Comments on Light Water and Graphite

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TSL for H_2O (H-in-H_2O): statement of problem (1)

2017 **Mini-CSEWG** (May 2017) :

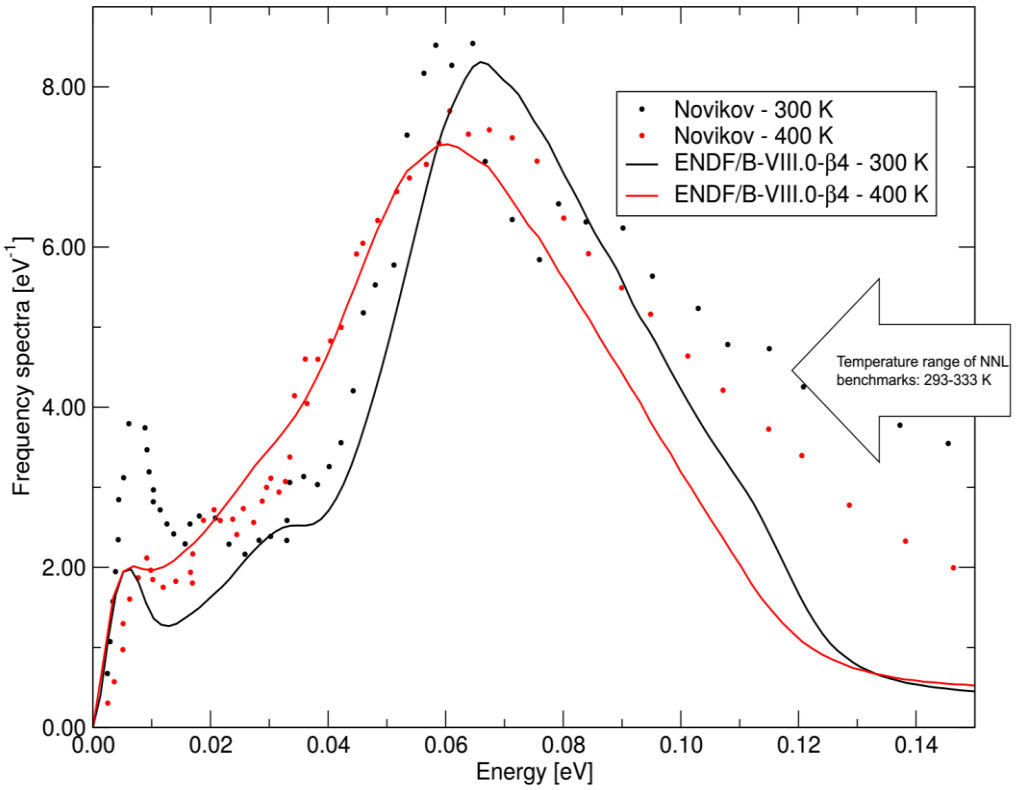
Naval Nuclear Laboratory (NNL) noted **anomalous behavior** in one of their proprietary benchmarks (Neptune benchmark). According to NNL analysis, it was caused by a reduction of the total cross section (σ_s(H-H_2O)) as function of T from 20 °C to 200 °C near $E \sim 20$ meV, which in turn was caused by the change of the frequency spectrum $\rho(\omega, T)$ with temperature.

2017 WPEC meeting (May 2017, **WPEC subgroup 43**):

We looked at the data and concluded that:

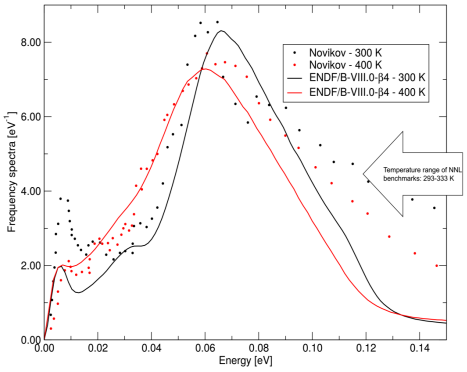
- The shift in the vibrational spectrum ρ with T is *real*; it is consistent with experimental data;
- The **reduction** in the total cross section with T is *real*; it is consistent with the only data set available (σ_{tot}(water) *vs.* E at elevated temperature T); **Dritsa, 1967**.

