MEMO: MODIFICATIONS IN H2O AND D2O TSL AFTER BETA4.

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TO: CSEWG EXECUTIVE COMMITTEE

Modifications in H_2O TSL after beta4:

NNL noted an anomalous behavior in one of their proprietary benchmarks. According to their research, this behavior was caused by a reduction of the total cross section from 20 °C to 200 °C, which in turn was caused by the change of the frequency spectrum with temperature. This was presented at mini-CSWEG 2017 [1].

We looked at the data and concluded that:

- The shift in the spectrum is consistent with experimental data (Fig. 1), and
- the reduction in the total cross section is consistent with the only data set available, measured by Dritsa in the 60's (Fig. 2).

(this was presented at WPEC 2017)

The remaining question was, what could be causing the anomalous behavior in the proprietary benchmark. To test the possible effects and solutions, and considering we could not access the conflictive benchmark, we asked NNL for a simplified benchmark with a similar physics but the request was denied. As an alternative, we prepared a simplified mock-up benchmark based on isolated arrays of LWR fuel pins (Fig. 4), following a previous work by Zerkle [4]. Considering that the temperature range of the proprietary benchmark was limited (27°C to 60°C), it was unlikely that the cause would be on the physics at 200°C, but we started to look at the temperature dependence.

What we found is that this type of isolated array critical systems is very sensitive to the way the thermal scattering data is prepared, and it has to be calculated from the LEAPR input at each temperature. Using ACE files interpolated with makxsf based on ENDF/B-VII data introduced changes even more important than using beta4 (black and blue lines in Fig. 5). We also found that in order to model them properly it is required to have a smooth behavior of the total cross section with temperature, and the models in beta4 had small oscillations caused by the numerical noise produced from running separate molecular dynamics simulations at each temperature.

The solution to this was to modify the frequency spectrum to obtain a smooth behavior of the total cross section with temperature (Fig. 3). This smoothed cross sections eliminated the trends of the multiplication factor in our mock-up benchmark (Fig. 5). Based on this we prepared two versions of the evaluation: Trial-A is beta4 with a improved interpolation scheme, and Trial-B implements the proposed changes. The proposed changes **do not** change criticality at room temperature.

These libraries were uploaded to the GForge server on June 19th. We have not received feedback from NNL.

Modifications in D_2O TSL after beta4:

In May, CNL reported artifacts in the angular distribution of deuterium and oxygen bound in heavy water. A bit later, NNL reported problems with the Skold coherent correction of O(D2O).

This was traced to an error in the Fourier transform routines used to compute the Skold correction factor from molecular dynamics. The problem was fixed (Fig. 6), and a new evaluation was prepared without the oscillations in the angular distribution.

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

References

[1] M. Zerkle, J. Holmes, D. Gill. *NNL Testing of ENDF/B-VIII.0(β4) H-H2O at Elevated Temperatures*. mini-CSEWG, 2017.

[2] A.G. Novikov, A.A. Vankov and L.S. Gosteva. *Temperature dependence of the general spectrum for water*. Journal of Structural Chemistry. **31**, 77 (1990).

[3] M. Dritsa, A. Kostikas. *Total cross sections of H2O at room temperature and 200C*. Report EANDC(OR)63 "L", 1967.

[4] M. Zerkle, T. Copinger. *Evaluation of an Unexpected Reflector Temperature Effectsfor Water Isolated Array Configurations*. ICNC-2015.

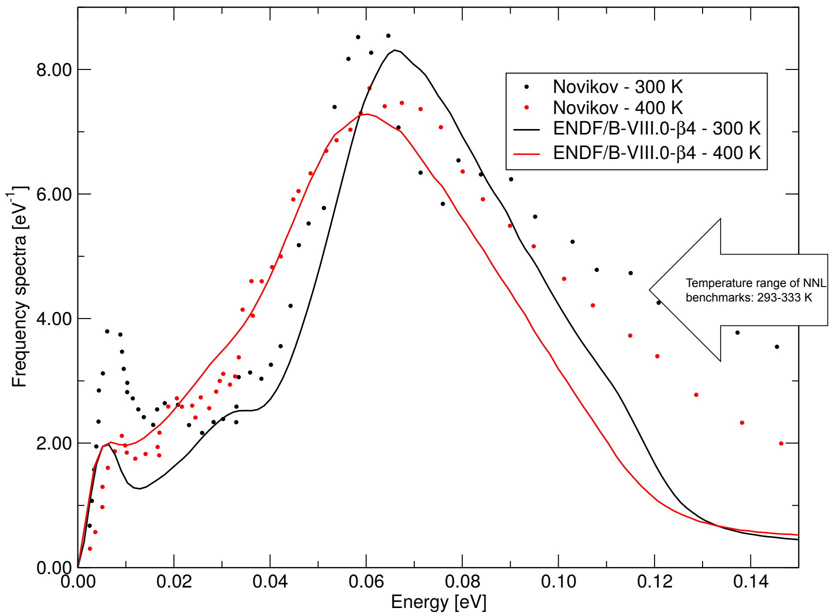

Figure 1: Comparison of ENDF/B-VIII.0-β4 frequency spectrum at 300 K with experimental data from Novikov [2].

