Summary Report of WPEC Subgroup 22

« nuclear data for improved LEU-LWR reactivity prediction »

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Purpose of the working group

- Investigate the underestimation of thermal LEU-LWR keff

  keff (~ 0.4-0.6%) observed with ENDFB/VI-8 – JEFF3.0 – JENDL3.3

  DL3.3

  lear data

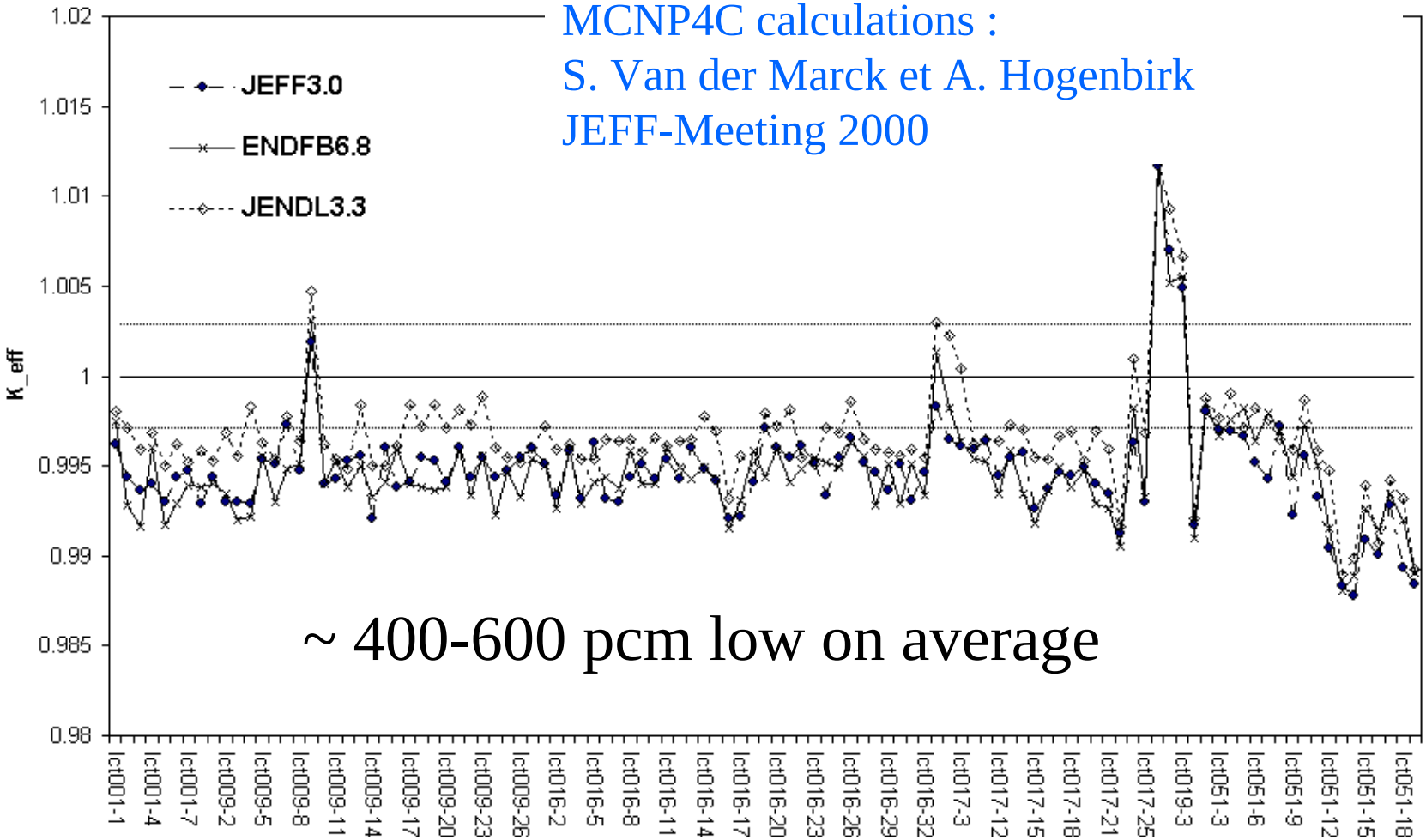
  in 2005.

  work done

  slides at www.nea.fr

The Problem !

Leu-Comp-Therm Benchmark from ICSBEP
MCNP4C calculations :
S. Van der Marck et A. Hogenbirk
JEFF-Meeting 2000



~ 400-600 pcm low on average

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 – Froehner [10 – 150 keV] JEFF3.0 : Froehner [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

