WPEC Subgroup-22

« nuclear data for improved LEU-LWR reactivity prediction »

Progress report to CSEWG

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Purpose of the working group

- Investigate the underestimation of thermal LEU-LWR keff (~ -0.4%) observed with ENDFB/VI-8 – JEFF3.0 – JENDL3.3
- focused on **U235 – U238 – H2O – O16 nuclear data**
- Subgroup-22 set-up in 2001 and expected to end in 2004.
- **These slides : progress since WPEC San-Diego meeting (May-2003)**
- For an overview of the past work, see WPEC slides in http://www.nea.fr/html/science/docs/2003/nsc-wpec-doc2003-293.pdf

Reactivity calculations

- K_{eff} bias was investigated as a function of:
  - U238, U235 capture and U235 fission rate
  - Leakage (ATLF), slowing down density
  - Pitch size, moderation ratio, U5 enrichments

- The « simplest » parameter is the U238 capture fraction. When we arrive at a fit to K_{eff} versus C8 which has a mean of 1.0000 and zero slope, it will be hard to argue with.

U8 (n,γ) Integral information

Trends from **P**ost-**I**rradiation **E**xperiments (A. Courcelle et al.)

- adjustment based on regression methods (RDN new code)
- Isotopic ratios (U-Pu-Am-Cm) measured in UO2 and UO2-PuO2 PWR.
- K_eff in LEU and HEU systems,
- U238 rate ratios meas. not included !
- Results with JEF2.2 for main actinides.

Energy range	change %	Std. Dev after adj	Std. Dev before adj
U235	capture		
12.00 keV - 454.0 eV	-6.3	9.5	10.0
454.0 eV - 22.6 eV	+12.9	3.1	10.0
22.6 eV - 4.0 eV	+12.8	3.6	10.0
4.0 eV - 0.54 eV	+12.4	3.7	10.0
0.54 eV - 0.1 eV	-0.7	1.6	2.0
< 0.1 eV	-0.1	0.8	1.0
U235	fission		
22.6 eV - 4.0 eV	-1.6	2.2	3.0
4.0 eV - 0.54 eV	-1.2	2.1	3.0
0.54 eV - 0.1 eV	-0.1	0.8	1.0
< 0.1 eV	-0.2	0.3	0.4
U235	ν		
22.6 eV - 4.0 eV	0.1	0.7	0.7
4.0 eV - 0.54 eV	0.2	0.7	0.7
0.54 eV - 0.1 eV	0.1	0.5	0.7
< 0.1 eV	0.1	0.2	0.4
U236	capture		
12.005 keV - 454.0 eV	-0.2	10.0	10.0
454.0 eV - 22.6 eV	-1.8	6.0	10.0
22.6 eV - 4.0 eV	-0.3	3.6	5.0
U238	capture		
12.00 keV - 454.0 eV	-0.1	2.2	2.2
454.0 eV - 22.6 eV	-0.5	1.6	2.0
22.6 eV - 4.0 eV	-0.7	1.7	2.0
4.0 eV - 0.54 eV	0.0	1.0	1.0
U238	n,2n		
19.6 MeV - 6.07 MeV	+6.3	2.1	10.0

Table 1: Adjustment results in % for uranium nuclear data

Results for U8 shielded ($\sigma 0 \sim 50$b) capture cross-section (JEF2.2)

Small changes linked with a slight overestimation of Pu239 build-up in PIE

Analyses of Hellstrand correlations

- U238 effective (shielded) resonance integral measurements compiled by E. Hellstrand (*1966 San Diego conference*)

  ⇒ compilation of 4 measurements

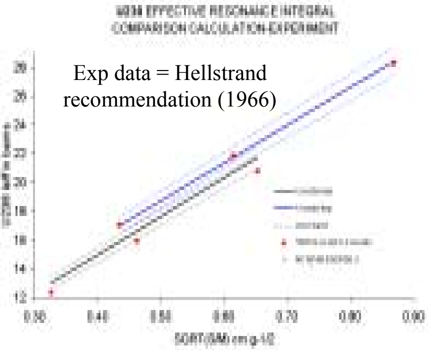
  ⇒ recommendations for U-metal and UO2 : I = a * sqrt(S/M) + b

- According to Hellstrand :

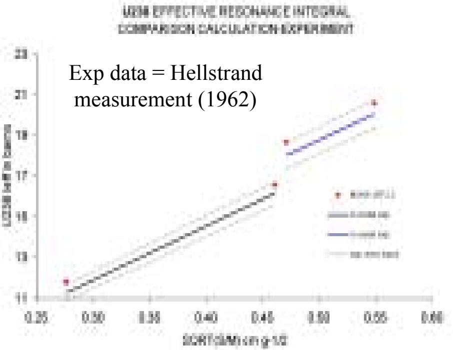
  « *limits of error below 3.5% could scarcely be obtained* »