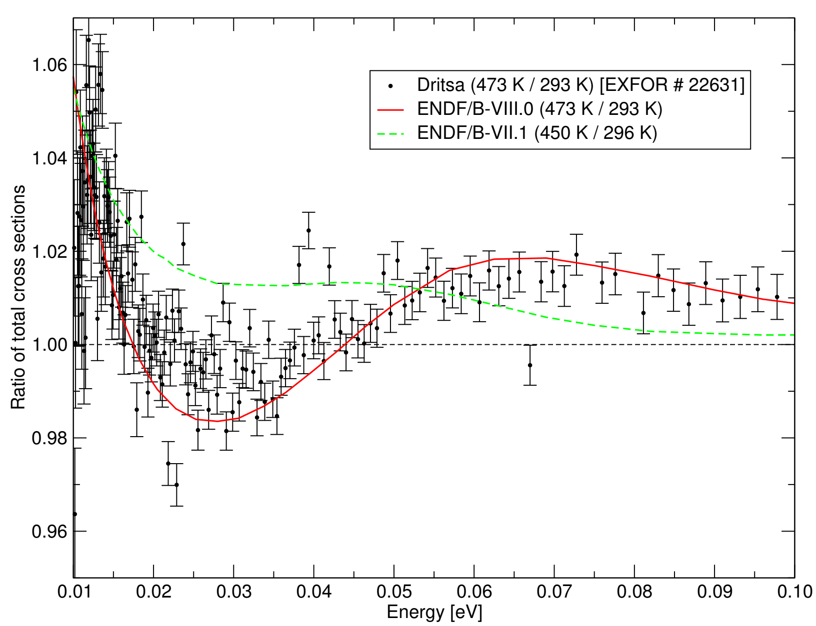

Figure 2: Ratio of total cross sections measured by Dritsa at 200°C and 20°C, compared with data from ENDF/B-VI.1 (450 K/293 K) and ENDF/B-VIII.0 (β4) (473 K/293 K).

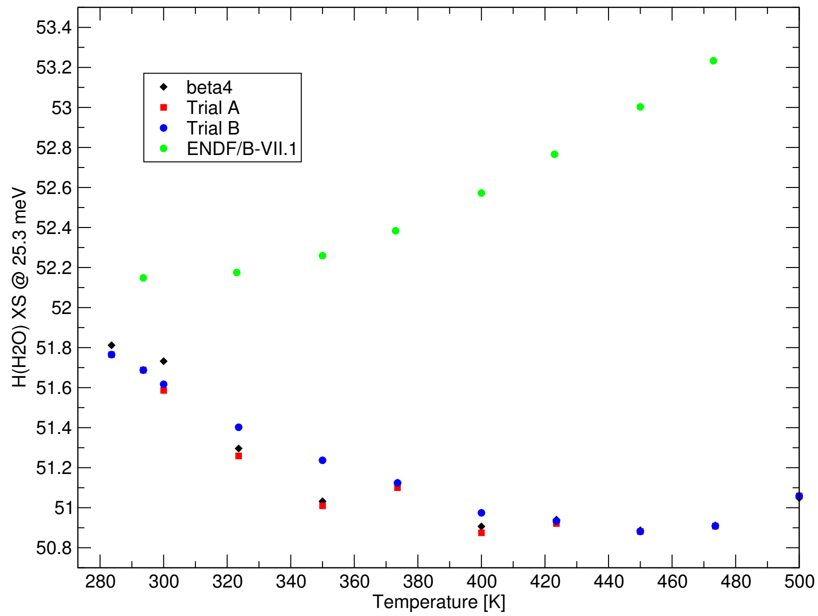

Figure 3: Scattering cross section computed for E = 25 meV using different models: ENDF/B-VII.0, ENDF/B-VIII.0β4 and the two trial evaluations: Trial A and Trial B. Trial A fixes the interpolated point at 300 K and simplifies temperature interpolation by fixing the energy grid of the spectrum. Trial B, includes the improvements of Trial A plus the smoothing of the spectrum.