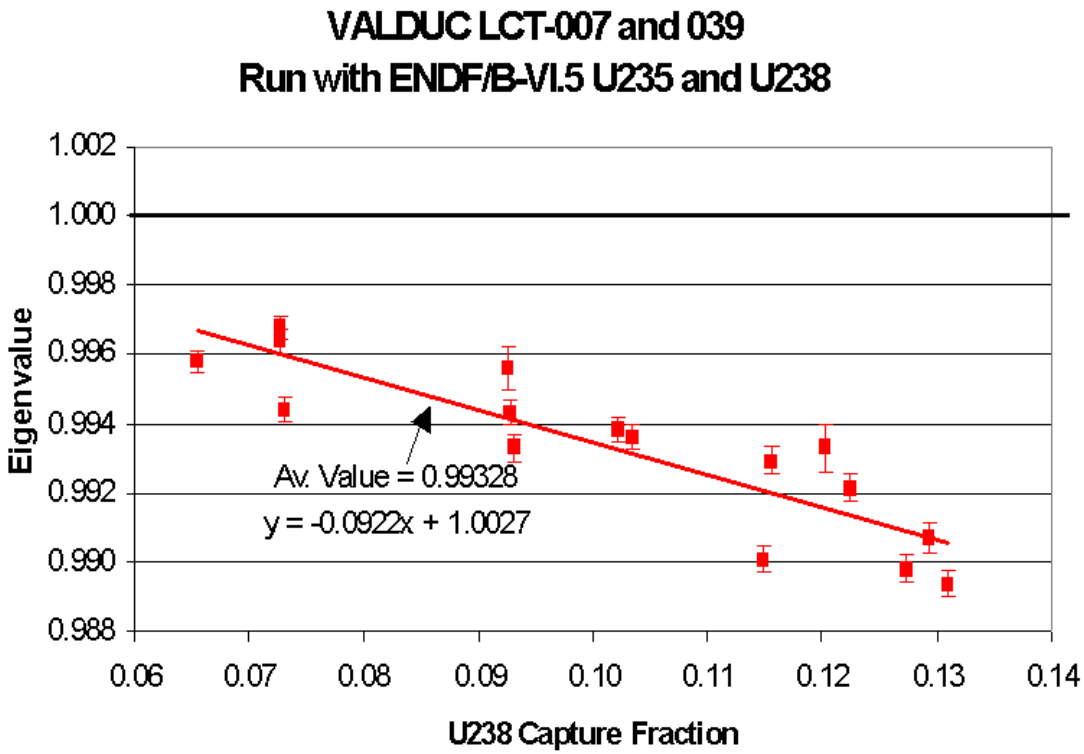
- Keff versus U238 capture fraction
- U238 Hellstrand correlations
- U238 spectral indices
- Production of Pu239 in Post-Irradiation Experiments

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

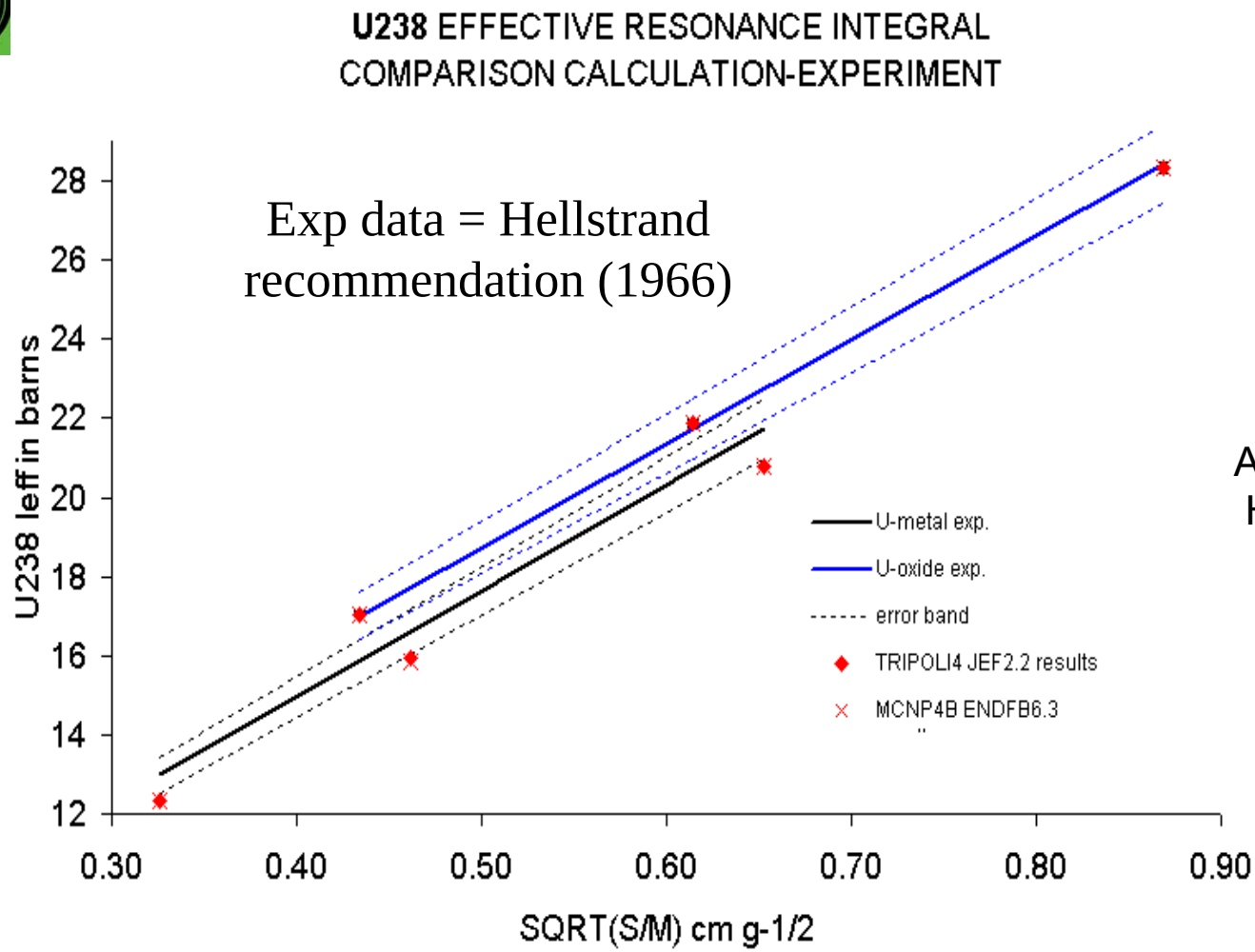
- U238 effective (shielded) resonance integral measurements compiled by E. Hellstrand (*1966 San Diego conference*)

