Nuclear Data Testing / Evaluating at CNL (Canada) and CAB (Argentina)

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CSEWG 2018

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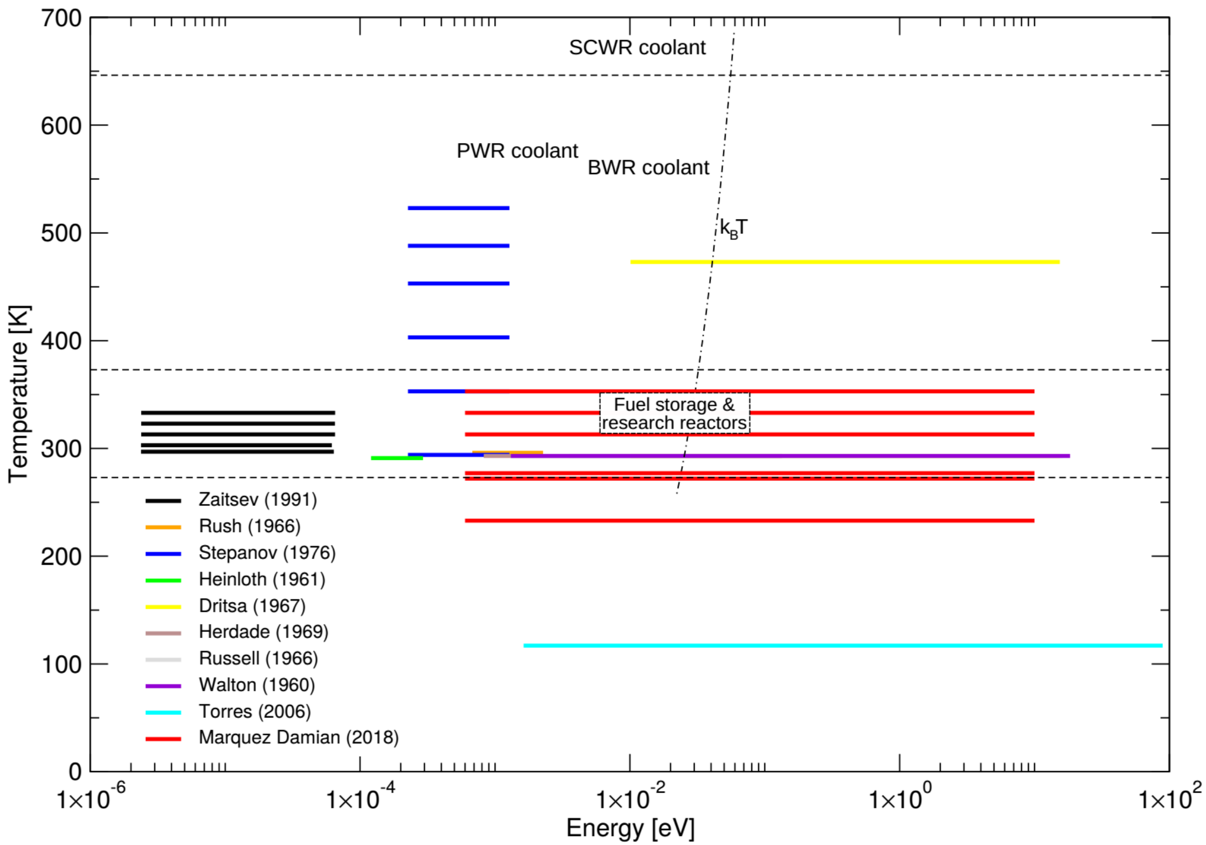
Plan

- *TSL for H_2O and D_2O : old/new experimental data for thermal scattering at T > T_room (293.6 K , p > 0.1 MPa); V&V .*

- *ND library for MCNP / SERPENT based on ENDF/B-VIII.0 : from LANL ace files (2018) to CNL version;*

- *ZED-2 reactor at CNL .*

TSL for H_2O : $\sigma_{tot}(E; T)$



Power reactor applications: T ~ 550 – 600 K, p ~ 15.5 MPa / p ~ 7.3 MPa

New measurements underway (data sets are not in EXFOR yet)