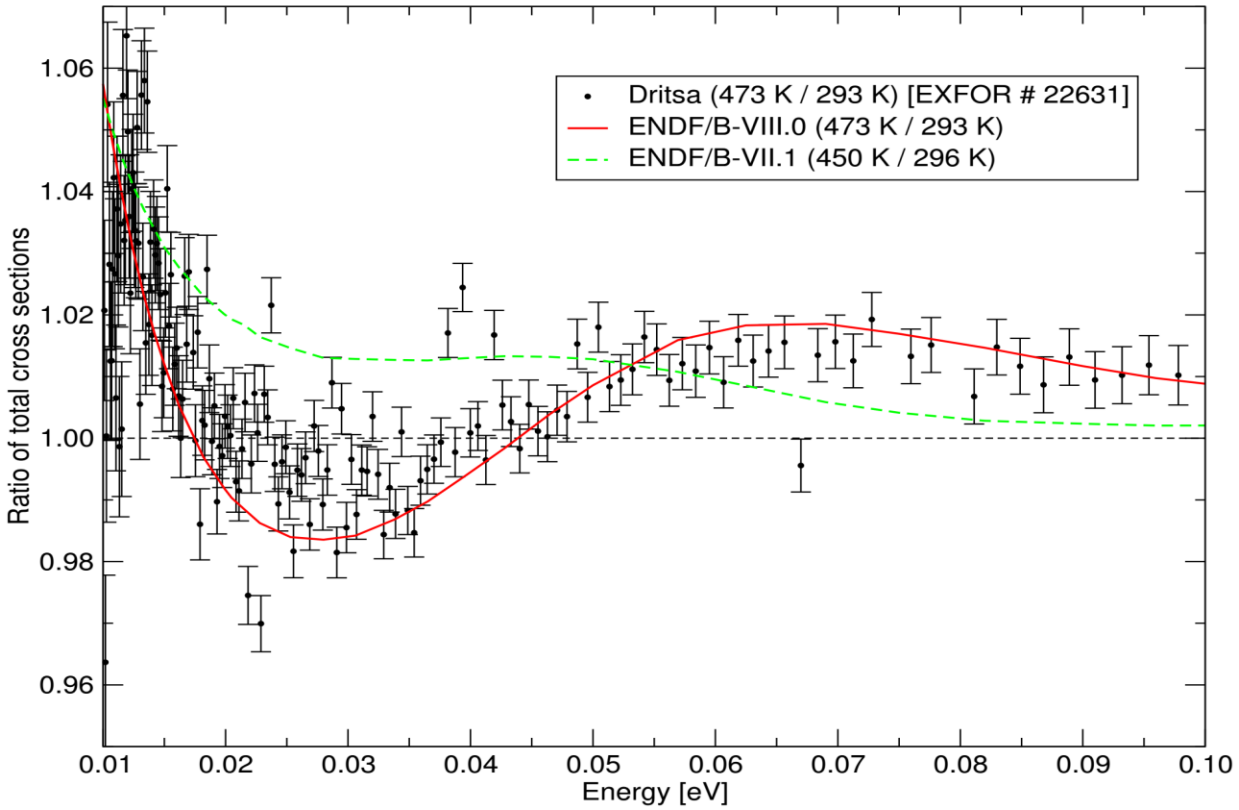
Vibrational Spectrum of H_2O



Comparison of ENDF/B-VIII.0_β4 frequency spectra at T = 300 K and 400 K with experimental data from Novikov (1990).

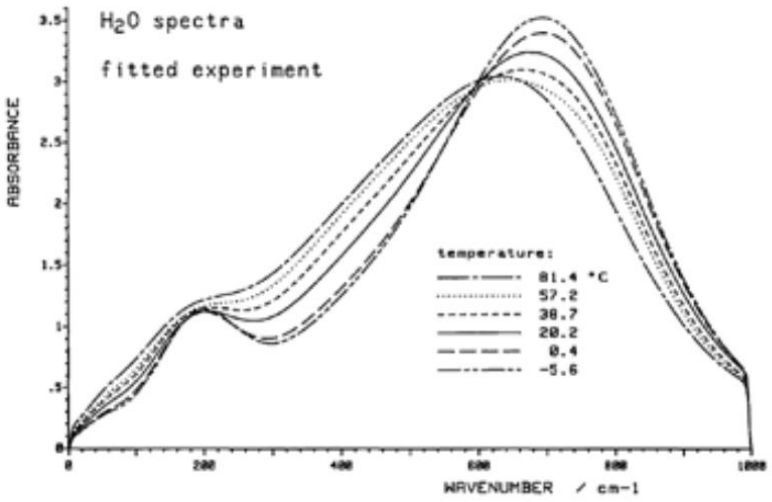
Vibrational Spectrum of H_2O and Ratio of $\sigma_{tot}(E)$ 2