  $\Rightarrow$ compilation of 4 measurements

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

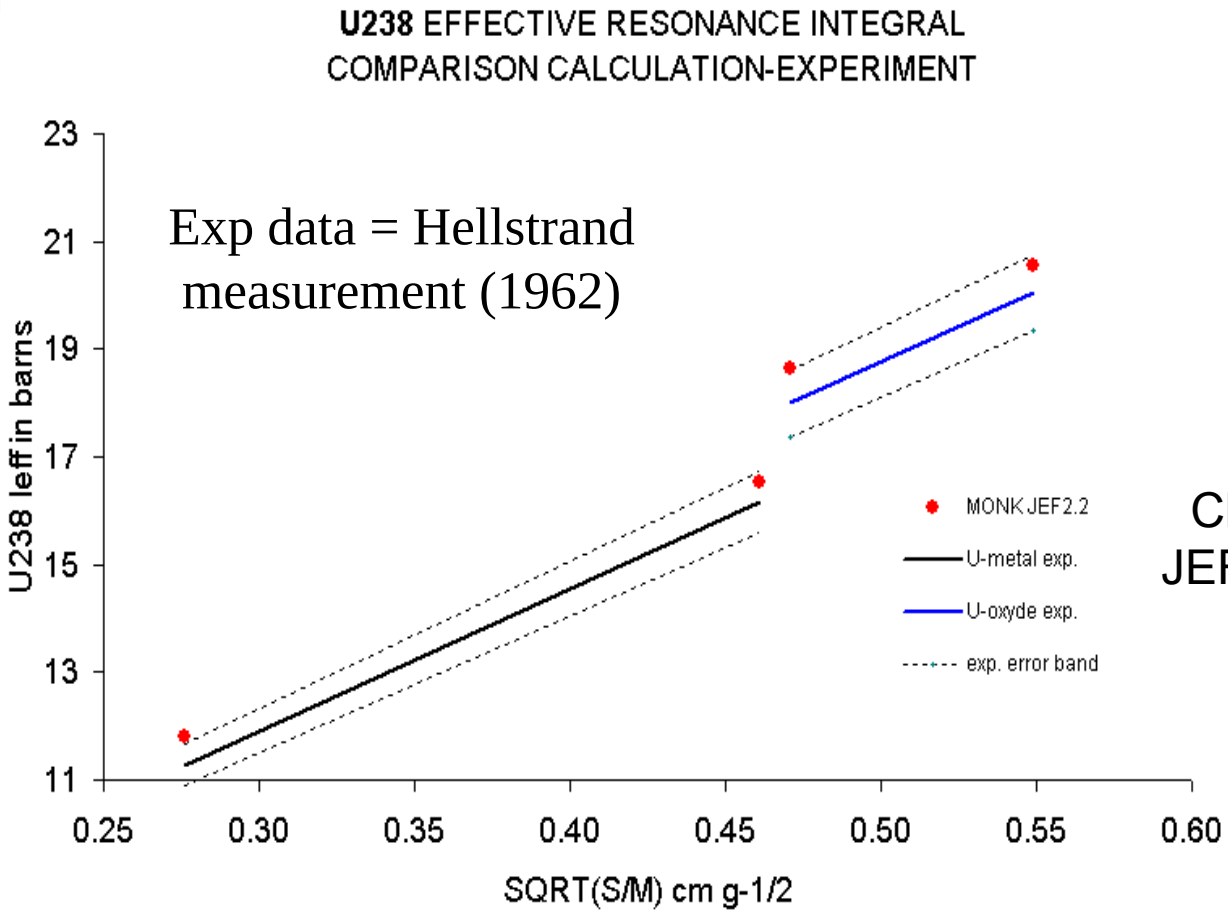
- According to Hellstrand :

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



A Courcelle
H.C. Huria et al.

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



David Hanlon
Christopher Dean
JEFF-Meeting 2002

- Calculations are within the experimental error bands
- Slight trend to U238 leff 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 (A. D. Santos et al., Physor 2002 – ENDF/BVI.5 [342],[345])

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%

Pu239 build-up in PWR

- Studies performed at CEA (C. Chabert, A. Santamarina et al.) demonstrate a systematic overestimation of Pu239 isotopic ratios in Post-Irradiation Experiments
- ~+1 % in UOX and ~+3% in MOX fuel
- Pu239 isotopic ratio is linked with U238 (n,γ).
- These results suggest a decrease (~ 1%) of the U238 shielded resonance capture integral

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 – 2.72 barns
  - Poenitz measurements : 2.68 +/- 0.019 b
  - Mughabghab 1984 & 2002 recommendation : 2.68 +/- 0.019 b
  - CSEWG « standards » 2.701 b
  - **ENDF-JEFF-JENDL value : 2.719 b** (negative-energy res's off a little)
  - 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