Experimental activities from CAB

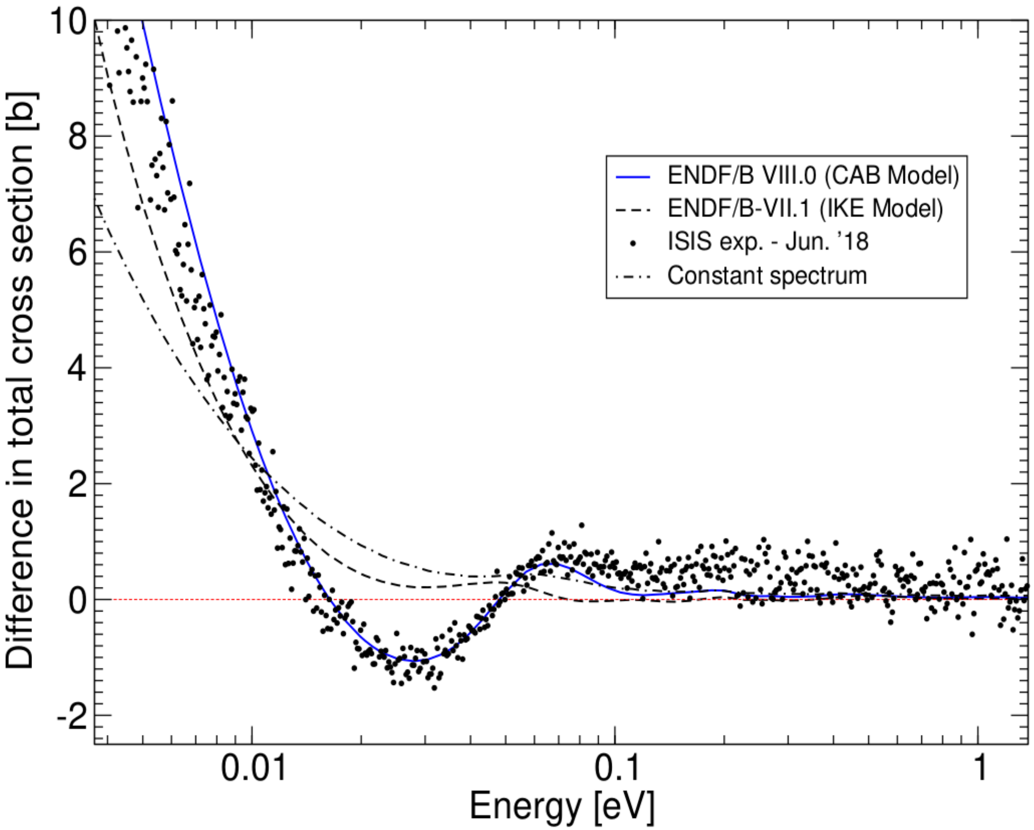
- In June 2018, researchers from Centro Atomico Bariloche performed an experiment at the VESUVIO spectrometer in the ISIS neutron source (UK).
- Samples of **light water**, ice, and three different types of graphite were used in transmission and diffraction experiments.
- Data is currently being analyzed and it will be published when ready.

Preliminary results for light water (H_2O)

- The experiment on light water was designed to test the temperature dependence of the total cross sections $\sigma_{tot}(E; T)$, as predicted by the CAB Model adopted in ENDF/B-VIII.0.

- The total cross section was measured at 10°C and 80°C, with high statistics over the whole thermal energy range, E ~ 1 meV - 1 eV .

Preliminary results for light water (H_2O)

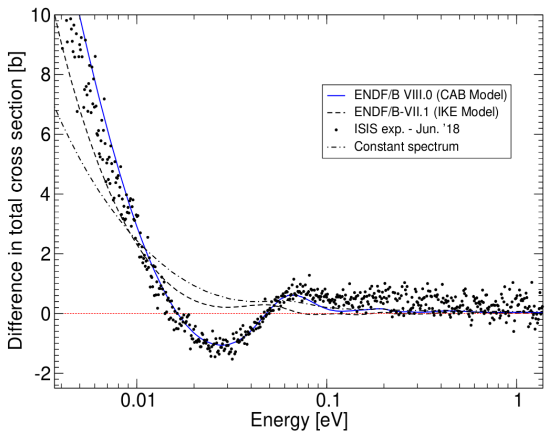


- Difference in total cross sections between 80°C and 10°C,

$\sigma_{tot}(E; T_2) - \sigma_{tot}(E; T_1)$ *vs.* E , $T_2 > T_1$

spectrum: $\rho_{ph}(\omega; T)$ for H-in-H_2O is "input parameter" in NJOY, leapr

Preliminary results for light water (H_2O), T < 100 °C



- Results confirm that the temperature dependence predicted by the ENDF/B-VIII.0 model is correct (reliable).
- Additional measurements were performed at T = 4, 20, 40, and 60 °C that confirm the trend.
- The sample was frozen and measurements were performed at T = -40 and -1 °C.

