Summary report of the WPEC sub-group-22 [May 2001 – May 2004]

« nuclear data for improved LEU-LWR reactivity prediction »

May 2004 Draft version

Coordinator : Arnaud COURCELLE (CEA)
Monitor : Richard Mc KNIGHT (ANL)

Contributors

Yung-An CHAO (Westinghouse)
Christopher DEAN (Serco Assurance)
Emmeric DUPONT (CEA-CAD)
Harish C. HURIA (Westinghouse)
Albert C. KAHLER (BAPL),
Cecil R. LUBITZ (KAPL),
Robert Mac Farlane (LANL)
Keisuke Okumura (JAERI)
Alain SANTAMARINA (CEA)
Andrej TRKOV (AIEA)
Steven VAN DER MARCK (NRG Petten)
and others…

Arnaud COURCELLE (CEA-CAD),
Hervé DERRIEN (ORNL),
Alfred HOGENBIRK (NRG Petten),
M. J. Lopez Jimenez (CEA-BRC)
Luiz C. LEAL (ORNL)
Michael C. MOXON
Benjamin MORILLON (CEA-BRC)
Pascal Romain (CEA-BRC)
Jean-Christophe SUBLET (CEA-CAD)
James P. WEINMAN (KAPL)

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 : Summary of the work done**

- For an overview of the past work,

→ see WPEC slides in http://www.nea.fr/wpec

Outline

- Short status of available uranium evaluations
- U238 integral trends (thermal and resonance range)
- Evaluation work
  - U238 thermal capture value
  - Resonance range
  - Inelastic scattering data
- New U238 complete files
- Status of U238 integral testing

BRIEF STATUS OF AVAILABLE URANIUM EVALUATIONS

U evaluations available in most recent libraries : ENDF\B-VI.8 - JENDL3.3 - JEFF3.0

data	description
U238 resolved range	same evaluation for ENDF\B-VI.8 - JENDL3.3 - JEFF3.0 : **Moxon et al. [0 – 10 keV]**
U235 resolved range	same evaluation for ENDF\B-VI.8 - JENDL3.3 - JEFF3.0 : **Leal, Derrien, Larson, Wright [0 – 2.25 keV]**
U238 unresolved range	ENDF\B-VI.8 – **Frohner [10 – 150 keV]** JEFF3.0 : **Frohner [10 – 300 keV]** JENDL3.3 : **JENDL eval. [10 – 150 keV]**
U238 and U235 « high energy »	JEFF3.0 = JENDL3.2 evaluation (Kawano et al.) JEF2.2 = ENDF\BVI-8 (N.B old evaluation) JENDL3.3 (Kawano et al.)

New preliminary U evaluation (available in ueval@nea.fr)

data	name	description
U238 thermal capture value		Evaluation (A. Trkov et al.)
U238 resolved range	**KAPL-22-1** **KAPL-22-2** **ORNL**	Adjustment of res par. (C. Lubitz) for sensitivity studies Adjustment of res par. (C. Lubitz) for sensitivity studies Preliminary Evaluation (H. Derrien, L. Leal) **[0 – 20 keV]**
U238 « high energy »	**LANL** **BRC** **Maslov** **KAPL-22-3**	Preliminary Evaluation (P. Young et al.) Preliminary Evaluation (M.J. Lopez Jimenez et al.) Evaluation by Maslov et al. Representation of (n,n') continuum for sensitivity studies
U235 unresolved range	**ORNL**	Evaluation by Leal et al.
U235 « high energy »	**LANL**	Preliminary Evaluation (P. Young et al.)
U235 prompt fission spectrum	**LANL**	Evaluation by D. Madland (WPEC/SG-9)

INTEGRAL TRENDS

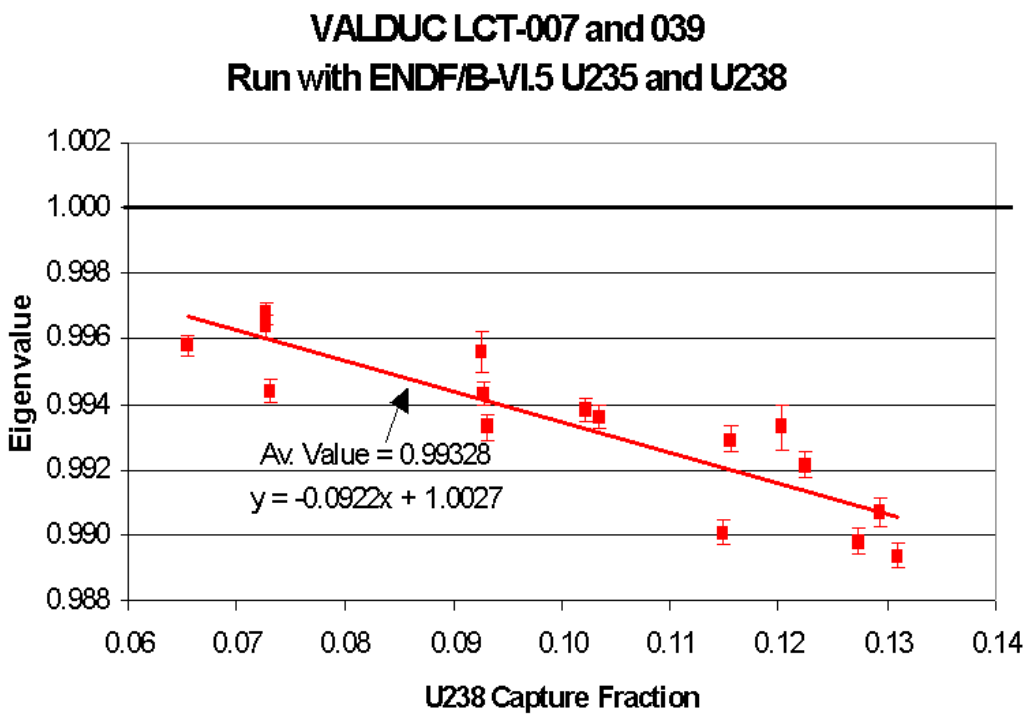
- Keff versus U238 capture fraction
- U238 Hellstrand correlations
- U238 spectral index
- Production of Pu239 in Post-Irradiation Experiments