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

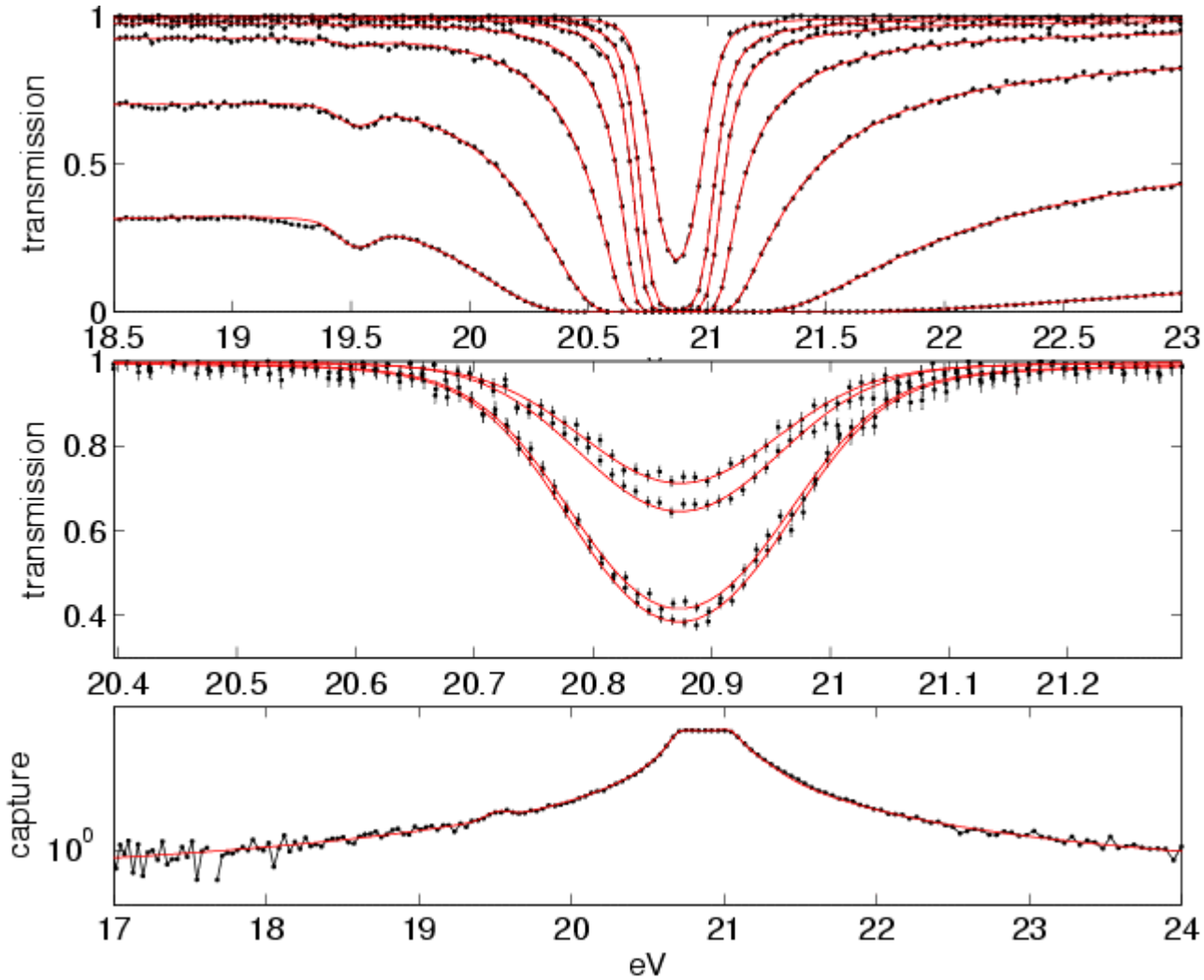
Previous work on U238 RRR
U238 resonance parameters of Moxon et al.

- NEANDC task force on U238 coordinated by Moxon and Sowerby.
- Led in 1990 to an improved evaluation up to 10 keV
- Adopted in ENDF/B-VI.8 - JEFF3.0 – JENDL3.3
- It was hoped it would solve the longstanding overestimation of the U238 (n,γ), which was ~2% in reactivity according to the U238 Brookhaven seminar in 1975. It brought it down, but not enough.

U238 resonance work at ORNL

- U238 evaluation from thermal **to 20 keV** in progress at ORNL (Derrien et al., [66]).
  - Present evaluation is preliminary (932 s-wave and 2354 p-wave resonances)
  - Includes for the first time the ORELA 1988 high resolution transmission experiments (J. Harvey et al. 1988) and complete (R. Macklin et al. 1988) capture data
  - Resolved range extended from 10 to 20 keV

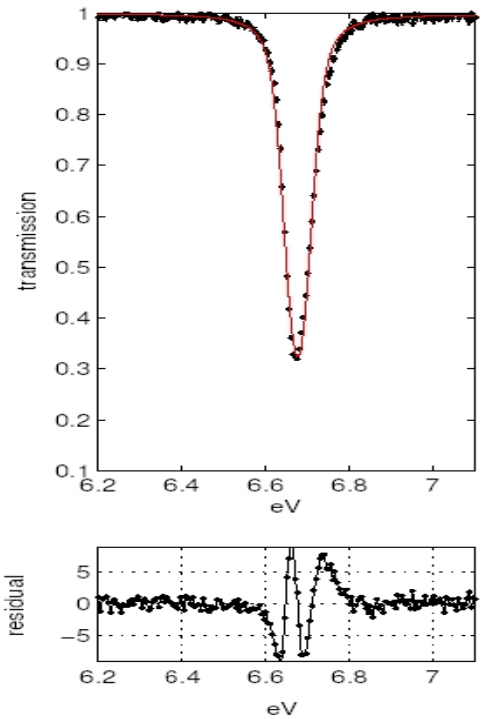
20.6 eV resonance



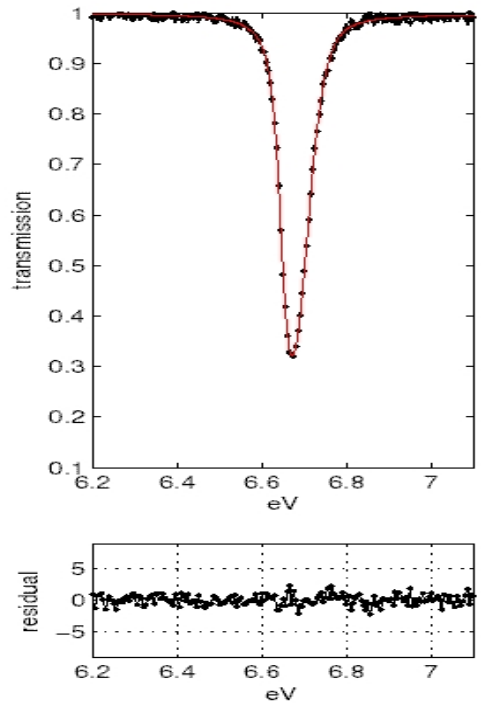
U238 fit with the Free Gas Model (FGM) and Crystal Lattice Model (CLM) of SAMMY