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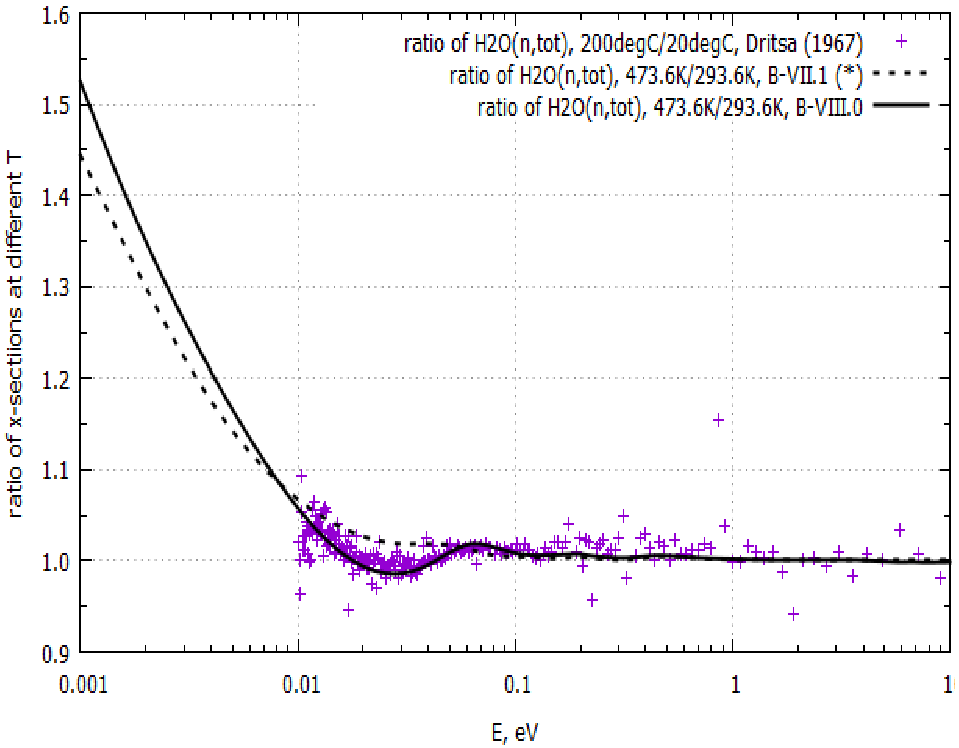
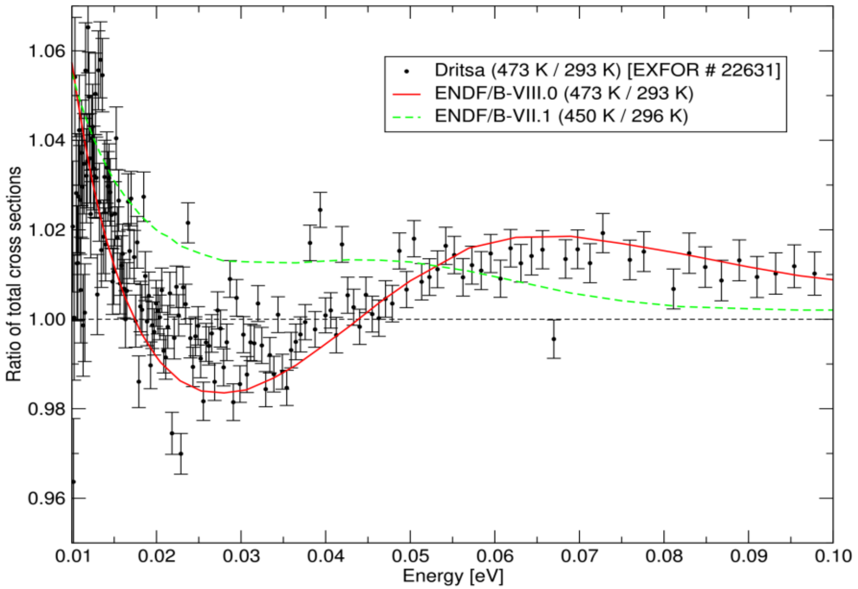
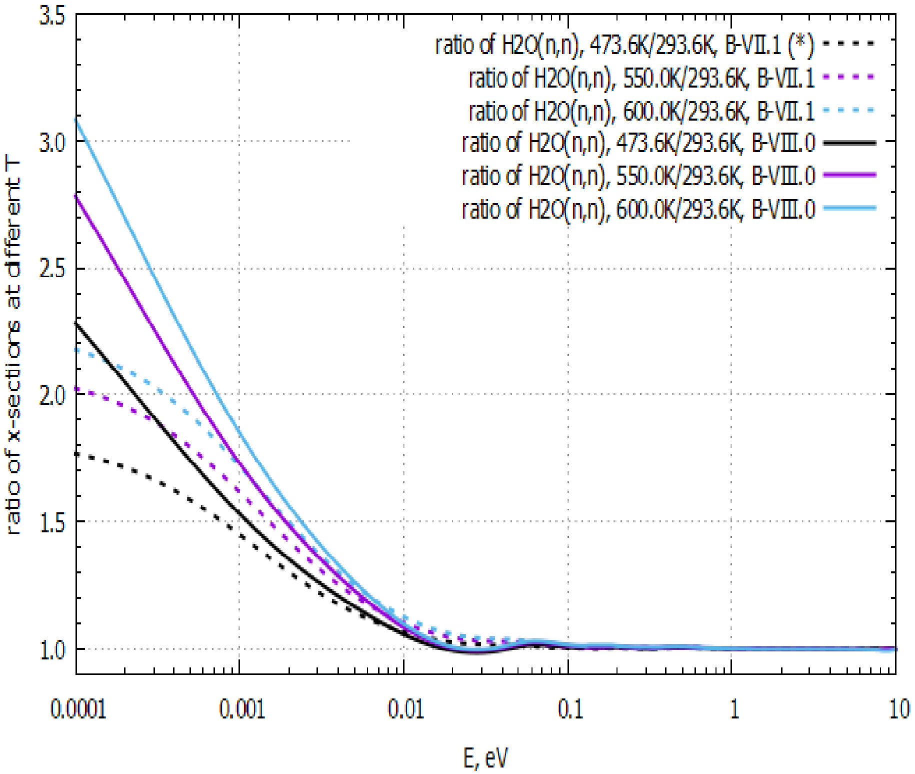
Results for light water (H_2O), **T > 100 °C**