Trends on LCT Keff

- Keff versus U238 capture fraction (Weinman, Kahler CSEWG 2003)
- Other parameters investigated : Epithermal fission fraction (ATTF) (Kahler CSEWG 2003), U5 capture and fission, (D.Hanlon – C. Dean JEFF Meeting 2003)

Ex :

Jim Weinman
CSEWG 2002



Analyses of Hellstrand correlations

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

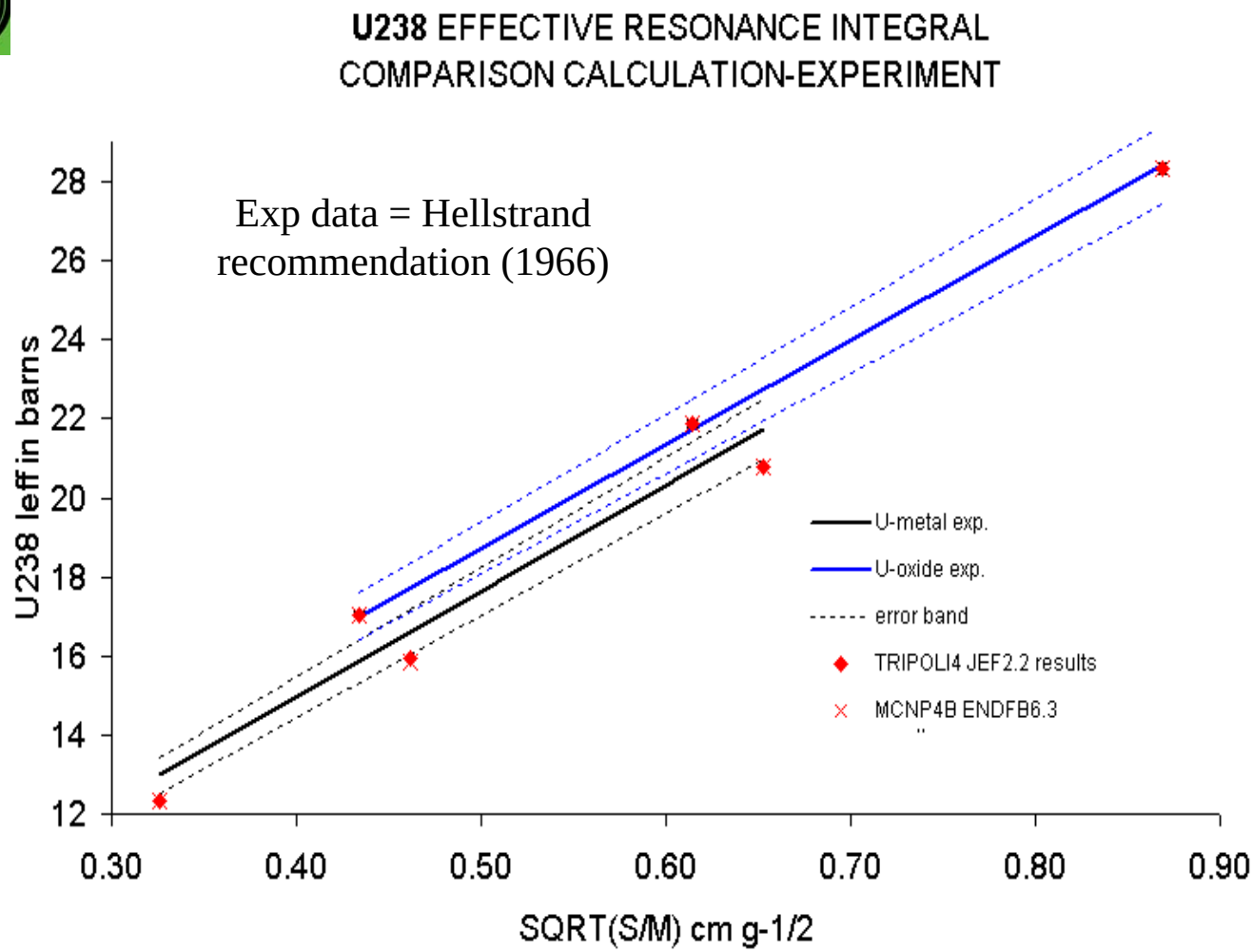
  $\Rightarrow$ compilation of 4 measurements

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

- According to Hellstrand :

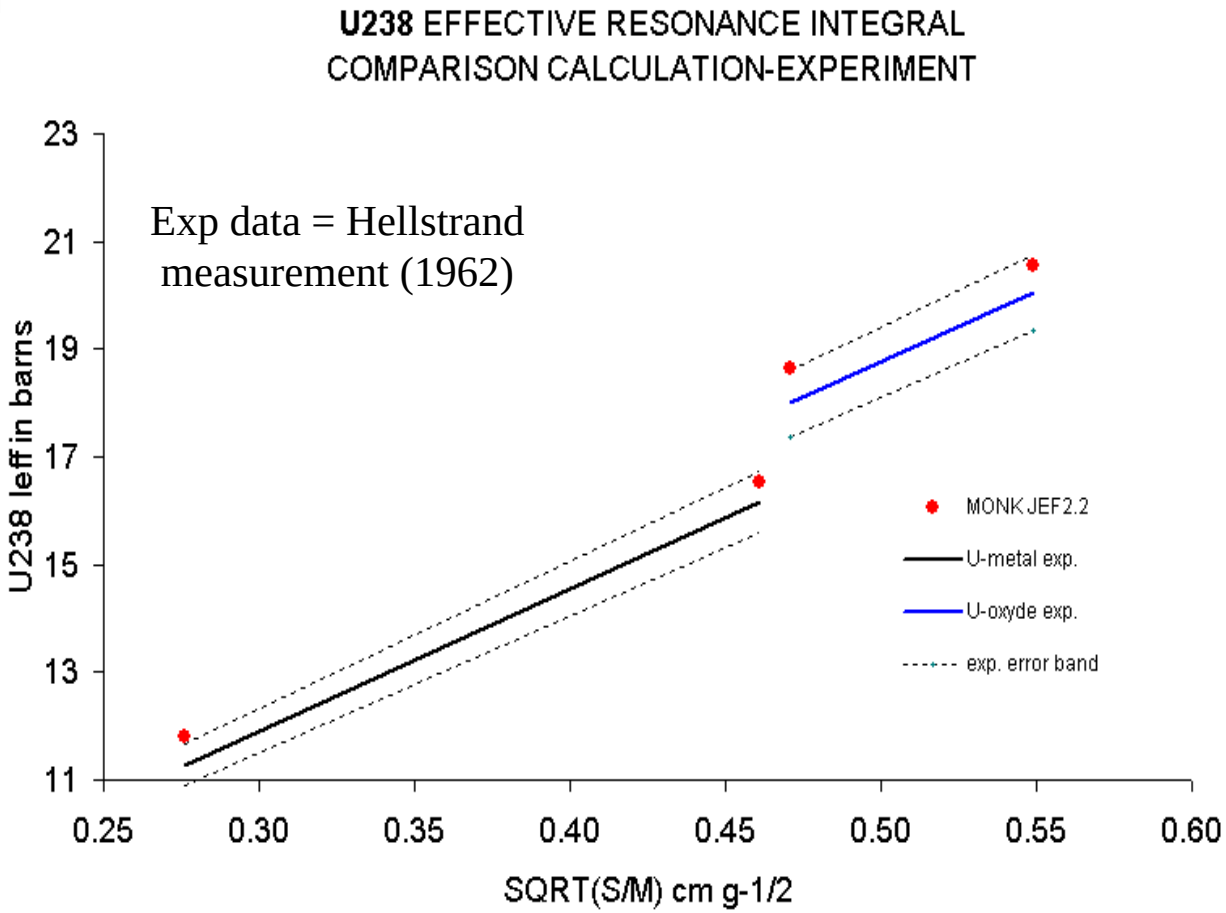
  « *limits of error below 3.5% could scarcely be obtained* »