→ test of SAMMY-CLM on U238 transmission (GEEL) at low and room temperature (Meister 1997) [215]

Ex :
UO2
thick sample
23.7K



FGM + adjT



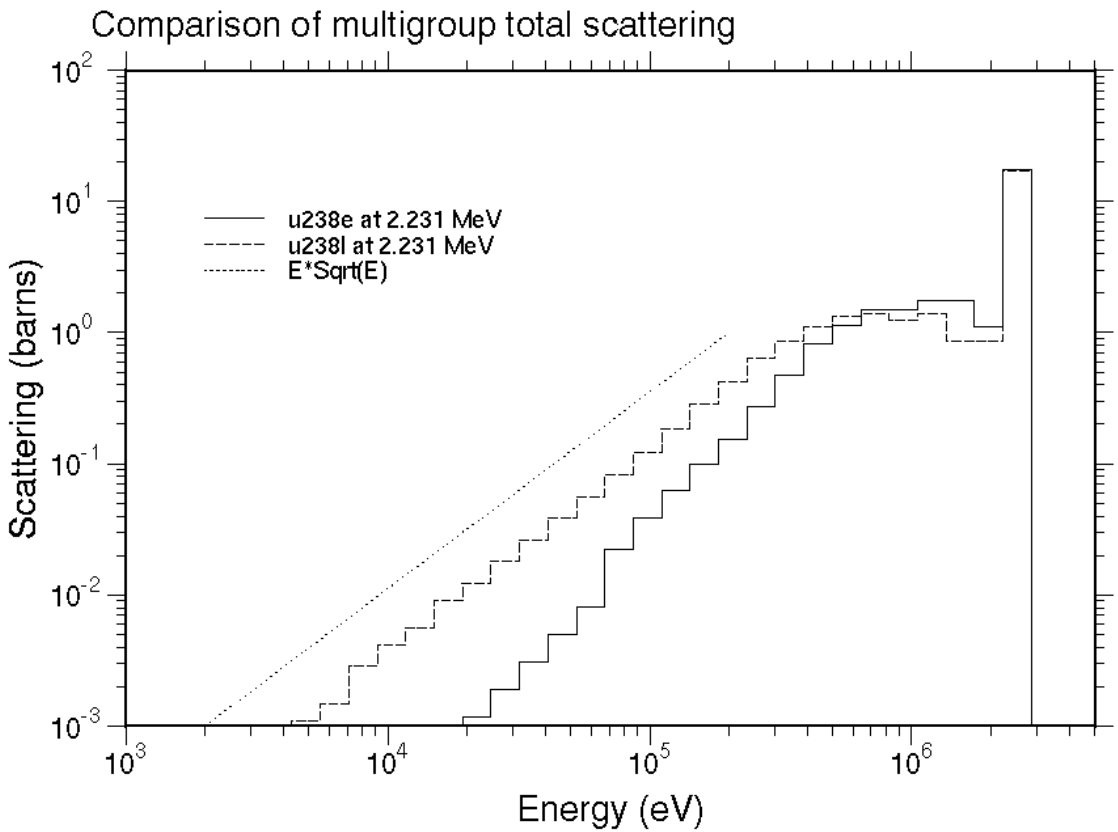
CLM with Dolling et al.
Phonon spectrum

U235-U238 inelastic scattering data evaluations

- 1989 : WPEC/Subgroup-4 «U238 capture and inelastic cross-section »
  - New measurements of inlelastic data
  - Improved evaluation (Kawano et al., Maslov et al.)
  - Raised reactivity but interest in U238 was not very high at the time.
- New preliminary U238 – U235 files from **LANL** (P. Young et al. may 2003 **[153])**
- New preliminary U238 **CEA-BRC** (M.J Lopez- Jimenez et al. oct 2003)
- U238 « Maslov » evaluation
- Improved modelling of inelastic data compared to older ENDF/B-VI.8 and JEF2.2 evaluations. Optical model + coupled channel calculations [150 keV – 30 MeV]