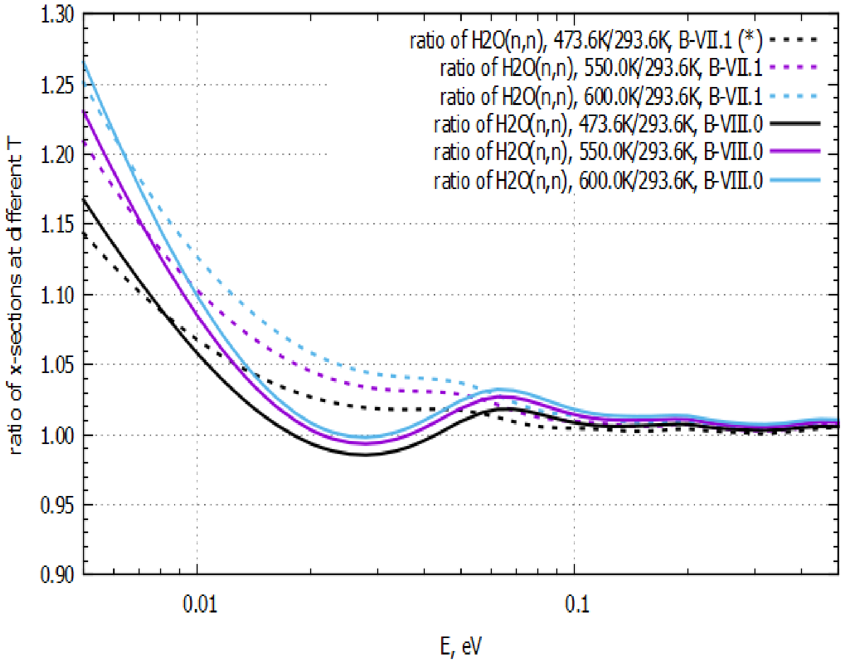




- EXFOR: Dritsa data sets at T = 200 °C and 20 °C (1967)
- Calculate the ratio, $\sigma_{tot}(E; T_2) \ / \ \sigma_{tot}(E; T_1)$, $T_2 > T_1$
- [$\sigma_{tot}(E; T)$: no new data in EXFOR as of October 2018]

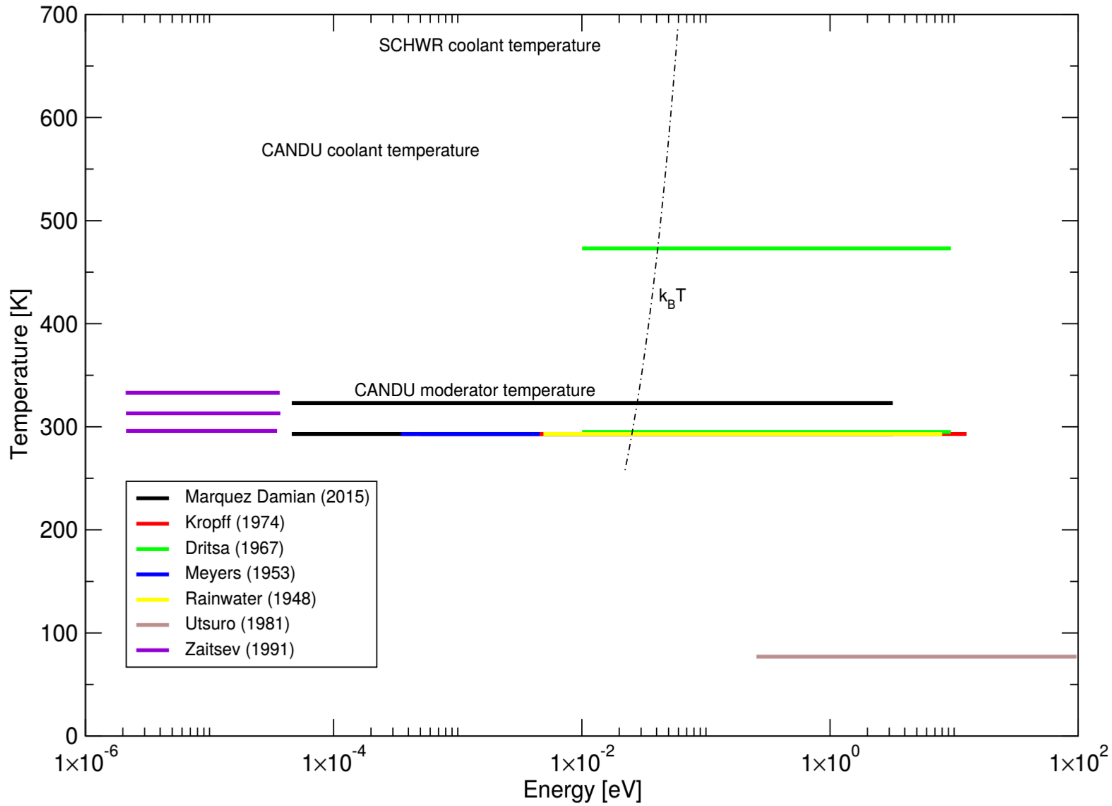
Results for light water (H_2O), **T > 100 °C**