- 2 different studies with MC codes :
  - Set-up of a simplified benchmark (*A. Courcelle et al. H. C. Huria et al.*) and comparison with Hellstrand recommendations (1966)
  - Detailed modelling of one particular experiment : Hellstrand et al. In 1962 (*David Hanlon and Christopher Dean*)

A. Courcelle H.C. Huria et al.



David Hanlon Christopher Dean



- Hellstrand et al. measurement (1962) different from Hellstrand recommendation (1966) based on 4 different experiments
- Calculations within the experimental error bands (±3.5%)
- Given the large experimental uncertainty, there is insufficient evidence to indicate a problem with U238 capture

Status of U8 (n,γ) Integral information

- **PIE study**: Overestimates Pu239 buildup in UO2 and UO2-PuO2 fuel
- **Spectral indices in reactors**: Previous studies suggested a decrease of shielded U8 (n,γ) by 1-1.5%
- **Hellstrand Measurements**: Calculations are within the experimental uncertainties.

Further analysis of benchmarks like TRX, BAPL, etc. could be useful but their experimental uncertainties may be too large for them to play an important role.

- Present resolved range U238(n,γ) agrees with integral experiments, but uncertainties allow for small changes.
- A ~0.7% reduction of shielded U8 (n,γ), consistent with differential measurements, would improve LEU keff and Pu239 prediction in PIE.

U238 thermal capture value

- Proposed capture σ_0 values in the range 2.68b – 2.74b
  - Poenitz measurements: 2.68 +/- 0.019 b
  - Mughabghab 2002 recommendation: 2.68 b
  - CSEWG Standards (ENDF-JEFF-JENDL): 2.708 b
  - Moxon survey of experimental data: ~2.74
- Measurements by G. Molnar et al. (unpublished)
- Evaluation by A. TrkoV et al supports 2.68
  - Based on the 5 most recent measurements
  - least-squares fitting in the log-domain to avoid PPP
  - Uncertainties and correlations between measurements are accounted for.

U238 resonance work at ORNL

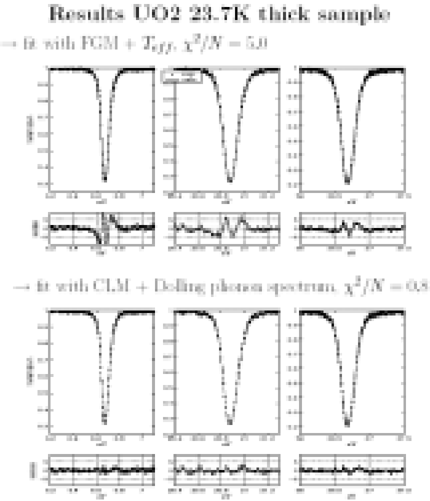
- U238 RRR evaluation (0 - 20 keV) by Derrien, Leal, et al.
- Includes ORELA 1988 transmission (J. Harvey et al.)
- Some data were lost: Part of de Saussure 1973 capture data; R. Macklin capture data.
- No reliable U238 capture measurements available
- Need for accurate capture meas. (priority thermal – 120 eV)
- U238 resonance parameters should ideally include integral trends (i.e recommended value of SRI). DOPUSH?
- See Luiz Leal presentation at this meeting
- Preliminary benchmark results: ~200-300 pcm increase in K_{eff}

Solid state effects on U238 resonance parameters

- Current evaluations use **F**ree **G**as **M**odel and effective **T**
- Recent study with DOPUSH **C**rystal-**L**attice **M**odel [Nabrejnev et al, *NSE 131, 222-229, 1999]*

  ⇒ Significant Biases on res. par. evaluation
- DOPUSH is now:
  - in REFIT (M. Moxon 1998)
  - in SAMMY (N. Larson 2001) :
- Test of SAMMY-DOPUSH using GELINA U238 transmission at low temperature in progress (A. Courcelle). Preliminary fit shows improvement.

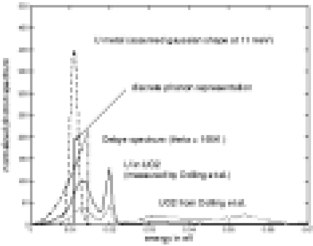
U238 SAMMY fit with FGM and CLM



First three U238 s-wave resonances transmission performed at GEEL in 1995

Complete analysis in progress with SAMMY + CLM (A. Courcelle)

The phonon distributions (total and weighted) measured with the phonon scattering method [*Dolling et al. Can. J. Phys. 43,8 (1965), Young et al. Nukleonik, 12 (1969)*]



