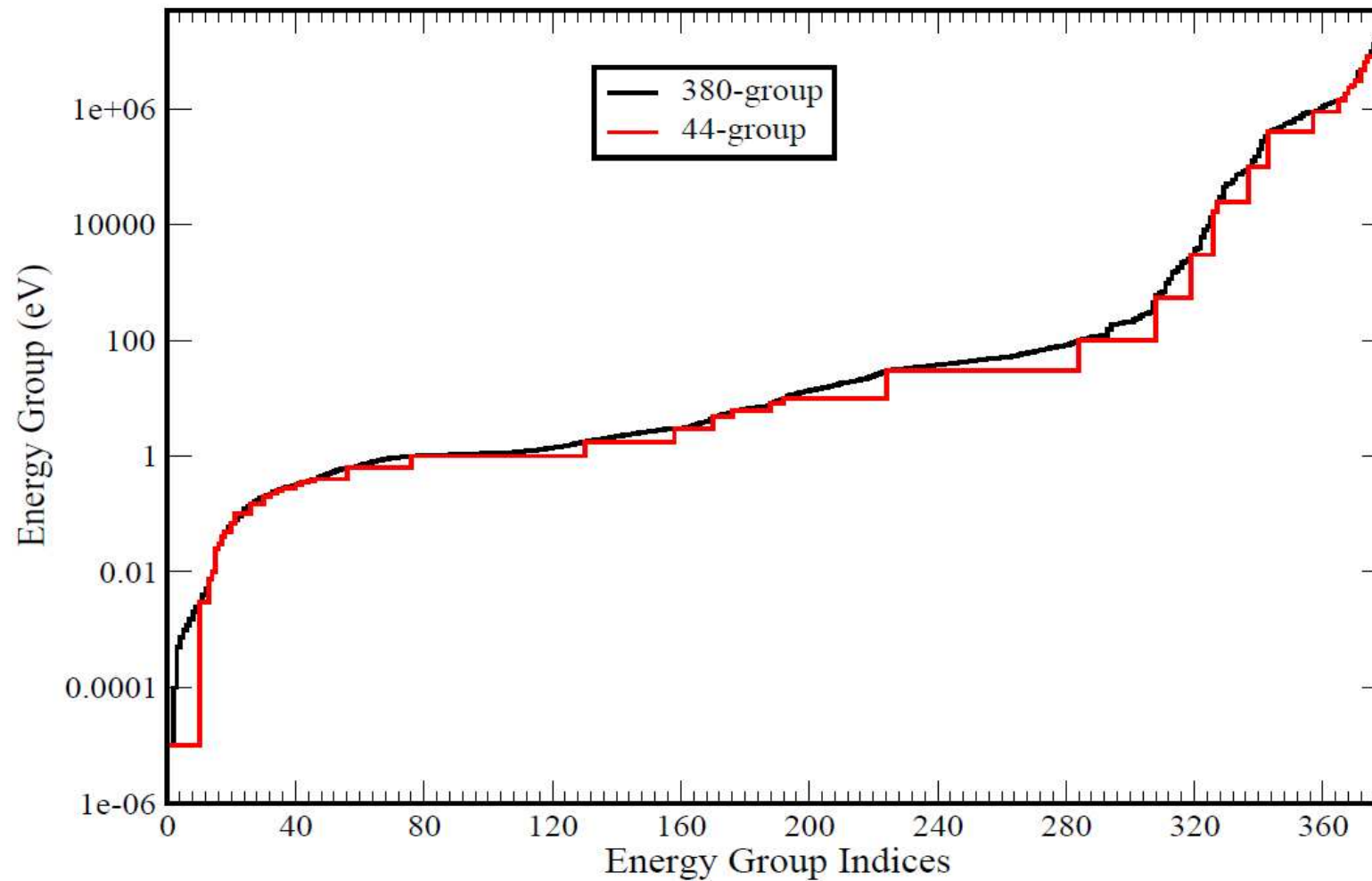
Cross section at thermal and capture resonance integral

Quantity	ENDF/B-VII.0	New ^{48}Ti Evaluation
σ_γ	7.84	8.32 ± 0.23
σ_s	4.36	4.04 ± 0.20
σ_t	12.20	12.35 ± 0.30
I_γ	3.68	3.78 ± 0.17