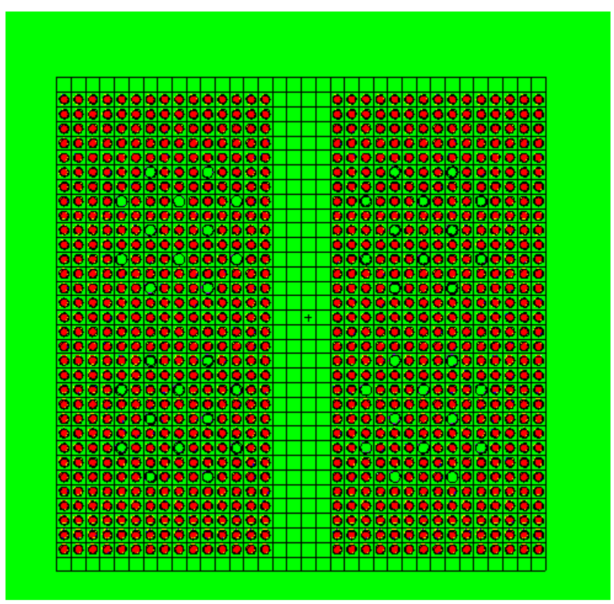

Figure 4: Geometry of the mock-up benchmark based on IPEN/MB-01.

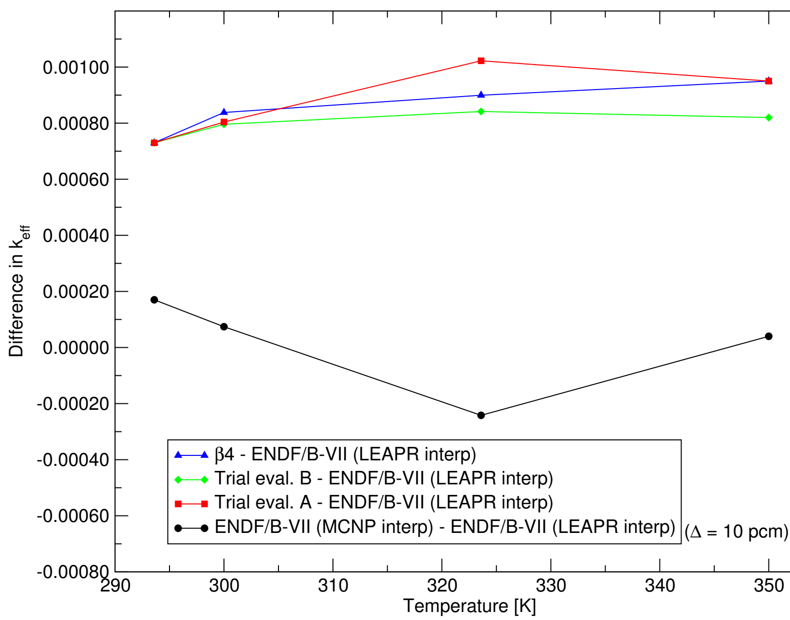

Figure 5: Results for the mock-up benchmark using different TSL libraries. Note that using makxsf for TSL interpolation (black line) introduces a significant bias in the calculation.

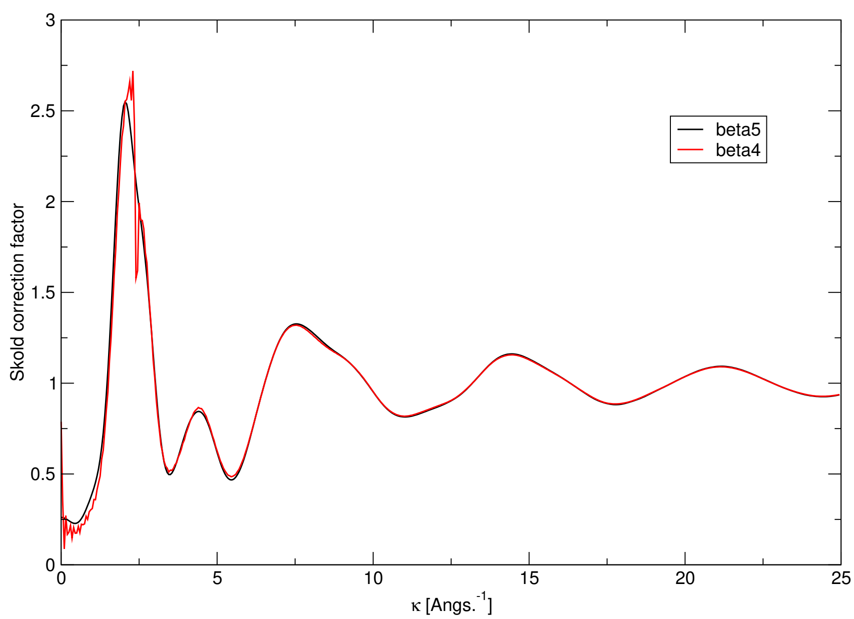

Figure 6: Skold correction factor for oxygen bound in heavy water at 350 K.