U238 resonance parameter adjustments

- 2 ENDF-formatted files generated by C. Lubitz for sensitivity studies
- Decreased average Γγ of U238 s-waves in ENDF6.5 by 1.35% : 22.96 → 22.65 meV (called version 22-1). Based on the Froehner URR analysis.
- Decreased Γn of U238 s-waves by 0.738% (version 22-2)
- The two adjustments give the same capture resonance integral : 276.6 b and thermal capture value : 2.708 b (« CSEWG Standards »)

E eV	**Moxon et al. Γγ meV**	**Moxon et al. Γn meV**	***22-1 Γγ meV***	***22-1 Γn meV***	**22-2 Γγ meV**	**22-2 Γn meV**
6.674	**23.00**	**1.493**	*22.69*	*1.489*	23.00	1.482
20.87	**22.91**	**10.26**	*22.60*	*10.24*	22.91	10.18
36.68	**22.89**	**34.13**	*22.58*	*34.08*	22.89	33.88
66.03	**23.36**	**24.60**	*23.04*	*24.57*	23.36	24.42
80.75	**23.00**	**1.865**	*22.69*	*1.863*	23.00	1.851
102.5	**23.42**	**71.70**	*23.10*	*71.64*	23.42	71.17

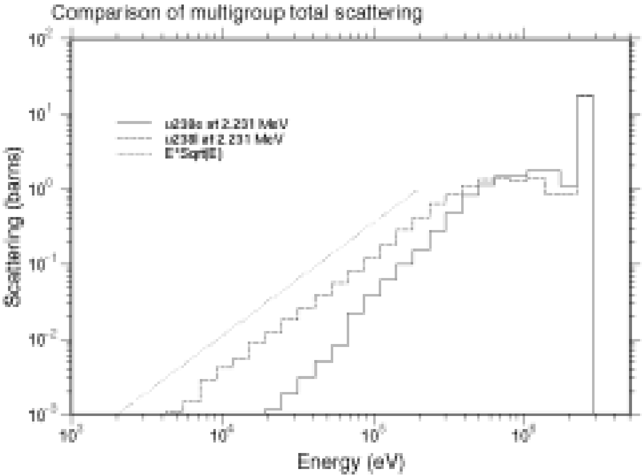
Exp + mod ratio	JEFF3.0 Keff (MC unc. pcm)	**22-1** Δ keff (pcm)	**22-2** Δ keff (pcm)
TCA-1.50	0.99575(20)	+142.8	+67.9
TCA-1.83	0.99592(15)	+110.2	+73.5
TCA-2.48	0.99659(15)	+105.1	+41.1
TCA-3.00	0.99669(15)	+92.5	+70.2

Quick integral tests on TCA exp.
(A. Courcelle MCNP4C-JEFF3.0)

U235-U238 LANL «above-URR» evaluation

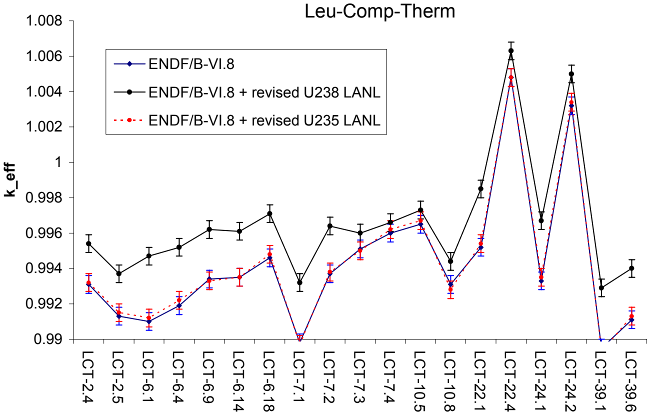
- Preliminary U8-U5 files from LANL (300 keV -30 MeV)
- Softer U238 (n,n’) secondary spectra than previous eval.
- Removes the keff biases on bare versus uranium reflected systems (MacFarlane, MCNP)
- Extensive tests against LEU and HEU benchmarks :
  - S. Van Der Marck, A. Hogenbirk, A. Courcelle (MCNP, JEFF3.0)
  - Bob MacFarlane (MCNP, ENDF\B-VI)
  - Skip Kahler (RCP, ENDF\B-VI)
- Effect of new Madland U235 fission spectrum needs to be separated from the cross section changes.