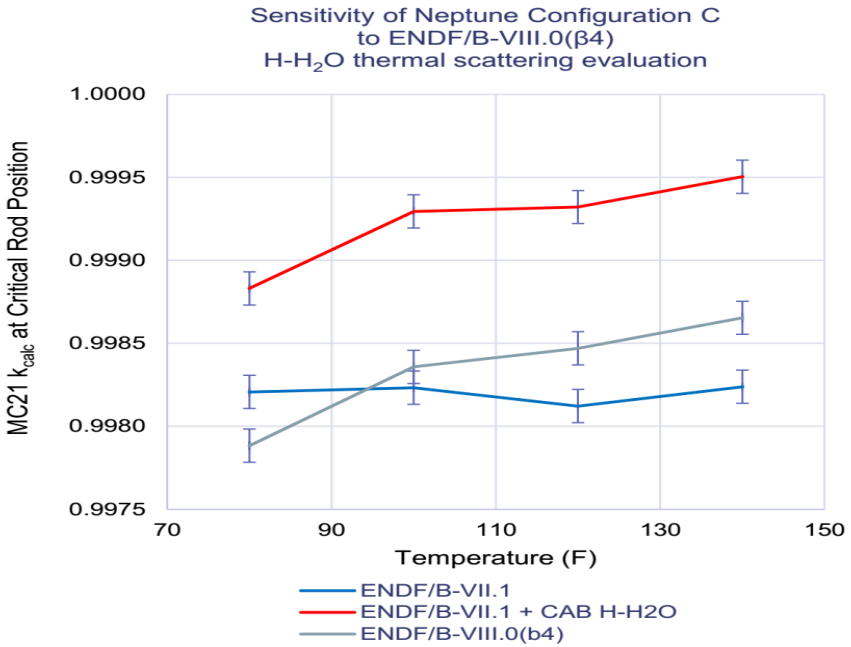




Ratio of total cross sections measured by Dritsa at 200 °C and 20 °C, compared with data from ENDF/**B-VII.1** (ratio of 450 K / 293 K) and ENDF/**B-VIII.0**_β4 (ratio of 473 K / 293 K)

How to resolve NNL “Neptune problem” ? 1





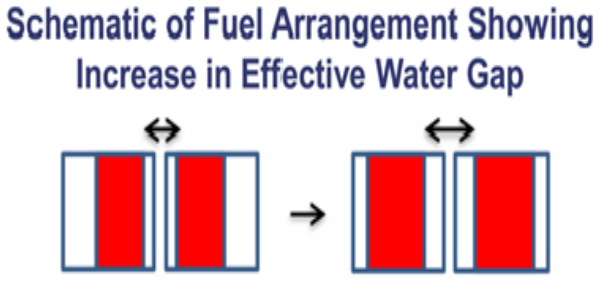
The temperature range of the Neptune (proprietary) benchmark was limited (26 °C to 60 °C),

and k_{eff} shows a *T*-dependent **bias,** up to ≈ +70 pcm **between 26 °C and 60 °C;**

and it is unlikely that the cause would be on the physics at 200 °C.

We started to look at the temperature dependence : $\rho(\omega, T) \rightarrow \sigma_s(E; T)$, $T <$ 100 °C, and we were in need of a simple benchmark …

How to resolve “Neptune problem” ? 2



Ref: S. Walley, et al., “Measurement of Positive Temperature Coefficients of Reactivity for Rack-like Arrangements of Reactor Fuel in the Neptune Zero Energy Facility,” Proc. RRFM-2016, pp. 287-296, Berlin, March 13-17, 2016.

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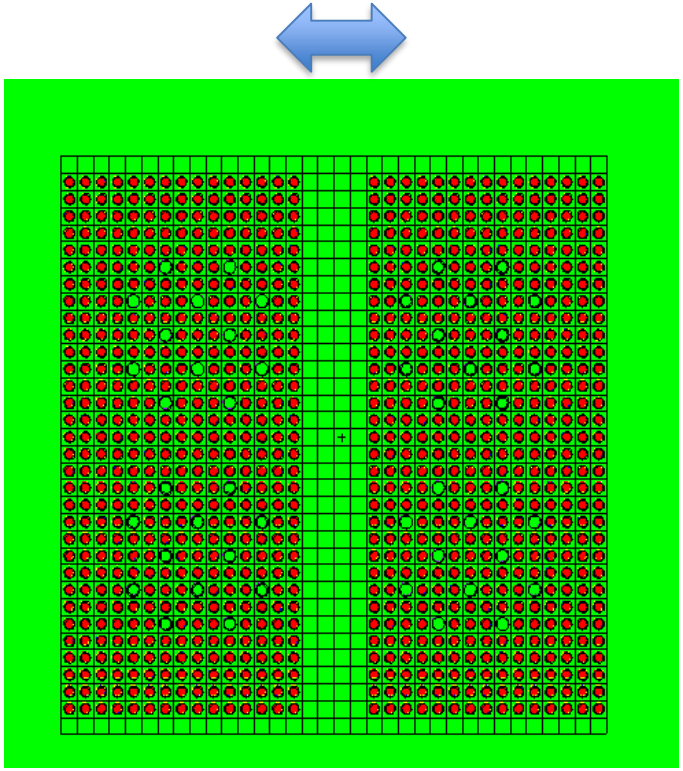
To produce reproducible results is one of the classical requirements for doing science & being a scientist …