- 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.

- Calculations within the experimental error bands (±3.5%)



David Hanlon
Christopher Dean

- Calculations within the experimental error bands
- Slight trends to U238 Ieff overestimation

U238 (n,γ) Spectral indices in Leu experiments

- EOLE (Physor 2002 – JEF2.2)

exp.	Meas.	C/E
– Mistral 1	C8/F	+2.2% ± 2.0%
– Mistral 2	C8/F	+2.3% ± 2.0%
– Erasme-S	C*=C8/F5	+1.6% ± 2.3%
– Erasme-R	C*=C8/F5	-0.2% ± 2.2%

- Calculations within the experimental error bands
- Slight trends to U238 capture overestimation

- IPEN/MB01 (Physor 2002 –ENDFB6.5)

ρ28	+2.3% ± 0.9%
C*=C8/F5	+2.4% ± 1.2%
C8/F	+0.9% ± 1.1%
(C8/F)epi	-2.7% ± 1.0%

U8 (n,γ) Integral information (thermal and resonance range)

Trends from **P**ost-**I**rradiation **E**xperiments (A. Courcelle et al. PHYSOR-2004)

- « adjustment » based on non linear regression method (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 in this work
- Results with JEF2.2 for main actinides in a 15 broad group structure.
- results for U8 shielded (dilution σ0 ~ 50b) capture cross-section (JEF2.2)

Small changes due to a slight overestimation of Pu239 build-up in PIE

Energy range	Modif In %	Incert. Post %	Incert. Prior %
U238	capture		
12.03 keV - 454 eV	-0.1	2.2	2.2
454 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**

Conclusions from U8 (n,γ) Integral information (thermal and resonance range)

- **Keff versus C8 fraction :** suggest a slight decrease of effective U8 (n,γ)
- **PIE study** :
  - C/E within the error bar of the measurements
  - Slight trend to overestimation (1-3%) of Pu239 build-up in UO2 and UO2-PuO2 fuel suggesting a reduction by 0.7% of shielded U8 (n,γ)
- **Reaction rate ratios** (spectral indices) measured in reactor :
  - Calculations within experimental uncertainties
  - Studies consistent with a small decrease of shielded U8 (n,γ) by 1-1.5%
- **Hellstrand correlations :** calculations are within experimental uncertainties

- So far, present resolved range U238 (n,γ) from Moxon et al. agrees well with integral experiments. C/E values are generally within exp. uncertainty margins.
- A slight reduction by ~0.7% of shielded U8 (n,γ) consistent with integral meas. would improve LEU keff and Pu239 prediction in PIE.

EVALUATION WORK

- U238 thermal capture value
- U238 Resonance parameters
- U238 inelastic scattering data

U238 thermal capture value

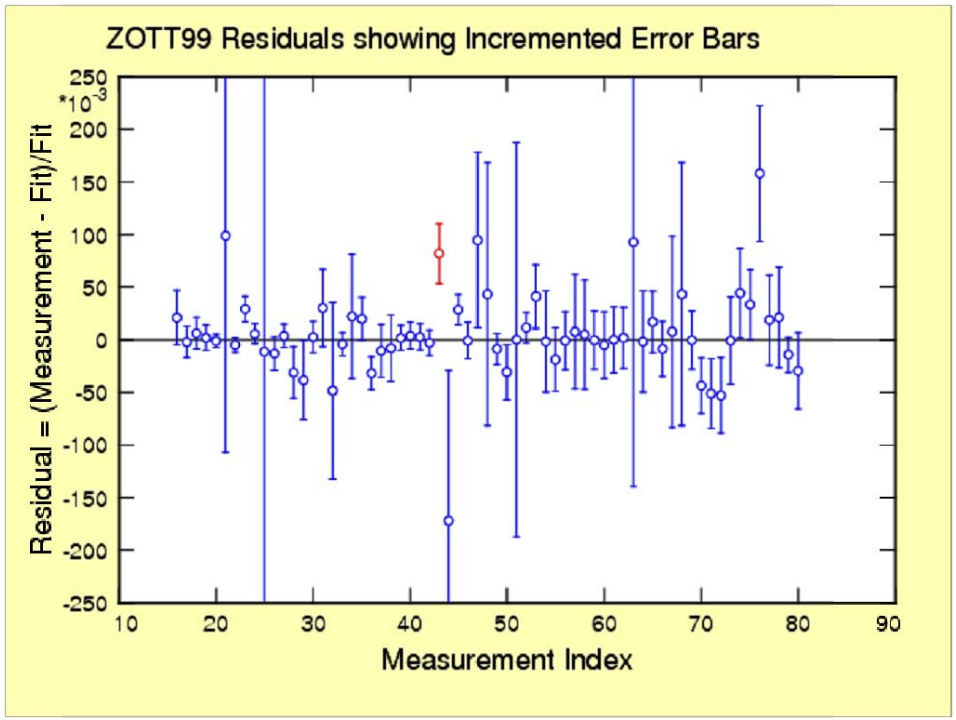
- Proposed capture σ_0 values in the range [2.68 b – 2.72 b]
  - Poenitz measurements : 2.68 +/- 0.019 b
  - Mughabghab 2002 recommendation : 2.68 b
  - CSEWG « standards » 2.701 b
  - **ENDF-JEFF-JENDL value : 2.719 b**
  - ORNL preliminary positive and negative resonance parameters : 2.679 b