U235-U238 inelastic scattering data evaluations

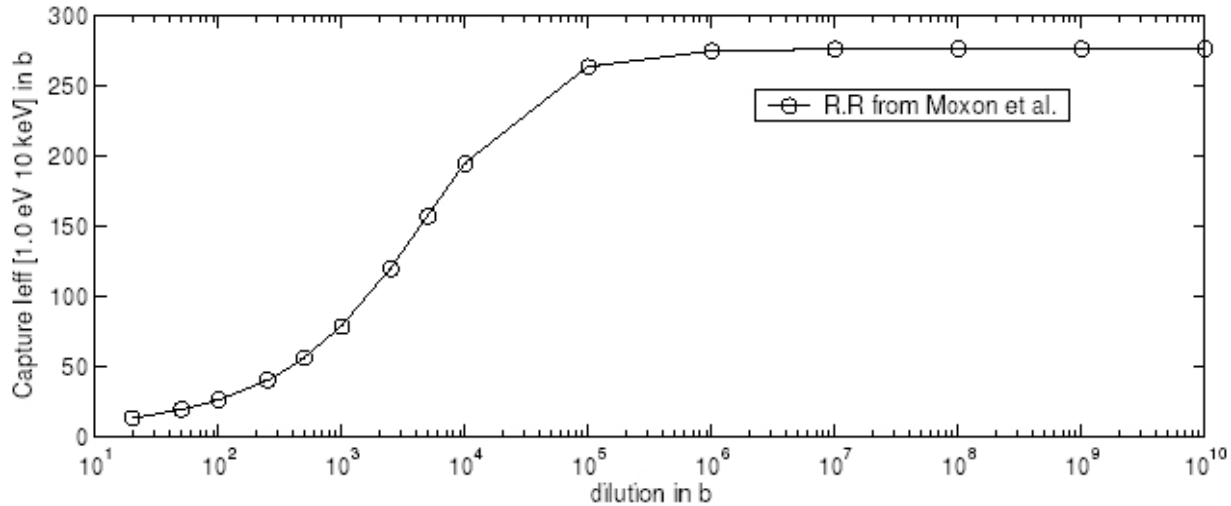
Softer LANL U238 (n,n') secondary spectra than in JEF2.2 and ENDF\B-VI.

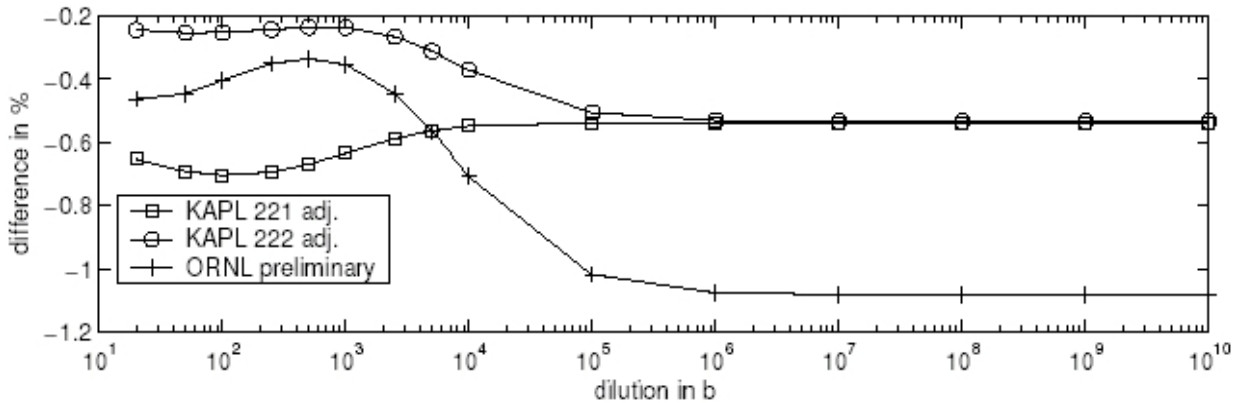


SUMMARY OF INTEGRAL TESTING (may 2004)

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 U235-U238 LANL and BRC inelastic data