CAB & CNL: Geometry of our mock-up benchmark based on **IPEN/MB-01** reactor core:

isolated arrays of LWR fuel pins (UO_2) in water;

all materials at the same temperature *T*;

with ≈ 6 cm of water in the middle of the core; k_{eff} ≈ 1.000 at room *T*, and *T* ↑↑↑

How to resolve “Neptune problem” ? 3

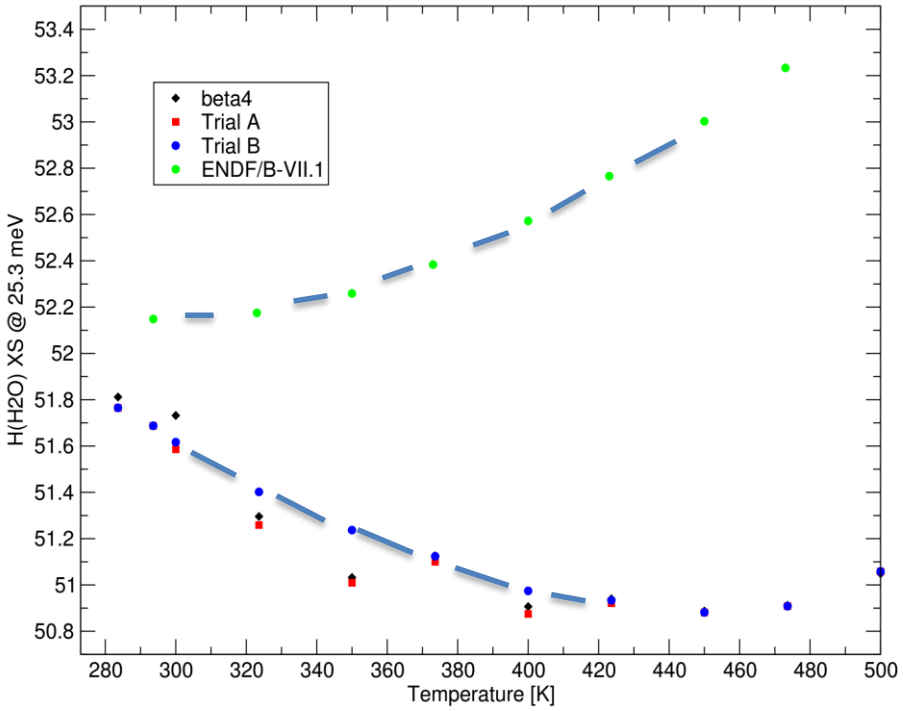
We found that, in order to model this temperature benchmark properly, it is required to have a smooth behavior of the total cross section with temperature *T*. For example, let us **fix** a (relevant) *E* and **check** $\sigma_s(T)$. However, the TSL models in β4 have small oscillations in $\sigma_s(T)$ caused by the numerical noise produced from running separate molecular dynamics simulations at each temperature *T*.

The solution to this problem was to modify the frequency spectrum $\rho(\omega, T)$ to obtain a smooth behavior of the total cross section with temperature.

This smoothed cross sections eliminated a trend of the multiplication factor k_{eff} *vs.* *T* in our mock-up benchmark.

Based on these observations, we prepared two versions of the TSL evaluation: Trial-A is β4 with a improved interpolation scheme (to generate TSL at *T*), and **Trial-B** implements the proposed changes in interpolation scheme **and** frequency spectrum $\rho(\omega, T)$