U238 thermal capture value

- New Evaluation work by A. Trkov et al.
  - Work submitted to *Nucl. Sci. And Eng*.
  - Review of U238 thermal capture cross-section measurements
  - Review of γ-ray emission probability (beta decay of Np239) (important for activation measurements)
  - Analysis of new measurement by Molnar et al. (Budapest) published recently
  - Simultaneous fit of measurements of U238 thermal cross-section and Np239 gamma-line production
  - least-squares fit with ZOTT99 in the log-domain to avoid PPP
  - Uncertainties and correlations between measurements are accounted for.

U238 thermal capture value

Simultaneous fit of measurements of U238 thermal cross-section and Np239 gamma-line production (A. Trkov et al. submitted to Nucl. Sci. And Eng.)



Final value : $\sigma_0 = 2.683 \pm 0.012$ b

Previous work on U238 RRR
U238 resonance parameters of Moxon et al.

- NEANDC task force on U238 coordinated by Moxon et al.
- Led in 1990 to an improved evaluation up to 10 keV
  - REFIT fits of selected capture and transmission measurements
  - New high resolution measurements performed (Capture of Macklin (1988) et al. Transmission from Harvey et al. (1988))
  - Improved modeling function
- Summary in the NEANDC report and WPEC/SG4 final report
- Adopted in ENDF/B-VI.8 - JEFF3.0 – JENDL3.3
- Expected to solved the longstanding overestimation of the U238 (n,γ) (see U238 Brookhaven seminar in 1975)

U238 resonance parameters adjustments

- 2 ENDF-formatted files generated by C. Lubitz for sensitivity studies
- Decrease average $\Gamma\gamma$ of U238 s-waves by 1.35% : 22.96 $\rightarrow$ 22.65 meV (called 22-1) : Based on the Frohner URR analysis
- Decrease Γn of U238 s-waves by 0.738% (version 22-2)
- The two adjustments give the same non-shielded capture resonance integral : 276.6 b and thermal capture value : 2.708 b (« CSEWG Standards »), scattering radius unchanged

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**	**ORNL prelim. Γγ meV**	**ORNL Prelim. Γn meV**
radius	**R' = 9.428 fm**						**R' = 9.450 fm**	
6.674	**23.00**	**1.493**	*22.69*	***1.489***	23.00	**1.482**	23.00	**1.475**
20.87	**22.91**	**10.26**	*22.60*	***10.24***	22.91	**10.18**	22.91	**10.02**
36.68	**22.89**	**34.13**	*22.58*	***34.08***	22.89	**33.88**	22.89	**33.55**
66.03	**23.36**	**24.60**	*23.04*	*24.57*	23.36	24.42	23.36	23.97
80.75	**23.00**	**1.865**	*22.69*	*1.863*	23.00	1.851	23.00	1.865
102.5	**23.42**	**71.70**	*23.10*	*71.64*	23.42	71.17	23.42	70.87

U238 resonance work at ORNL

- U238 evaluation from thermal **to 20 keV** in progress at ORNL (Derrien, Leal et al. PHYSOR-2004).
  - Present evaluation is preliminary (932 s and 2354 p resonances)
  - Includes for the first time the ORELA 1988 high resolution transmission experiments (J. Harvey et al. 1988)
  - Resolved range extended to 20 keV
  - Part of De-Saussure 1973 and R. Macklin 1988 capture data were not available for this evaluation
  - FGM + adjusted T is used for this preliminary evaluation
- Need for accurate U238 capture meas. (ideally thermal – 1 keV, priority : thermal – 120 eV)

Solid state effect and U238 resonance parameters

- Current evaluation with **F**ree **G**as **M**odel and **adjusted T**
- Study with DOPUSH code [*Nabrejnev et al, NSE 131, 222-229, 1999*] $\Rightarrow$ Significant Biases on res. par. Evaluation in some cases

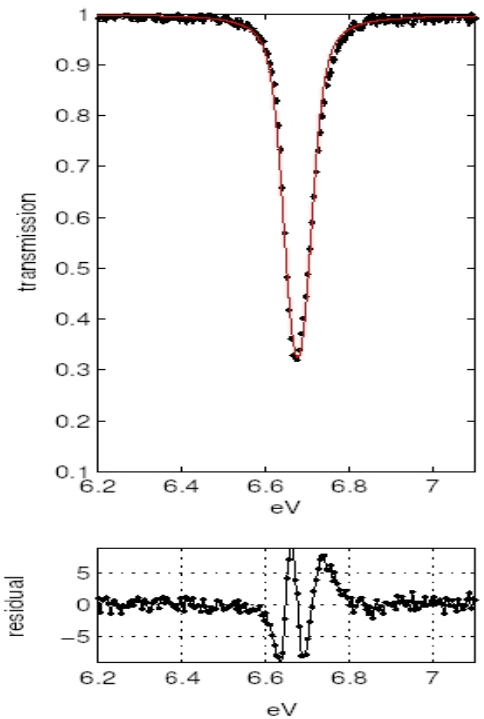
- DOPUSH is now available in :
  - REFIT (M. Moxon 1998)
  - SAMMY (N. Larson 2001) :

- Test of SAMMY-DOPUSH using GELINA U238 transmission at low temperature (A. Courcelle)
- Final version of ORNL R.R fit will include CLM for the low energy resonances.