- 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

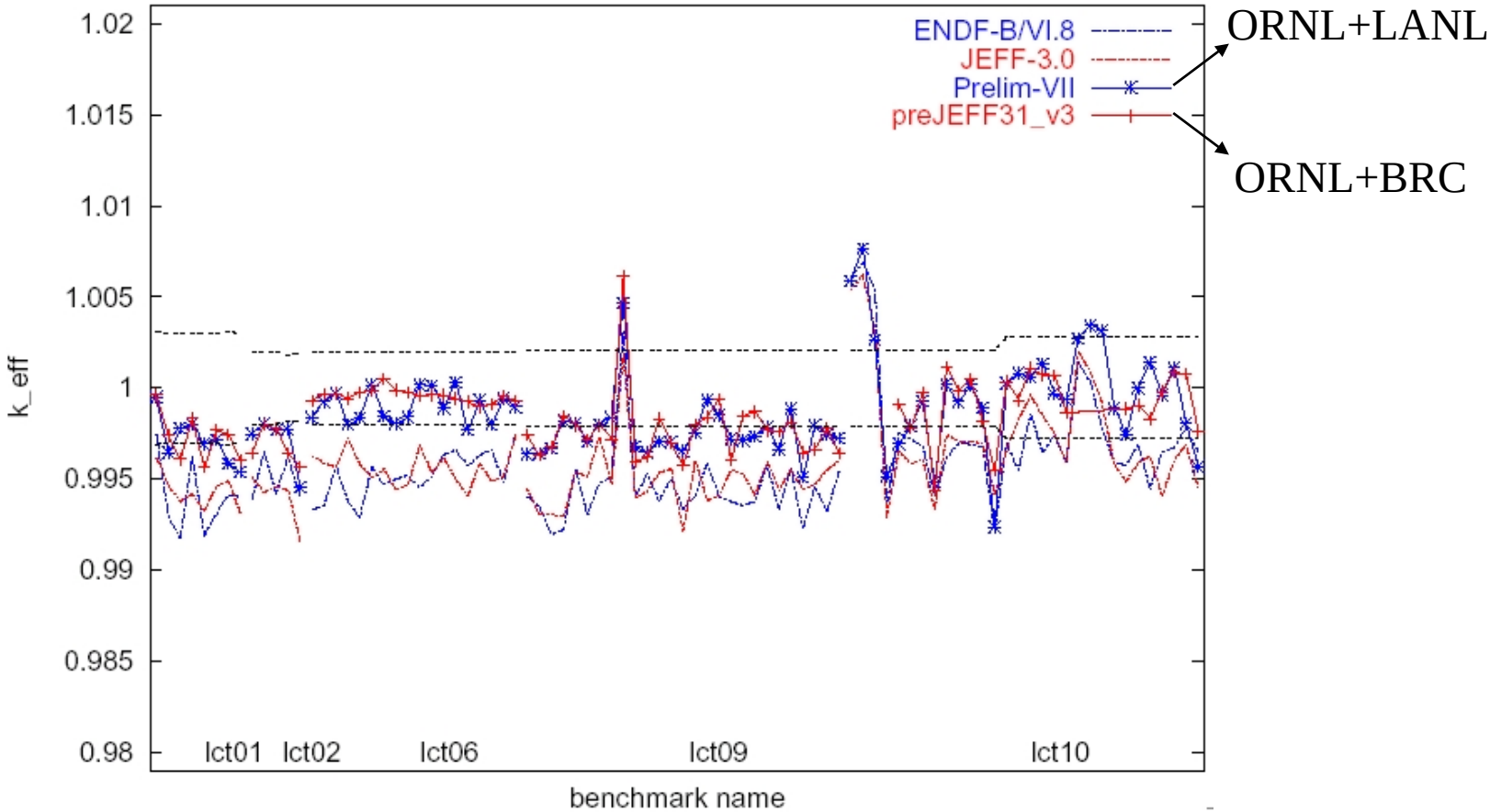
preliminary U238 complete files

- ORNL preliminary resolved range + unresolved range of Froehner + LANL fast range
- ORNL preliminary resolved range + unresolved range of Froehner + BRC fast range
- New LANL U235 and U238 just released

Integral testing of new U238 files

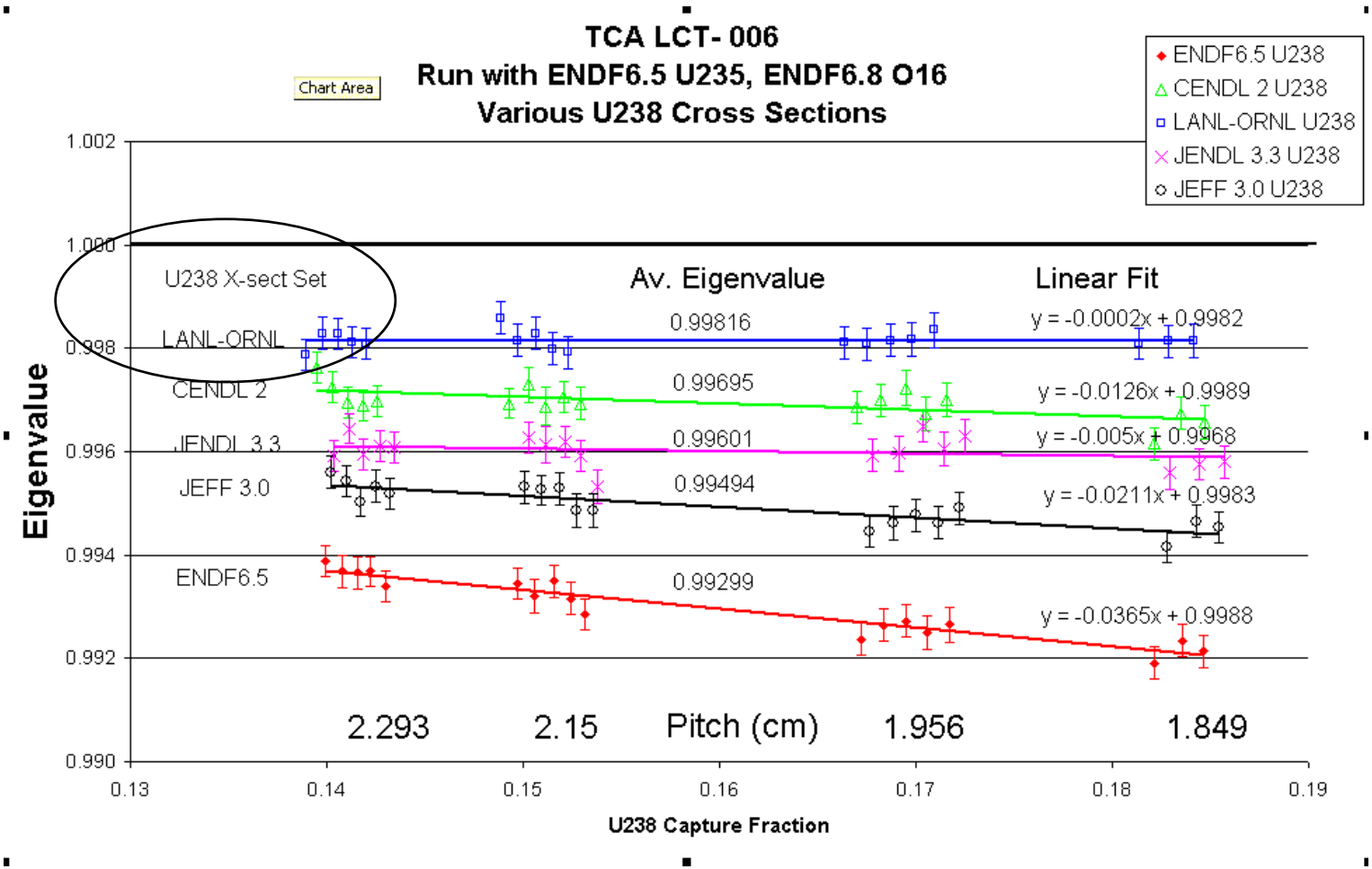
- Kahler (RCP Monte Carlo)
- Weinman (RACER, Monte Carlo)
- Van der Marck, Hogenbirk (MCNP4)
- Mac Farlane (MCNP5, Monte Carlo
- Trkov (WIMS, Deterministic)
- M. Jimenez, Morillon (TRIPOLI4, Monte Carlo)
- Courcelle (MCNP4-5, Monte Carlo)
- Sublet et al. (TRIPOLI4, Monte Carlo)
- Dupont et al. (ERANOS, deterministic)
- …