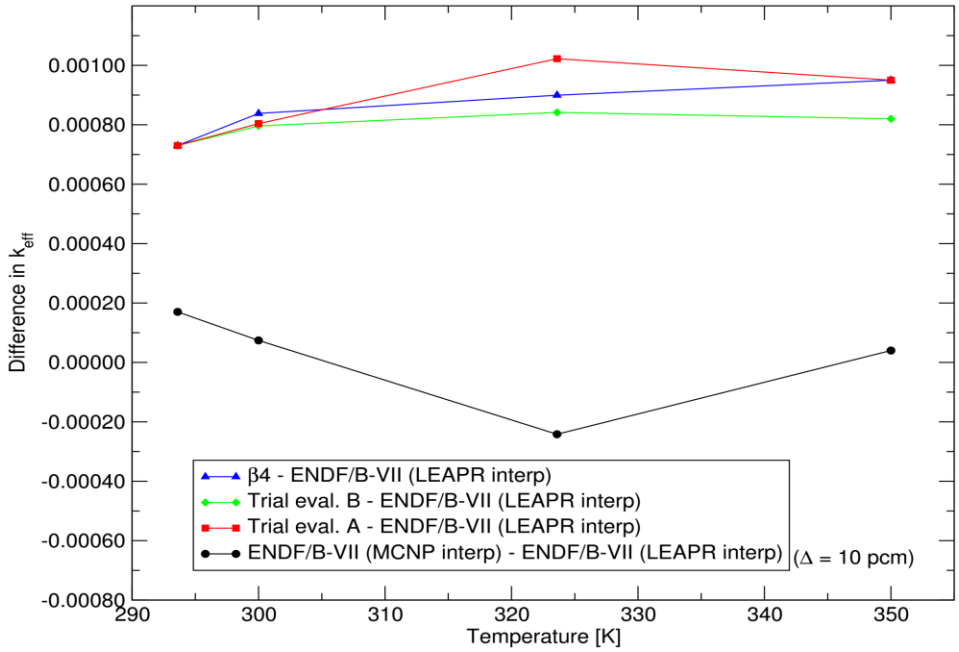
How to resolve “Neptune problem” ? 4



Scattering cross section σ_s(H-H_2O) computed for E = 25.3 meV using different models: ENDF/B-VII.0, ENDF/B-VIII.0_β4 , and the two trial evaluations: Trial A and **Trial B**. Trial A fixes the interpolated point at 300 K and simplifies temperature interpolation by fixing the energy grid of the spectrum.

Trial B includes the improvements of Trial A plus the smoothing of the spectrum ρ

How to resolve “Neptune problem” ? 5



There is a bias between k_{eff} (H-H_2O = ENDF/B-VII.0) and k_{eff} (H-H_2O = ENDF/B-VIII.0_β),

but, do we observe a temperature-dependent bias? (It is desirable to have a constant bias.)

NOTE: k_{eff} *vs.* T has to be calculated using thermal (ace) files for H-H_2O generated from the LEAPR input at each temperature T_i (T_1, T_2, T_3, …)

It is important **HOW** the thermal scattering data are prepared at each T_i of the refined temperature grid (if used). For example, using ACE files interpolated with **makxsf** (part of MCNP) can introduce a bias in calculations.

Recall that we discuss the effects of ~ 10 pcm upon ΔT ~ 10 °C …

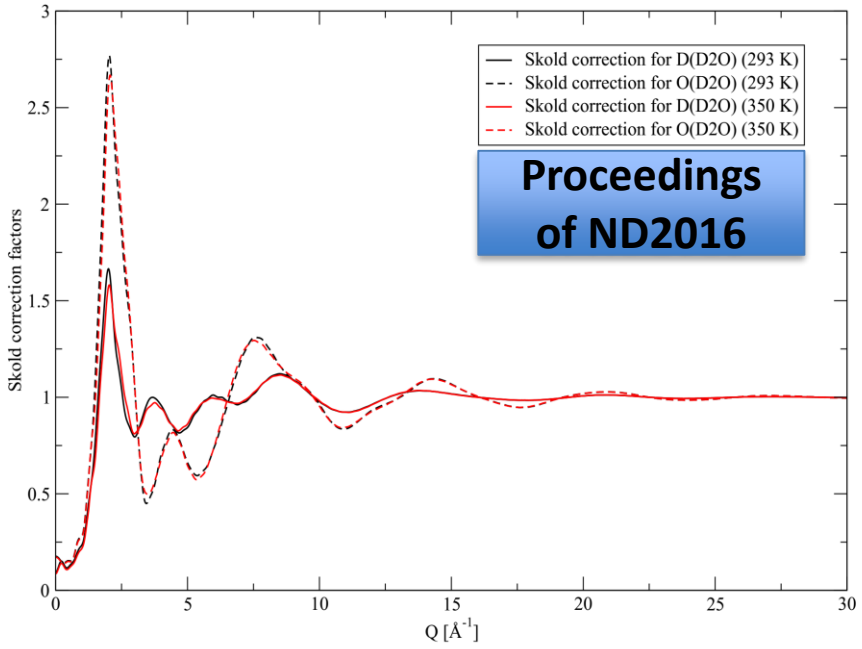
Trial A and Trail B, improved TSL for H-in-H_2O