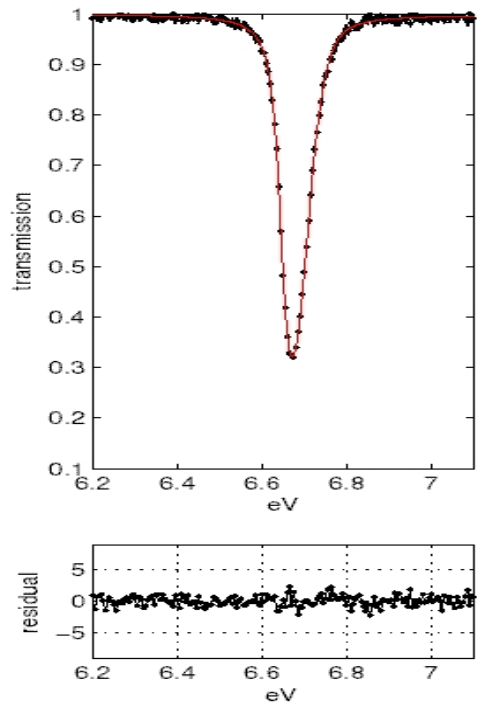
U238 fit with the Free Gas Model (FGM) and Crystal Lattice Model (CLM) of SAMMY

→ test of SAMMY-CLM on U238 transmission (GEEL) at low and room temperature (Meister 1997)

Ex :
UO2
thick sample
23.7K



FGM + adjT



CLM with Dolling et al.
Phonon spectrum

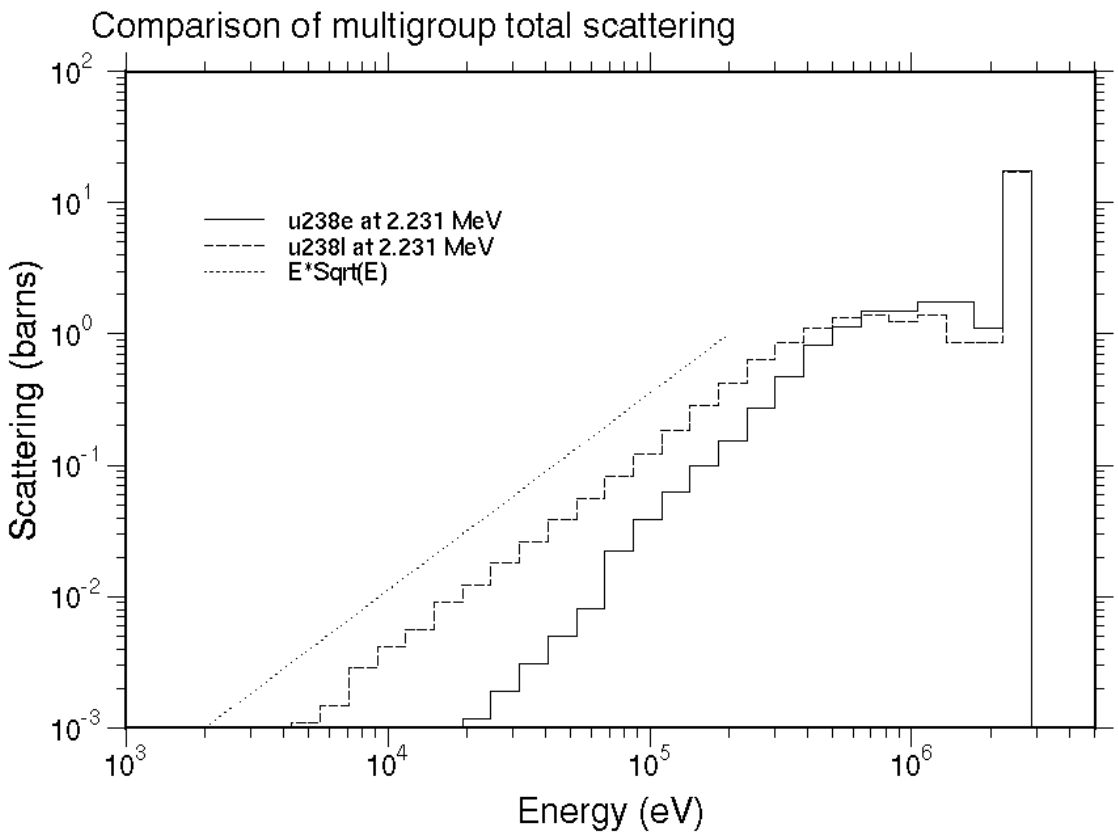
U235-U238 inelastic scattering data evaluations

- 1989 : WPEC/Subgroup-4 «U238 capture and inelastic cross-section »
  - New measurements of inelastic data
  - Improved evaluation (Kawano et al., Maslov et al.)

- New preliminary U238 – U235 files from **LANL** (P. Young et al. may 2003)
- New preliminary U238 **CEA-BRC** (M.J Lopez- Jimenez et al. oct 2003)
- Optical model + coupled channel calculations [150 keV – 30 MeV]
- Improved modeling of inelastic data compared to older ENDF/B-VI.8 and JEF2.2 evaluations

U235-U238 inelastic scattering data evaluations

Softer LANL U238 (n,n') secondary spectra than in JEF2.2 and ENDF\B-VI.