- $\sigma_{tot}(E; T_2)$ / $\sigma_{tot}(E; T_1)$ *vs.* E
- TSL for H-in-H_2O : ENDF/B-VIII.0 *vs.* ENDF/B-VII / JEFF-3.3
- **V&V** : ND-2019

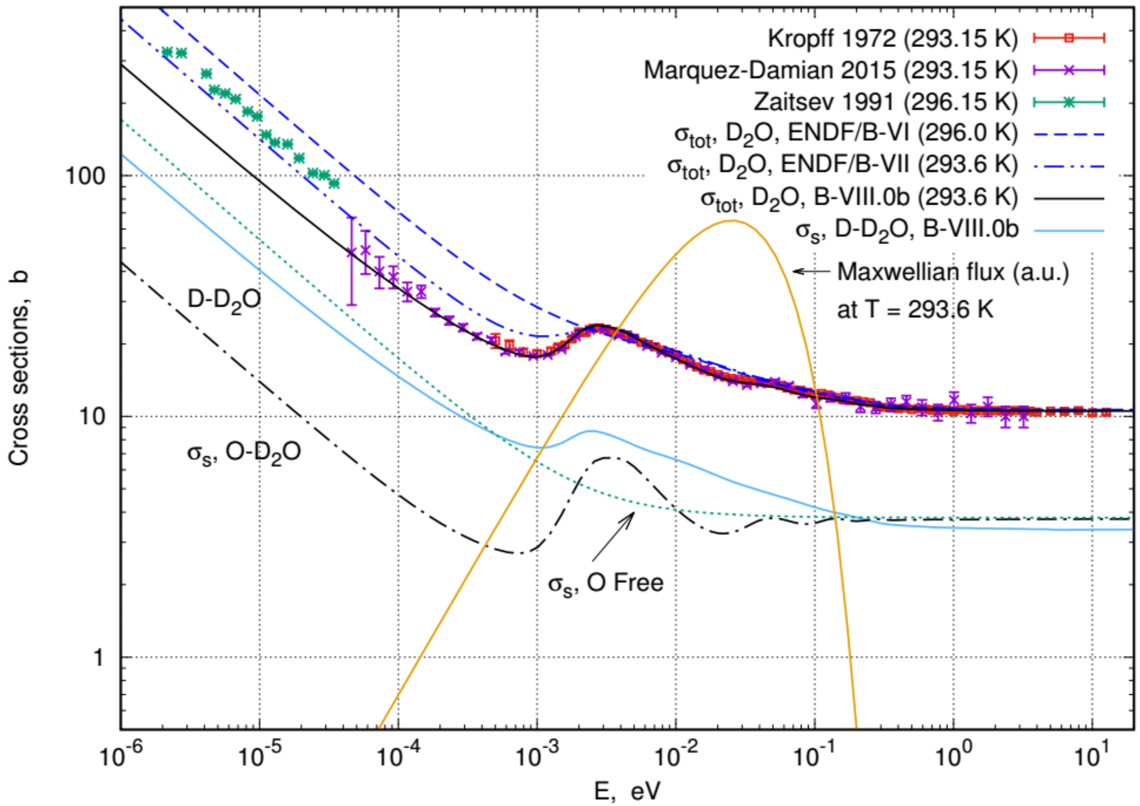
TSL for D_2O : $\sigma_{tot}(E; T)$



Power reactor applications: T ~ 550 – 600 K, p ~ 10 MPa (D_2O coolant).

New measurements underway : ?