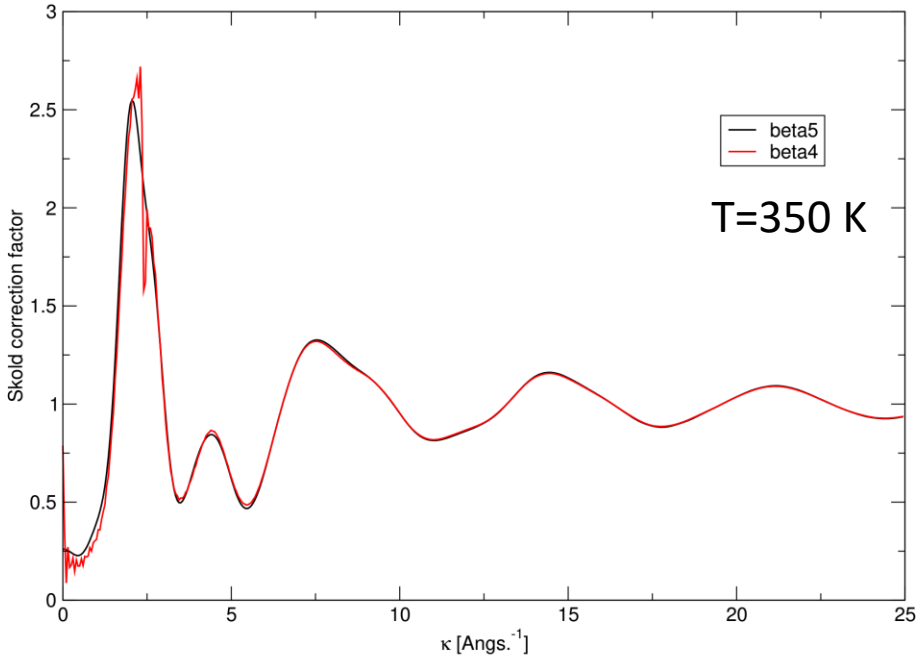
These libraries were uploaded to the GForge server on June 19th, 2017.

The proposed changes **do not** change estimates of criticality at room temperature.

Do we need a simple *temperature benchmark* to test & verify the effects found by NNL ?

TSL for D_2O: improvements of numerical quality





In May 2017, some artifacts in the angular distribution of deuterium and oxygen bound in heavy water were observed at T > 300 K;

NNL reported problems with the Sköld coherent correction of O(D2O).

The problem was *fixed* (MD results → *Fourier transform* → $S_{ij}(q; T)$);
see Sköld correction factor for oxygen bound in heavy water at 350 K in **β5**

Graphite

The proposed evaluations for coherent solids from NCSU

cannot be fully reproduced from the LEAPR inputs available in the GForge server.

This affected the ability to test the data and data processing,
and to compute scattering cross sections at other temperatures (from LEAPR)

(*e.g.*, from LEAPR model to MF7 file and then to thermal ACE file at a given *T*).

For mono-atomic solids,

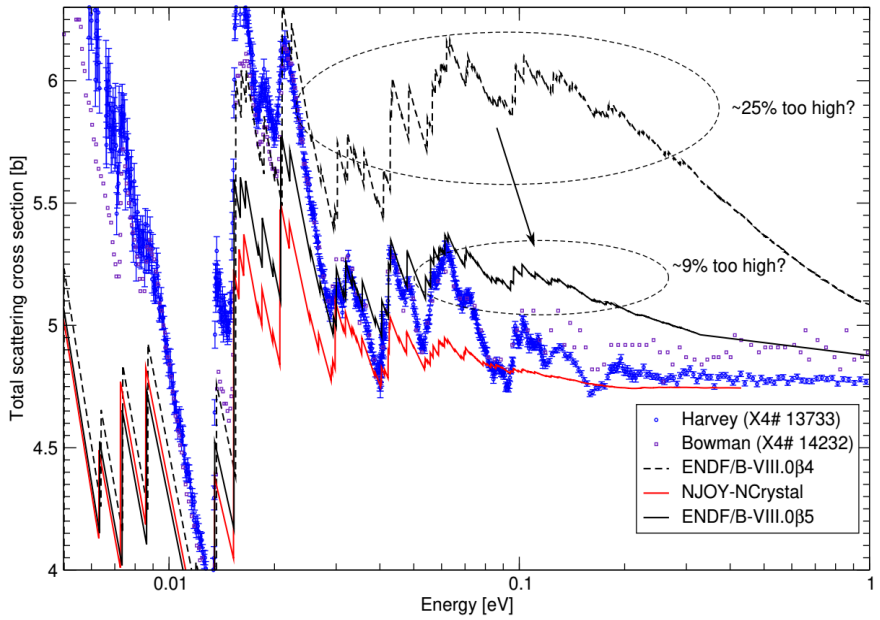
LEAPR (NJOY) has a capability to generate coherent elastic cross sections, and also has a potential for improvements / modifications)