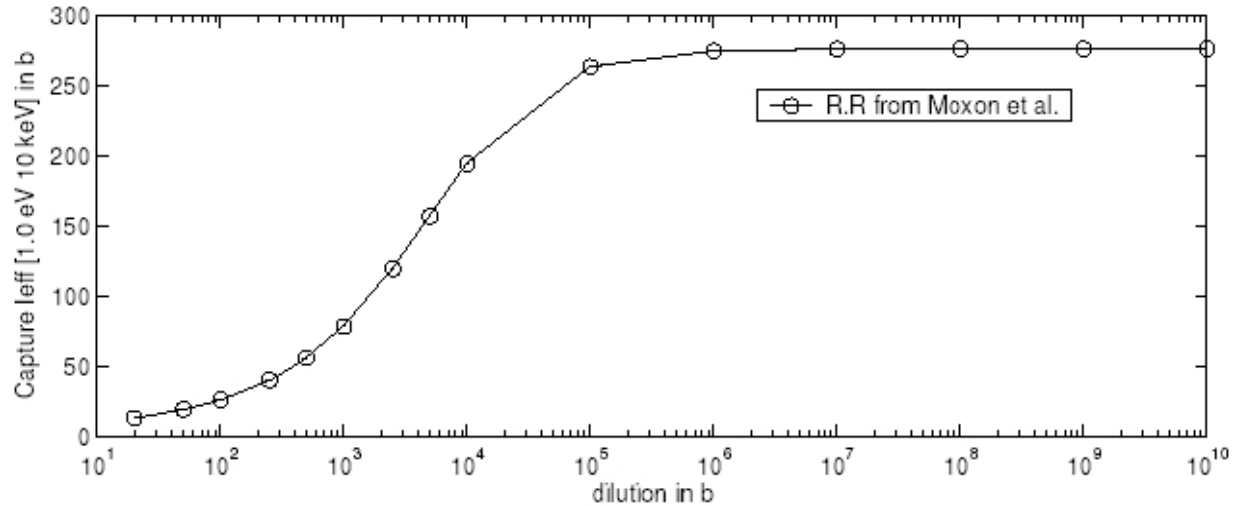
U235 thermal fission spectrum

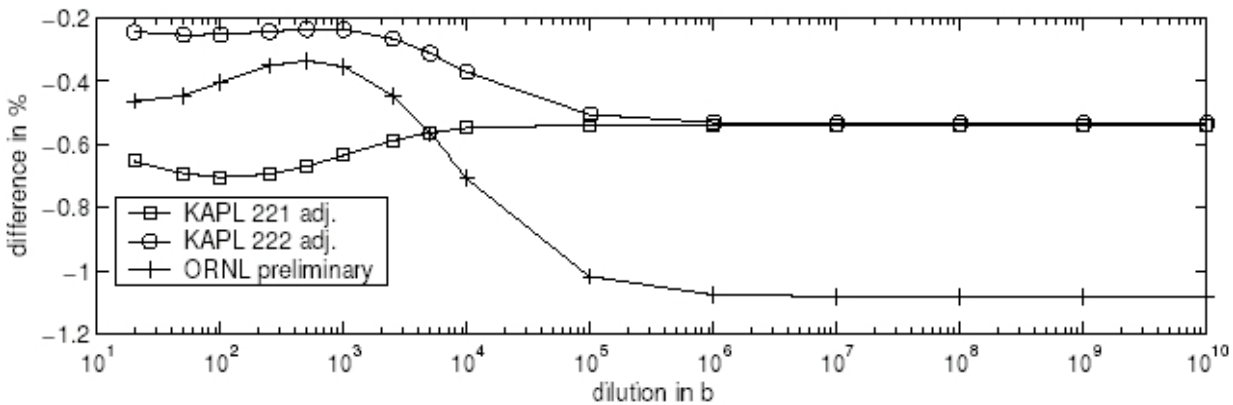
- New U235 fission spectra (D. Madland 2003, WPEC/SG-18)
- Modified Los-Alamos Model based on simplified modeling of fission fragment decay.
- According to WPEC/SG-18 work :
  - Inconsistencies in 2 recent measurements for U235 for thermal incident energy
  - Needs for measurements !
- Sensitive issue in HEU and high leakage benchmarks
- Temporary U235 thermal spectrum : $\bar{E}$ slightly larger than ENDF/B-VI value

SUMMARY OF INTEGRAL TESTING (may 2004)

Integral tests of U238 resonance range Effective resonance integral

$$I_{eff} = \int_{E_{min}}^{E_{max}} \sigma(E)\varphi(E)\frac{dE}{E} = \int_{u_{min}}^{u_{max}} \sigma(u)\varphi(u)du$$





LWR dilution range : [20 – 50b]

Integral tests of U238 resonance range

(R. Mac Farlane - Skip Kahler – A. Hogenbirk –
S. Van Der Marck – A. Courcelle)

Integral tests of U235-U238 LANL and BRC inelastic data

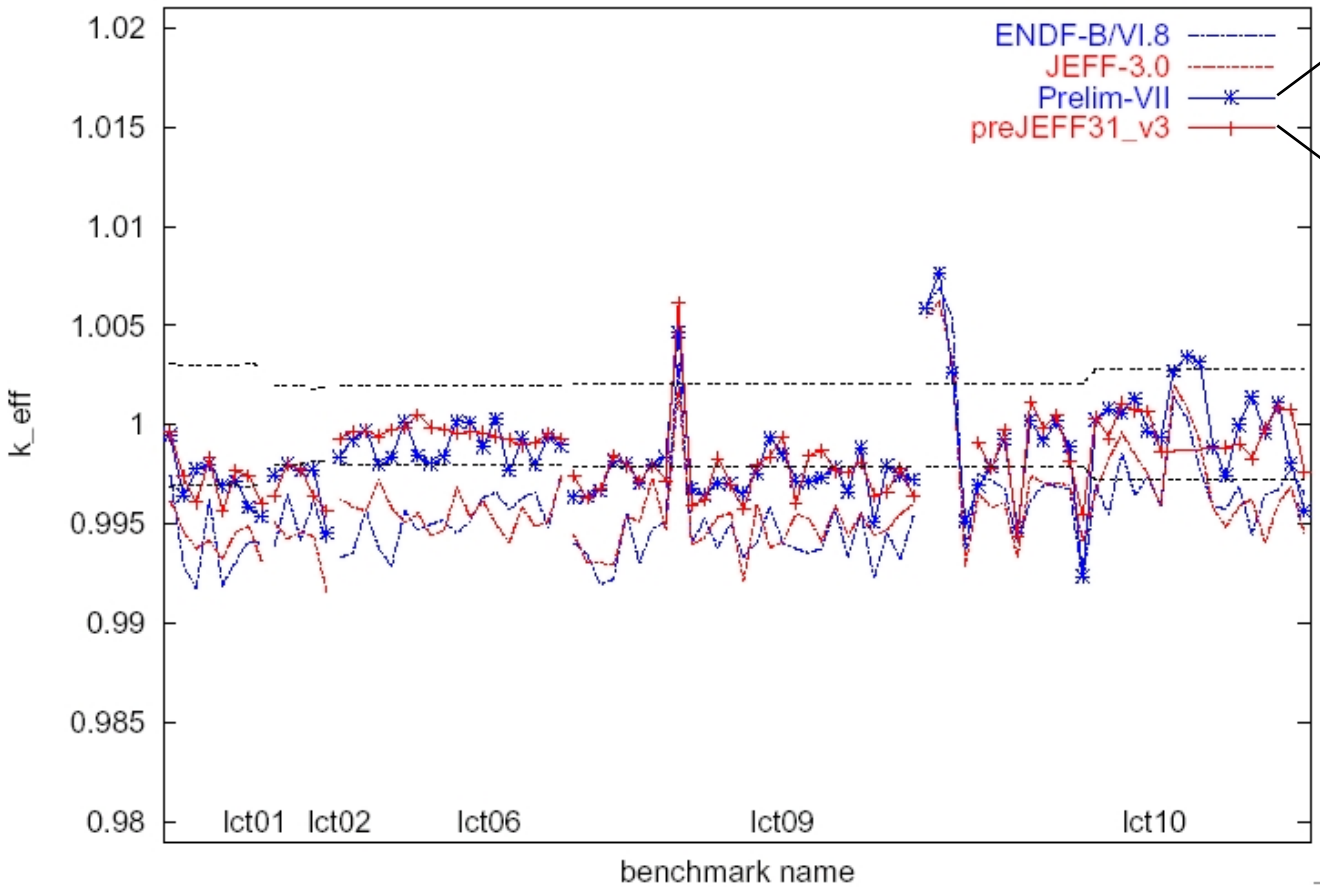
(R. Mac Farlane - Skip Kahler – A. Hogenbirk – S. Van Der Marck – A. Courcelle)