TSL for D_2O : $\sigma_{tot}(E; T)$, T ~ 20°C

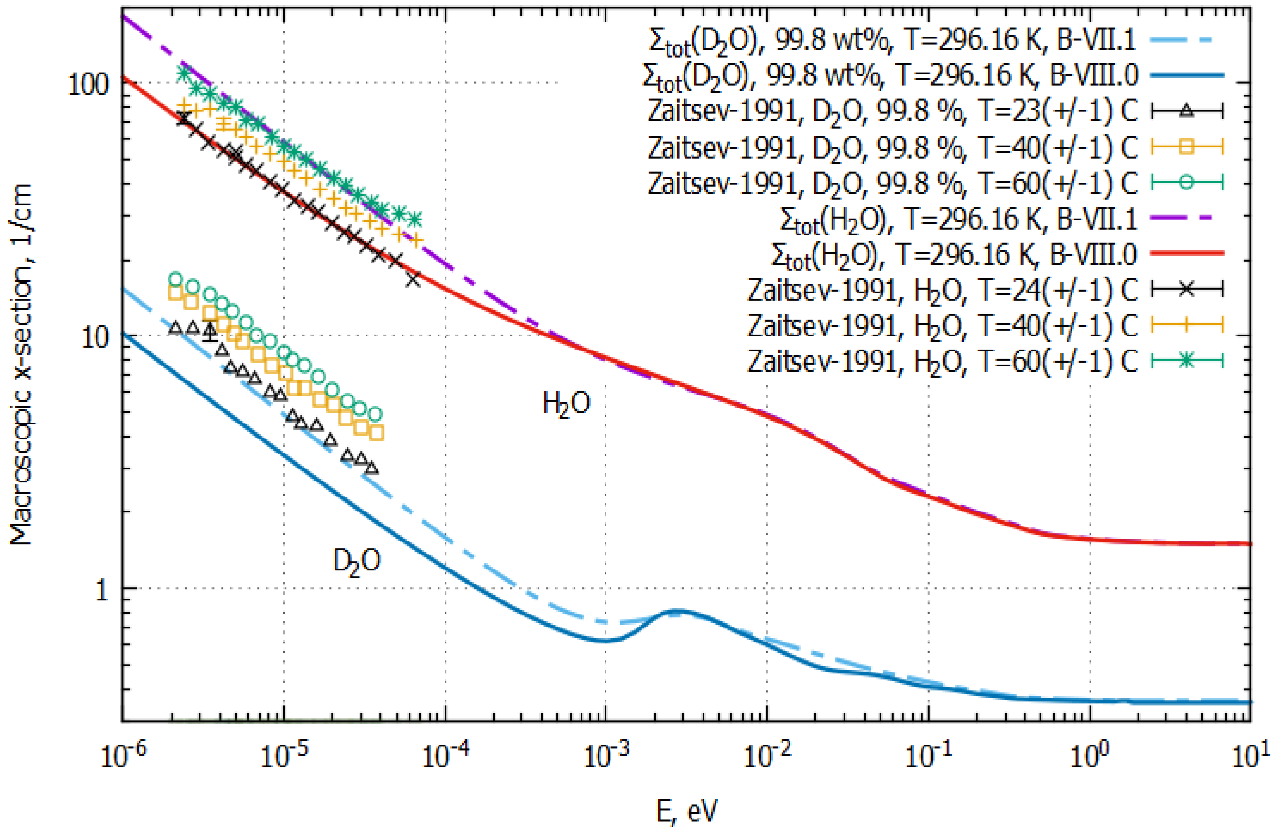


Room Temperature data:

For Zaitsev data set for D_2O (Zaitsev 1991), agreement with ENDF/B-VIII.0 is poor.

Model or data ?

TSL for D_2O : $\Sigma_{tot}(E; T)$



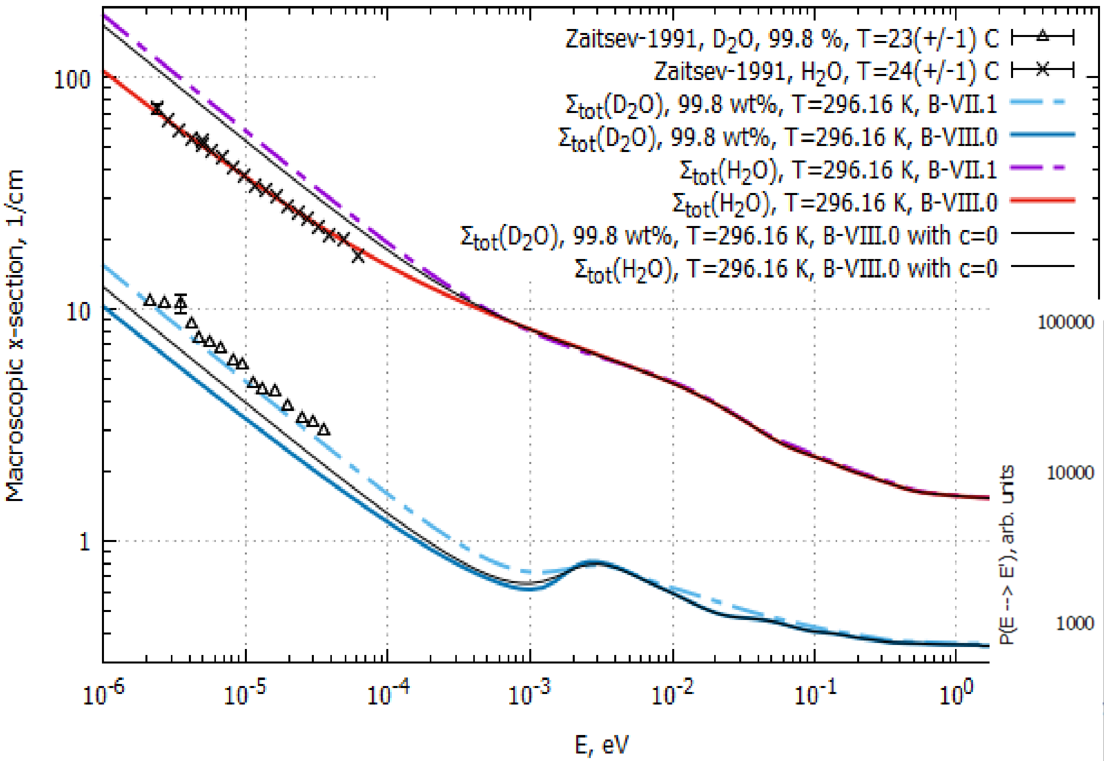
Zaitsev data for H_2O, D_2O, at 20 °C < T ≤ 60 °C