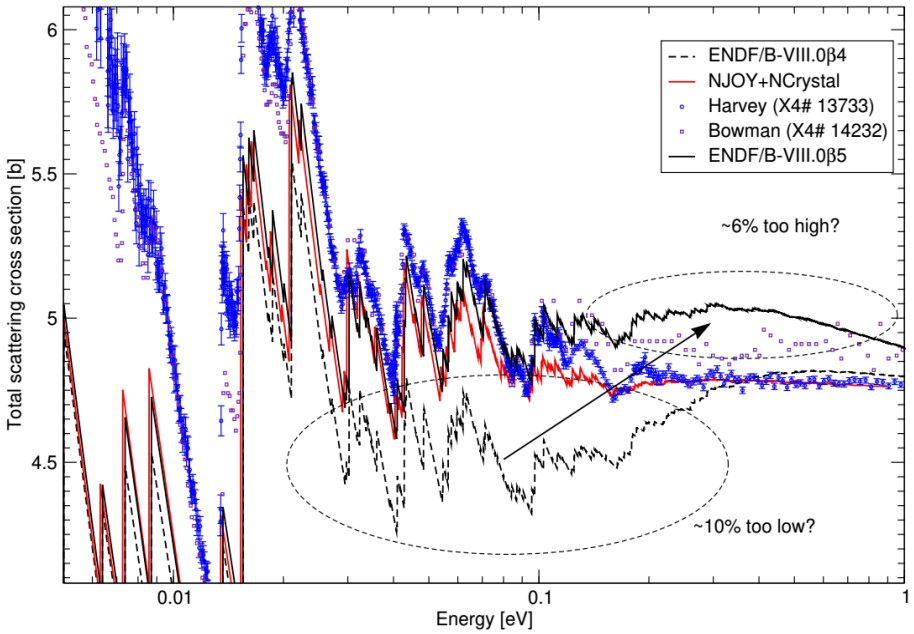
C-Graphite (both evaluations)

noticeable differences in criticality (crit. thermal benchmarks) were observed from β4 to β5

Why? (new *results* in physics usually require interpretation / rationalization)

C-Graphite in lower epithermal region





Total cross section for the **reactor graphite** model (left) ↑

Total cross section for the **crystalline graphite** model (right)

At $E >> kT_D$ (~ 63 meV) , $\sigma_s \approx \sigma_{free}(1 + C_1/E + \ldots)$, Plazek (1952), Granada (1984) : valid in β5 (?)

The total cross section calculated

with the ENDF/B-VIII.0_β4 models for crystalline graphite and reactor graphite show

"bumps" and "valleys" in the asymptotic epithermal energy range (~ 0.1 – ~ 1.0 eV).

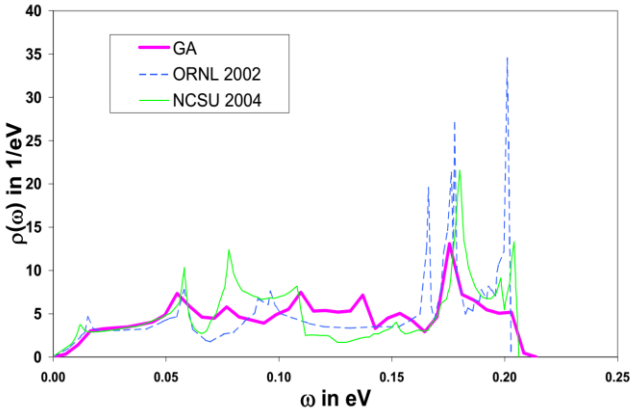
C-Graphite in lower epithermal region

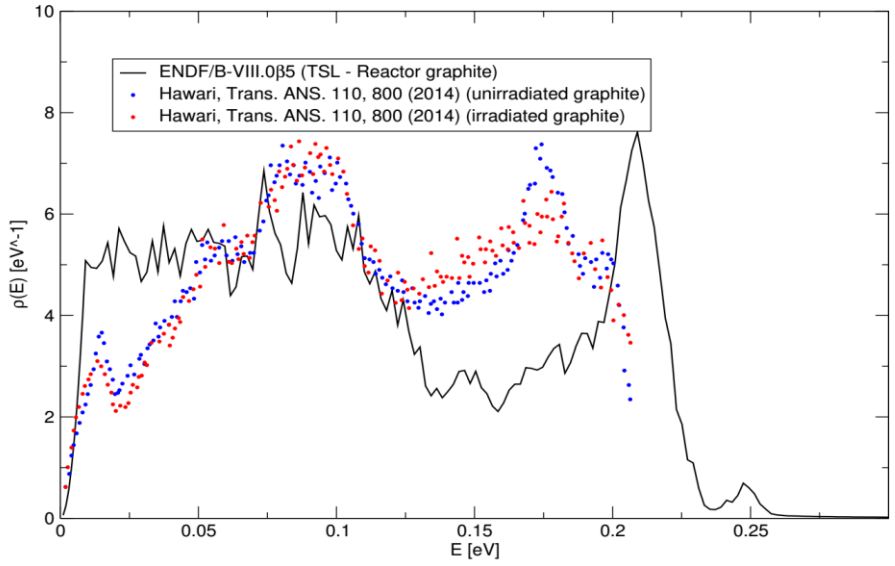
It seems that these anomalies are caused by
an **inconsistency between the evaluation of the inelastic and elastic components of MF7** :
the rise of the ***inelastic*** *scattering cross section* is not compensated
by the decrease of the ***elastic*** *scattering cross section*.