- U235 LANL file has a small impact (except U5 fission spectrum) on LEU and HEU benchmarks
- U238 LANL file improves keff prediction for small size Leu-Comp-Therm benchmarks (+200 - 300 pcm : reduction of leakage with a softer secondary inelastic spectrum)
- U238 BRC produces similar keff improvement as LANL for Leu-Comp-Therm benchmarks

Two preliminary U238 complete files

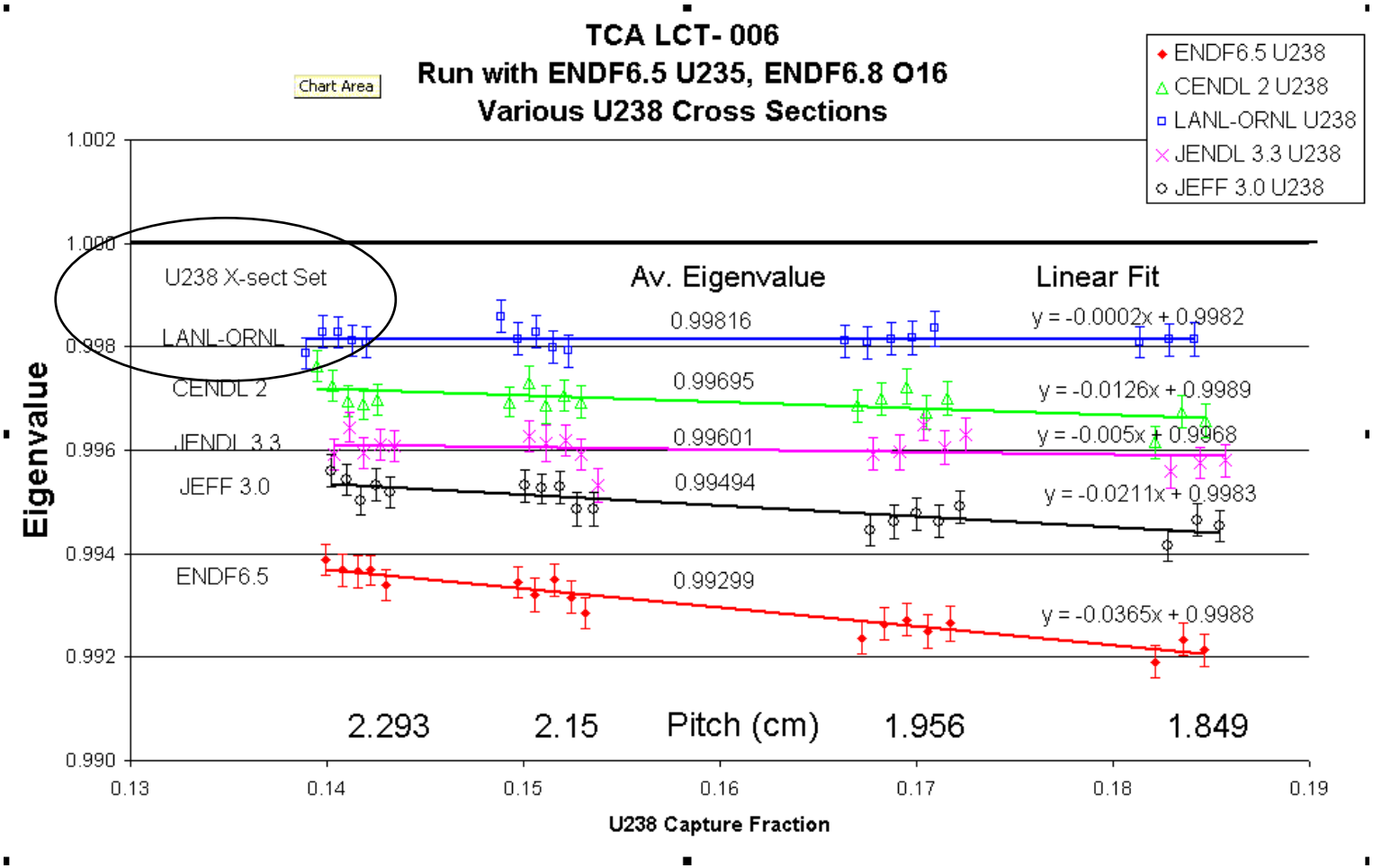
- ORNL Preliminary Resolved range + Unresolved range of Frohner + LANL fast range
- ORNL Preliminary Resolved range + Unresolved range of Frohner + BRC fast range

Integral testing of new U238 files



S.C. Van Der Marck et al. (MCNP4C) JEFF-Meeting May - 2004

Integral testing of U238 files



Jim Weinman (KAPL) : correction of the slope : keff versus C8

Integral testing of U238 files Substitution analysis (J. Weinman)