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)

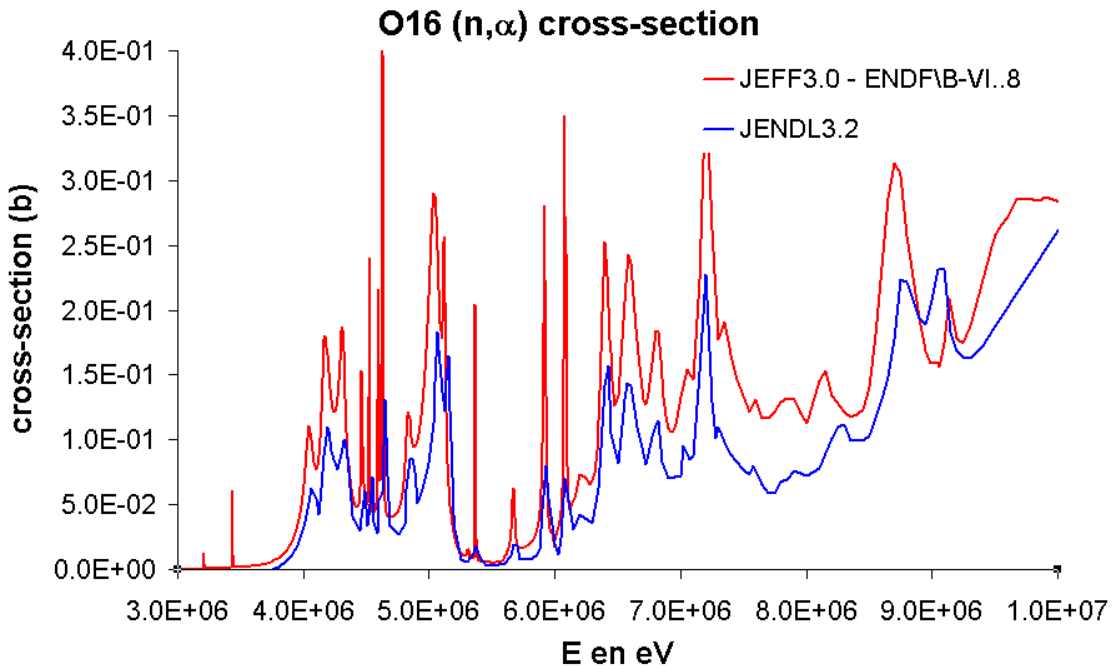
New LANL inelastic substituted

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	

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 but not anticipated.
- Small but non-negligible effect on LEU-COMP-THERM k_{eff} : ~ 80 pcm
- GEEL believes the experiment would be very time-consuming and does not plan to do it.



Arnaud Courcelle WPEC meeting, may 2004 -- CSEWG nov 2004 update

SOME CONCLUSIONS

Tentative Conclusions

- ~400-600 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 calculational methods (use of CEMC)

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

- 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's. However, there are few (no?) benchmark-quality models of commercial reactors in the public domain.

Tentative Conclusions, continued

- A new thermal (2200 m/s) U238 capture value : 2.683 ± 0.012 b
- The integral experiments (Pu239, spectral indices, Hellstrand) do not *require* a lowering of the Moxon-Sowerby resonance-capture cross sections. However, they are statistically *compatible* with a reduction of 0.5 to 1.0%
- Derrien's work at ORNL, and the subsequent SAMMY analysis by Derrien, Courcelle, et al, show that credible fits to the microscopic data can be achieved within this envelope of uncertainty.
- Such a reduction would improve the calculated LEU criticality, so it is not unreasonable to consider that information as part of the "prior" and adopt the set which improves the eigenvalues.
- Finally, the combination of new inelastic data (LANL or BRC) with the preliminary ORNL RRR gives a good correction of the LCT keff underestimation

Work in progress

- U238 RRR evaluation still in progress at ORNL (ARNL?)
- LANL and BRC still preliminary and additional modifications may be made.
- Role of U235 fission spectrum to be investigated
- O16 (n,a): needs a hard look at the existing database. Can a crude measurement decide between ENDF6 and E5/JENDL?
- More integral testing with new files would be beneficial, preferably in the 1-2% accuracy range and not 3-5%
  - Pu239 production – spectral indices (thermal and fast range)
  - Thick sample transmission and self-indication measurements.
  - keff of systems reflected by depleted uranium
  - Pulsed sphere exp. : neutron leakage spectra measurements.

Work in progress, continued

• Incorporation of coherent scattering length into ARNL calculations. Mughabghab (1984) 8.55 f / 9.38 b; Austrian Universities / Bouef 8.407 f / 9.08 b; ORNL/SAMMY 9.41 b.

• Incorporation of direct capture contribution. SAMMY does Reich-Moore and this omits direct capture. Mughabghab (1984) 80 mb at .0253 eV; ~ 50 mb of unexplained background in capture fits, unfortunately pretty flat in energy.

• Incorporation of non-statistical capture. Looking at using REFIT or SAMMY, or Chrien's method from the 1975 Seminar on U238. Contributions welcomed.

MANY THANKS TO THE CONTRIBUTORS OF THIS WORK

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

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