In the evaluations proposed for β5, the anomaly in the total cross section of reactor graphite was partially reduced, and the anomaly in crystalline graphite reversed in sign.

These changes have a significant effect in reactor calculations (e.g., critic. of thermal systems).

Phonon spectrum is also **subject for discussion:**



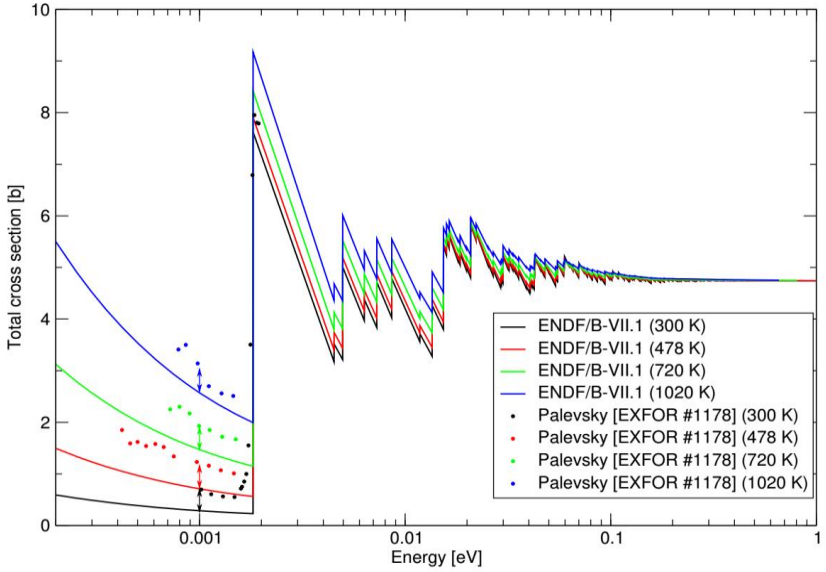


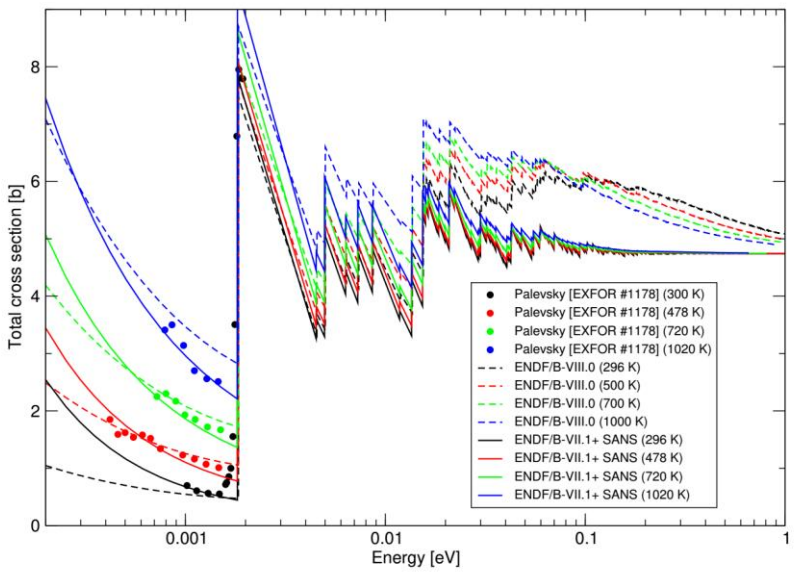
C-Graphite in sub-Bragg region

Palevsky (1955) measured the total cross section of graphite below the lowest Bragg edge at different temperatures, and there is a discrepancy between what the current ENDF/B-VII model predicts and what is actually measured…

Different approach (from ENDF/B-VIII.0β graphite models) :

the differences in the total cross section at low energy ($E < 2$ meV) is caused by elastic small-angle neutron scattering caused by pores and cracks present in real (non-crystalline) graphite; for example, SANS model by Petriw (2010): ↓





Conclusion

ENDF/B-VIII.0_β5 has
modified & improved TSL for **H_2O** (H-H_2O) and
D_2O (D-D_2O, O-D_2O); available from June 2017 from Gforge.

The proposed modifications should **not** change the estimates of criticality / benchmarking results **at room temperature**.

For H-H_2O, **Trial B** is subject for testing in *temperature benchmarks*.

We expect (and hope) that it will reduce the temperature dependent bias in k_{eff} reported by NNL in May 2017 (mini-CSEWG / WPEC 2017).

For detail, see **memo_tsl.pdf** and **memo_graphite.pdf** (Nov 2017)