New inelastic SED LANL

New RRR ORNL

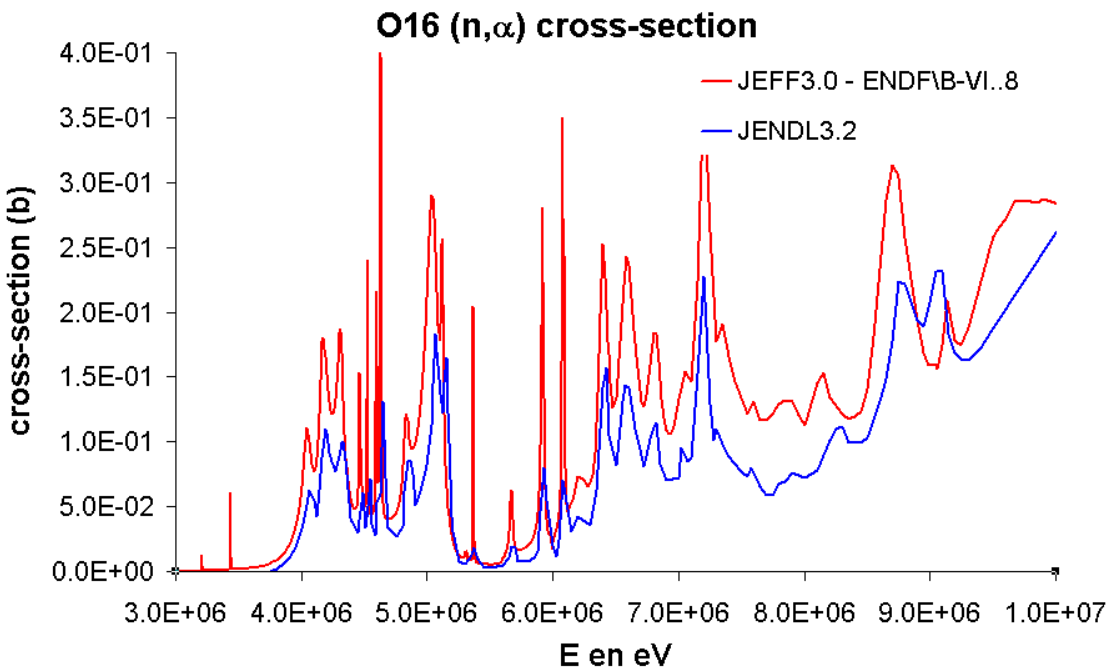
International Handbook of Evaluated Criticality Benchmark Experiments						
LEU-COMP-THERM-006 CASE 1						
TCA - Tank Type Critial Assembly - JAERI						
Run with ENDF6.5 U235 and ENDF6.8 O16						
Results of U238 Cross Section Substitution Calculations						
LANL-ORNL U238 into ENDF6.5 U238						
Case Description	Eigenvalue	95% CI	Change in Eigenvalue relative to Base Case	95% CI	Change in Eigenvalue for Reaction Type	95% CI
Base Case ENDF6.5 U238	0.99191	0.00032				
ENDF6.5 with LANL-ORNL inelastic transfer matrix	0.99465	0.00031	274	0.00045	274	0.00045
Previous substitution plus inelastic cross sections	0.99413	0.00030	222	0.00044	-52	0.00043
Previous substitution plus elastic cross sections	0.99329	0.00033	138	0.00046	-85	0.00045
Previous substitution plus elastic moments	0.99376	0.00029	185	0.00043	47	0.00044
Previous substitution plus disappearance cross sections	0.99701	0.00032	510	0.00045	325	0.00043
Previous substitution plus fission cross sections	0.99762	0.00031	571	0.00045	62	0.00045
Run with LANL-ORNL U238	0.99809	0.00030	618	0.00044		
			in pcm		in pcm	

Integral test of new U235 fission spectrum
(A. Trkov – R. Mac Farlane - Skip 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.

O16 (n,α) evaluations

- Large ≠ between evaluations : exp. database poor and discrepant : O16 (n, α) deduced by reciprocity from old C13(α,n) measurements
- **O16 (n, α) measurements** in the 3-6 MeV needed
- Small effect (but non-negligible) on Leu-Comp-Therm k_{eff} : ~ 80 pcm



FIRST CONCLUSIONS

First Conclusions

1. ~400 pcm underestimation of keff of LCT is confirmed with ENDFB/VI.8, JEFF3.0 and JENDL3.2 and is not likely the consequence of numerical approximations in reactor calculation methods (use of CEMC)

2. Given the large number of independent LEU exp. investigated (mostly from ICSBEP), the present bias is not believed to come from exp. errors in criticality measurements

3. The problem has been studied on small size configurations (high neutron leakage rate) and so far, is not demonstrated (with CEMC) for large commercial PWR

First Conclusions

4. So far, no significant bias on present U238 (n,γ) (Moxon et al.) is demonstrated with integral experiments (Pu239 production, spectral indices, Hellstrand correlations). C/E value are in the uncertainty margin of integral experiments. However, a slight reduction by ~0.7% of shielded U8 (n,γ) is consistent with U238 integral measurements and would correct the LEU keff discrepancy and overestimation of Pu239 build-up in PWR.
5. A new evaluation of thermal (2200 m/s) U238 capture cross-section is proposed : 2.683 ± 0.012 b
6. Preliminary ORNL R.R featuring a lower thermal capture value (-1.4%) and a lower effective resonance integral (-0.4%) corrects partly the LCT underestimation (+150 - +250 pcm)
7. New eval. of U238 inelastic scattering data contribute towards the correction of the problem

First Conclusions

8. The combination of the new inelastic data (LANL or BRC) with the preliminary ORNL R.R. gives a satisfactory correction of the LCT keff underestimation

9. New differential measurements are recommended :
   - U238 (n,γ) in the resolved range (ideally from thermal to 1 keV). Priority is thermal – 120 eV
   - O16(n,α) in the range 3-6 MeV
   - U235 prompt fission spectrum for incident neutron at thermal energy as recommended by the WPEC/Subgroup-9

Future work

- U238 R.R still in progress : inclusion of Macklin data, CLM model… U238 unresolved range is also planned at ORNL.
- LANL and BRC still preliminary and additional modifications are expected.
- More integral testing with new files would be beneficial
  - Pu239 production – spectral indices (thermal and fast range)
  - Thick sample Transmission and self-indication meas.
  - keff of systems reflected by depleted uranium
  - Pulsed sphere exp. : neutron leakage spectra meas.

✓ propose to extend the sg22 duration : 1 year to strengthen the present conclusions.

Other Topics

- O16 (n,α)
- U235 prompt spectrum (SG-18)
- U235 prompt multiplicity (fluctuations in the resonances)
- U238 unresolved range
- New thermal standards (work in progress SG-7 - U235 fission, H1(n,n) [4eV – 25 keV])

Any comments ? !Use ueval mailing list ! : ueval@nea.fr

http://www.nea.fr/lists/ueval.html