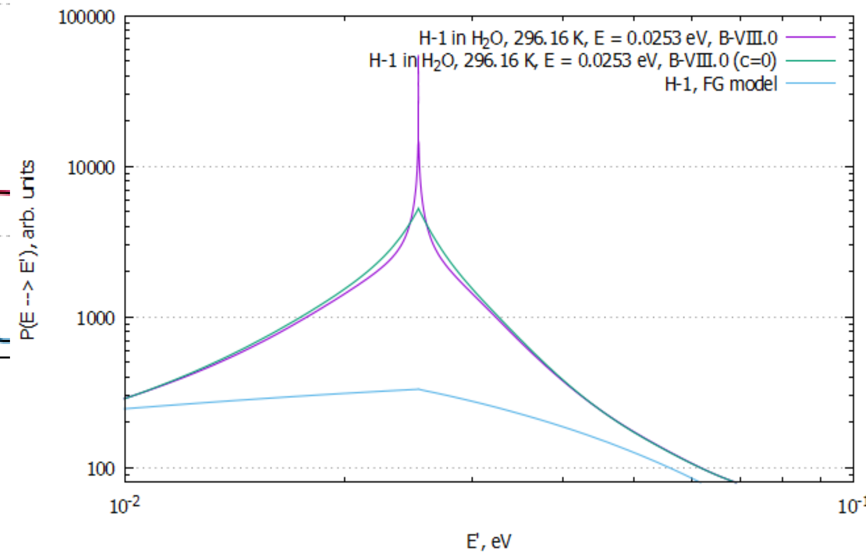
Zaitsev data for D_2O, purity 99.8%, in EXFOR (41622003) :