U235-U238 LANL «above-URR» evaluation



Tests of U238 – U235 LANL evaluations

(Skip Kahler Sept 2003)



U235-U238 LANL «above-URR» evaluation

- U235 LANL file has a small impact (except U5 fission spectrum) on LEU and HEU benchmarks
- U238 LANL file significantly increases keff for small size LEU benchmarks (reduction of leakage with a softer secondary inelastic spectrum)
- U238-U235 LANL evaluations do not entirely correct the LEU keff biases. ORNL resonances help greatly.
- Similar tests are in progress with CEA-BRC and Maslov U238 evaluations to check these trends

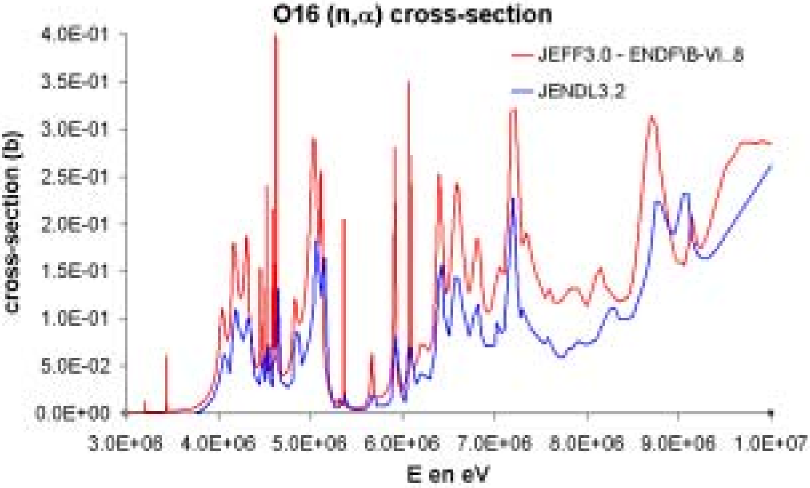
U235 thermal fission spectrum

- New U235 fission spectra (D. Madland 2003, WPEC/SG-18)
- According to WPEC/SG-18 work :
  - Inconsistencies in the meas. for U235 for thermal incident energy
  - Need for measurements
- Sensitive issue in HEU and high leakage benchmarks
- Temporary U235 thermal spectrum : $\bar{E}$ slightly larger than ENDF/B-VI value
- Several Tests against LEU and HEU benchmarks :
  - Van Der Marck, A. Hogenbirk, A. Courcelle (MCNP, JEFF3.0)
  - Bob Mc Farlane (MCNP, ENDF\B-VI), Skip Kahler (RCP, ENDF\B-VI)

Integral tests of new U235 fission spectrum
(Trkov – MacFarlane - Kahler)

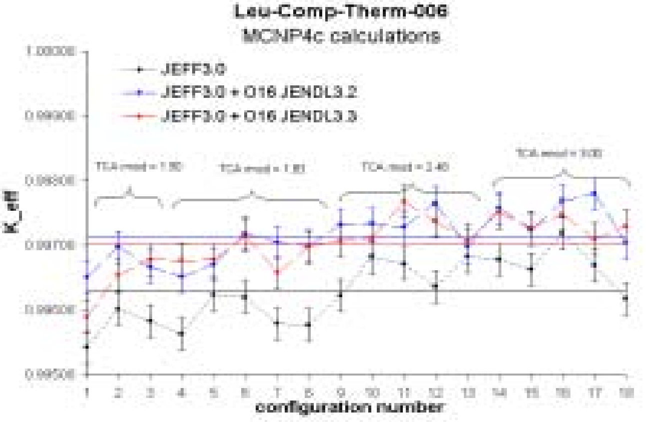
- Minimal impact on the reactivity of low-leakage systems
- Causes eigenvalue decreases of ~300 pcm for high-leakage Heu-Sol-Therm systems. Would require compensating changes in other cross sections to remove leakage trend.
- Decreases Leu-Comp-Therm keff by ~50-150 pcm. Would require additional compensation from other cross sections.
- These integral results do not tell whether the new U-235 thermal fission spectrum is better or not, but its adoption would require re-adjusting other cross sections, so there would have to be some advantage to using it.

O16 (n,α) evaluations



O16 (n,α) evaluations

- Large ≠ between evaluations; exp. database poor and discrepant
- Deduced by reciprocity from old C13(α,n) measurements
- **O16 (n, α) measurements** in the 3-6 MeV region needed
- Non-negligible effect on Leu-Comp-Therm keff ~ 80 pcm



Main Conclusions

Two main issues are being investigated with top priority :

- U238 (n,γ) in the thermal and resolved range
- U238 inelastic data

- So far, no significant bias on present U238 (n,γ) (Moxon et al.) is demonstrated.
- However, a slight reduction by ~0.7% of shielded U8 (n,γ) is compatible with integral experiments and would reduce the size of the eigenvalue discrepancy
- New LANL nn' data and ORNL parameters (with «lower» 2200m/s capture) significantly improve the eigenvalues.
- A combination of lower O16(n,α) and crystal-lattice broadening could probably bridge any remaining gap.

Future work

- U238 spectral index benchmarks (TRX, BAPL…)
- Trend analyses (keff bias as a function of parameters) with new files (U238, O16, DOPUSH)
- Testing of the CEA-BRC and «Maslov» U238 evaluations and comparisons between these, LANL, JENDL, and CENDL.
- Testing of the ORNL resonance parameters
- Influence of continuum (n,n’) representation on reactor calc.