FILE32 to FILE33 Conversion

- AMPX modules used: PRELL, PRILOSEC, PUFF, and COVCONV
- Energy Groups: 44-group and 380-group
- In the resonance range up to 400 keV:
 - 35-group of the 44-group
 - 343-group of the 380
- Three Cross Section Libraries:
 - RPCM_LIB: FILE32
 - CSCM_44LIB: FILE33 44-group
 - CSCM_380LIB: FILE33 380-group
 - BOXER and COVERX format

380-group (black line) and the 44-group (red line)



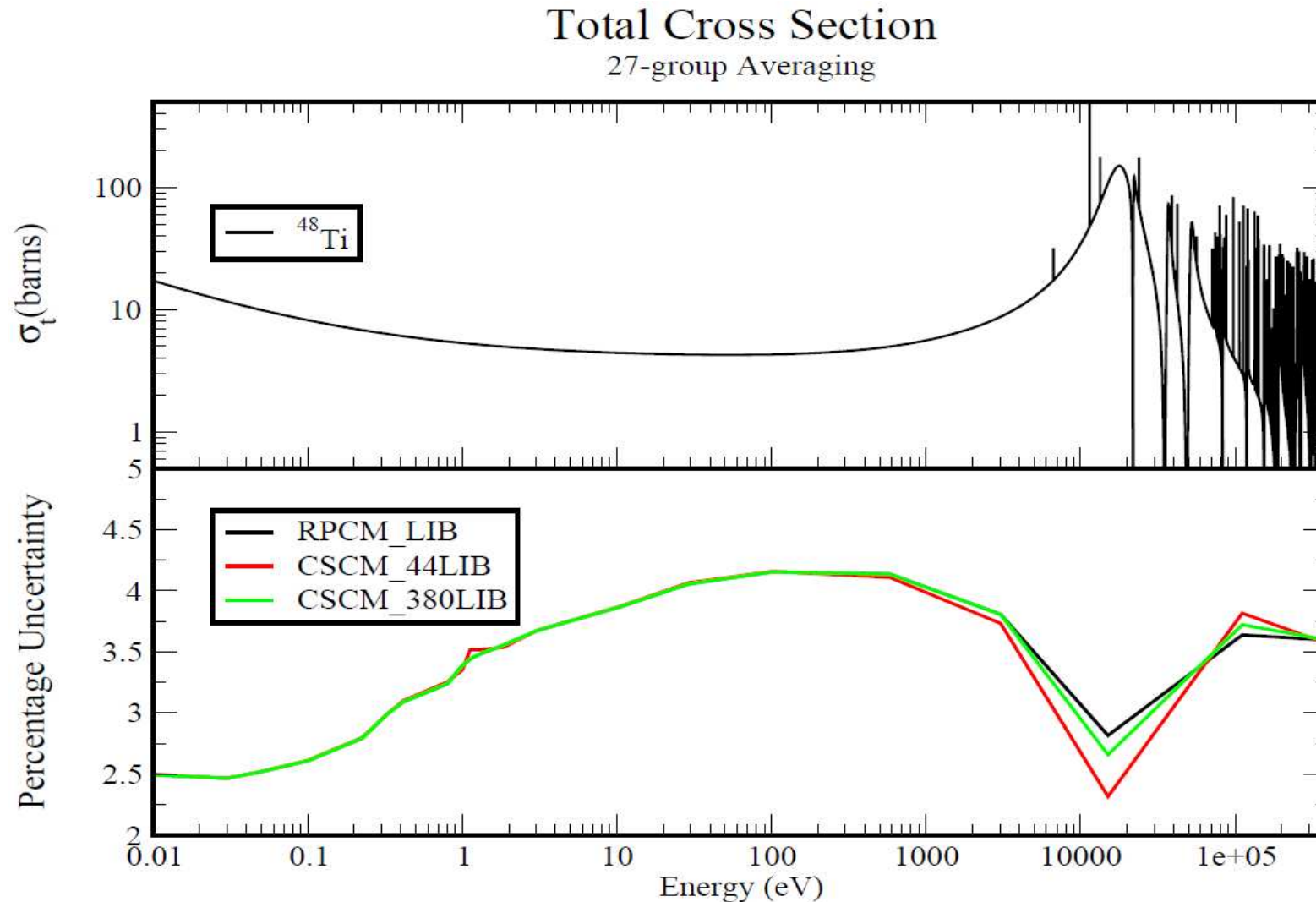
Covariance Libraries Computer Storage

Library	Size
RPCM_LIB	904 KB
CSCM_44LIB	95 KB
CSCM_380LIB	7.2 MB

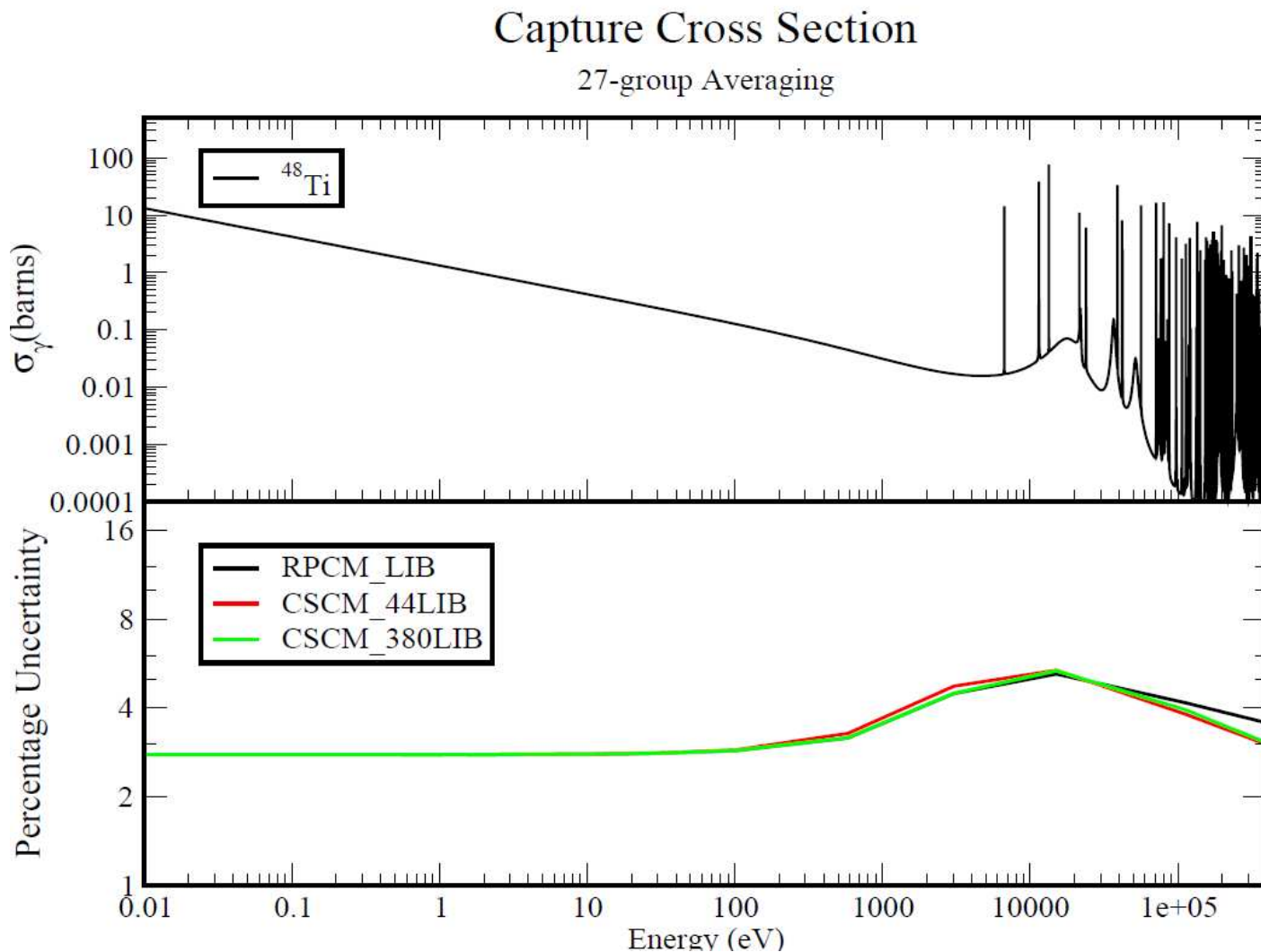
Test and Results

- 27-group and 238-group used for calculating averaged cross section and covariance
- Constant energy neutron flux
- Three Cross Section Libraries:

Test and Results: 27-group calculated covariance for the total cross section

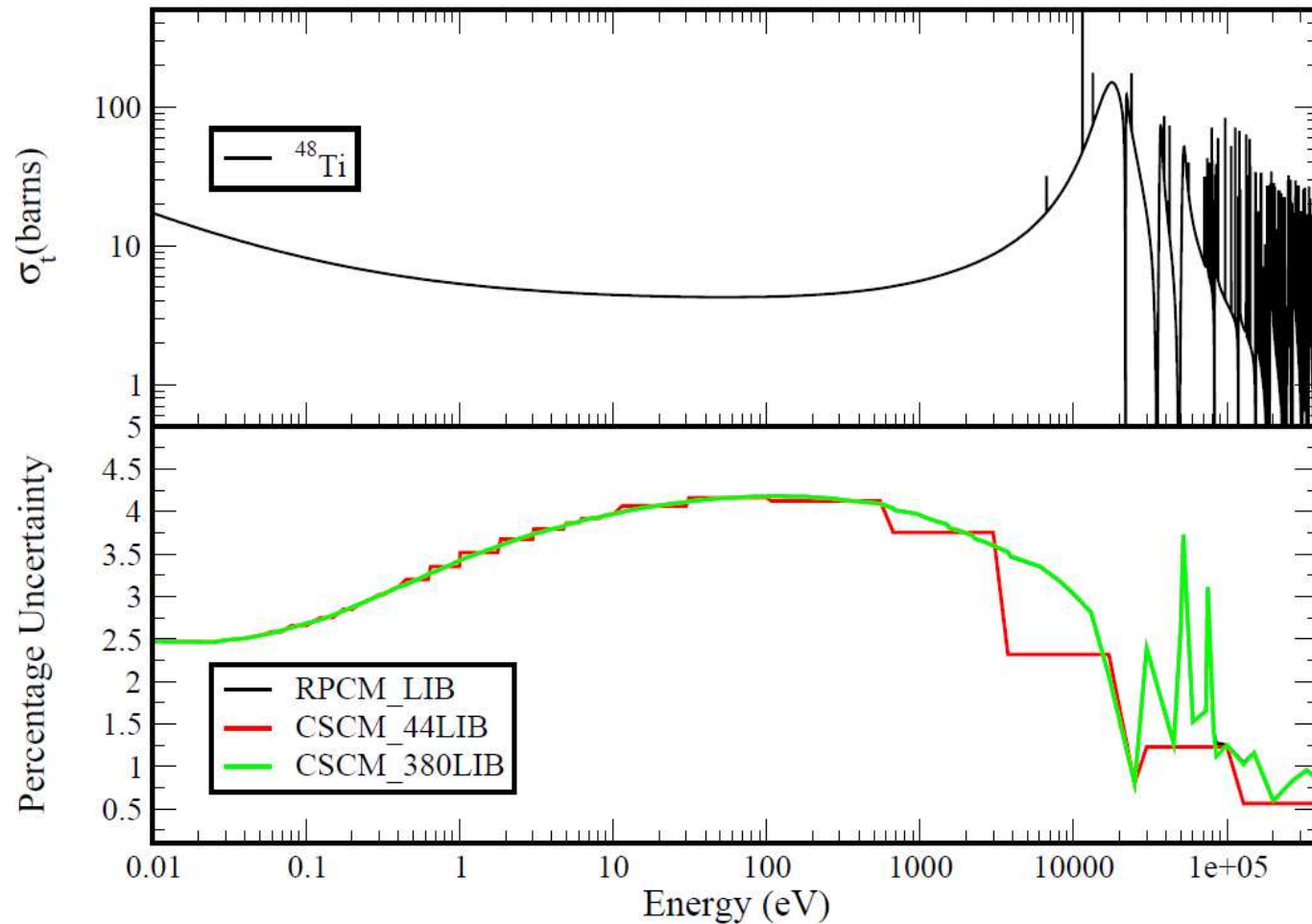


Test and Results: 27-group calculated covariance for the capture cross section



Test and Results: 238-group calculated covariance for the total cross section

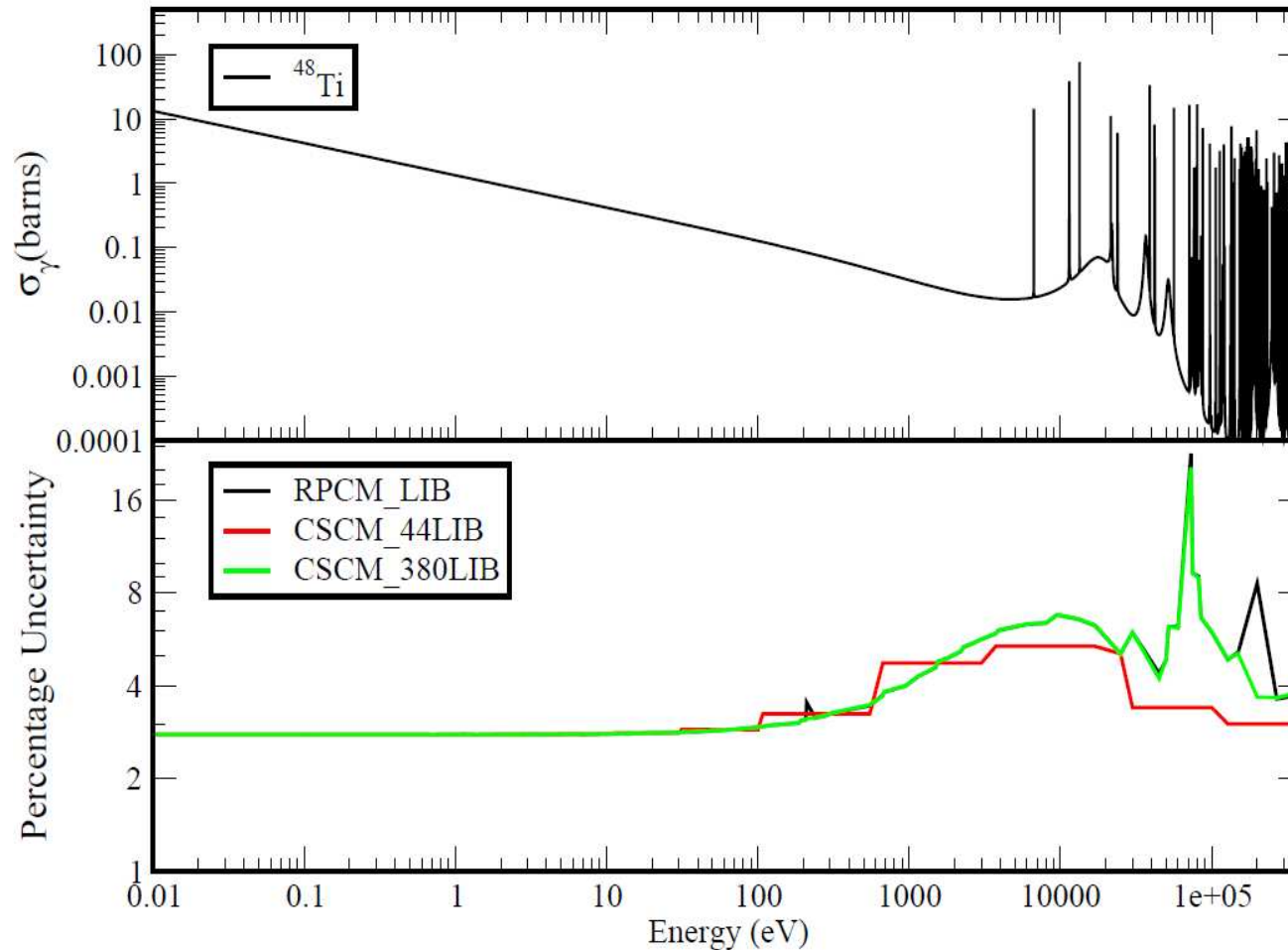
Total Cross Section
238-group Averaging



Test and Results: 238-group calculated covariance for the capture cross section

Capture Cross Section

238-group Averaging



Conclusions

- Care must be taken when using few-group covariance representations. It may be appropriate for the energy range where the data are smooth and the resonances are not present as for instance in the high energy region
- For a detailed covariance results the use of the RPCM is recommended
- Conversion of the RPCM to CSCM using a fine energy-group structure must be examined so as to assure that the computer allocation size is not overwhelming larger than that of the RPCM
- In the resonance region few-group representation is acceptable when a general overview of the impact of covariance results is sought

Food for Thought

- Impact of the weighting spectrum in the covariance conversion from RPCM to CSCM
- Impact of the cross section energy self-shielding
- Impact of the cross section on the temperature effect