Σ_{tot} (in cm^{-1}, not ARB-UNITS) *vs.* λ (in MILLI-MU = nm ; 1 nm = 10 Å),

D_2O : 4 nm < λ < 20 nm → $2*10^{-6}$ eV < E < $5*10^{-5}$ eV

TSL for D_2O : $\Sigma_{tot}(E; T)$



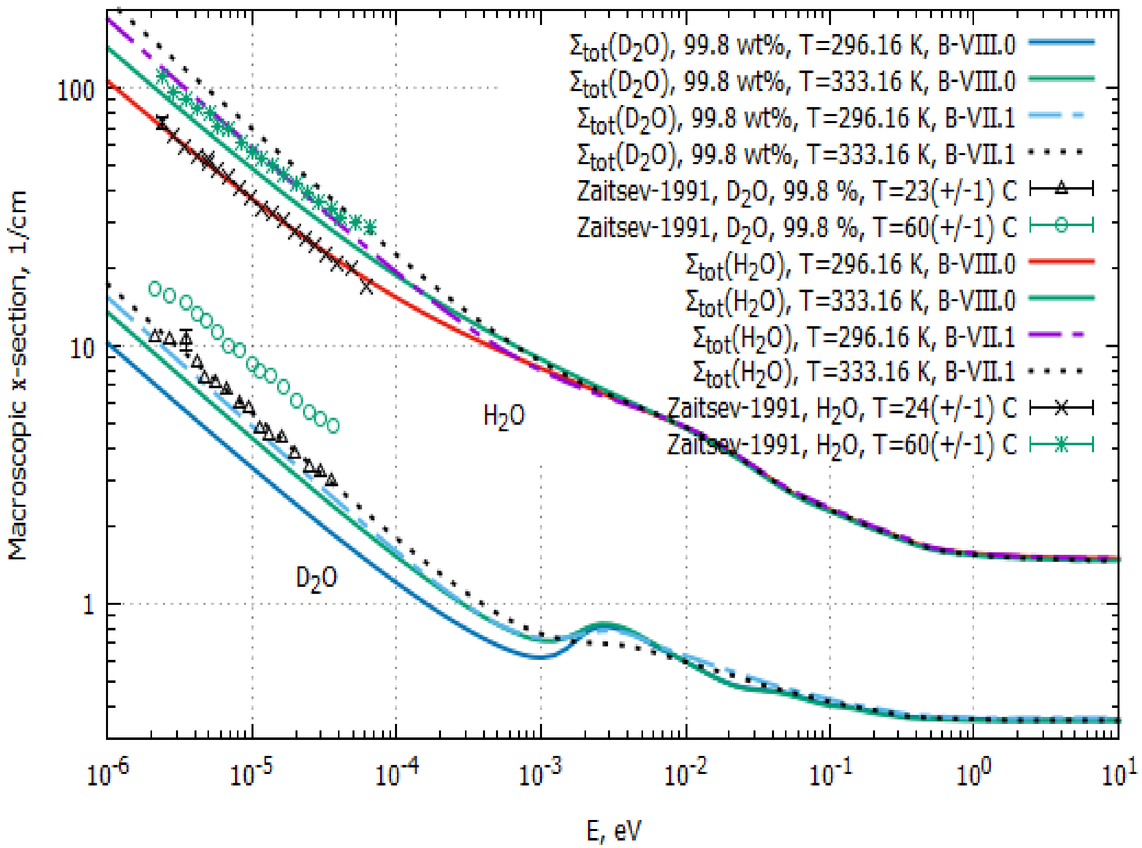


Zaitsev data for H_2O, D_2O, at T= 23 °C.

Test: *how* Σ_{tot} changes if Egelstaff diffusion model is **not** used (black lines); also compare $P(E \to E')$ *vs.* E' at $E = 0.0253$ eV; see figure on the right.

Here, c = 0 means: in leapr, we have card13 = twt, 0, tbeta .

TSL for D_2O : $\Sigma_{tot}(E; T)$

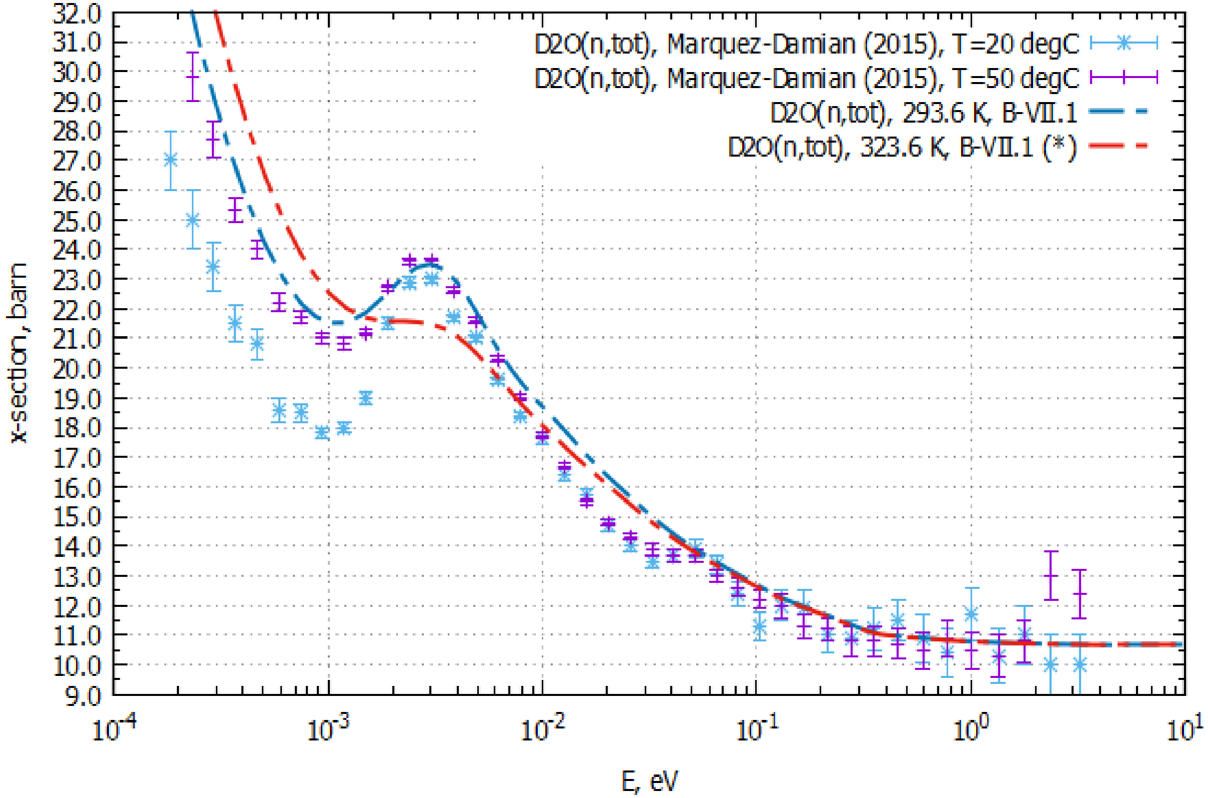


Zaitsev data for H_2O and D_2O, at 20 °C < T ≤ 60 °C

Zaitsev data for D_2O, at T > T-room : ?

(no **overlap** with other measurements ?)

TSL for D_2O : $\sigma_{tot}(E; T)$, T = 20 → 50 °C

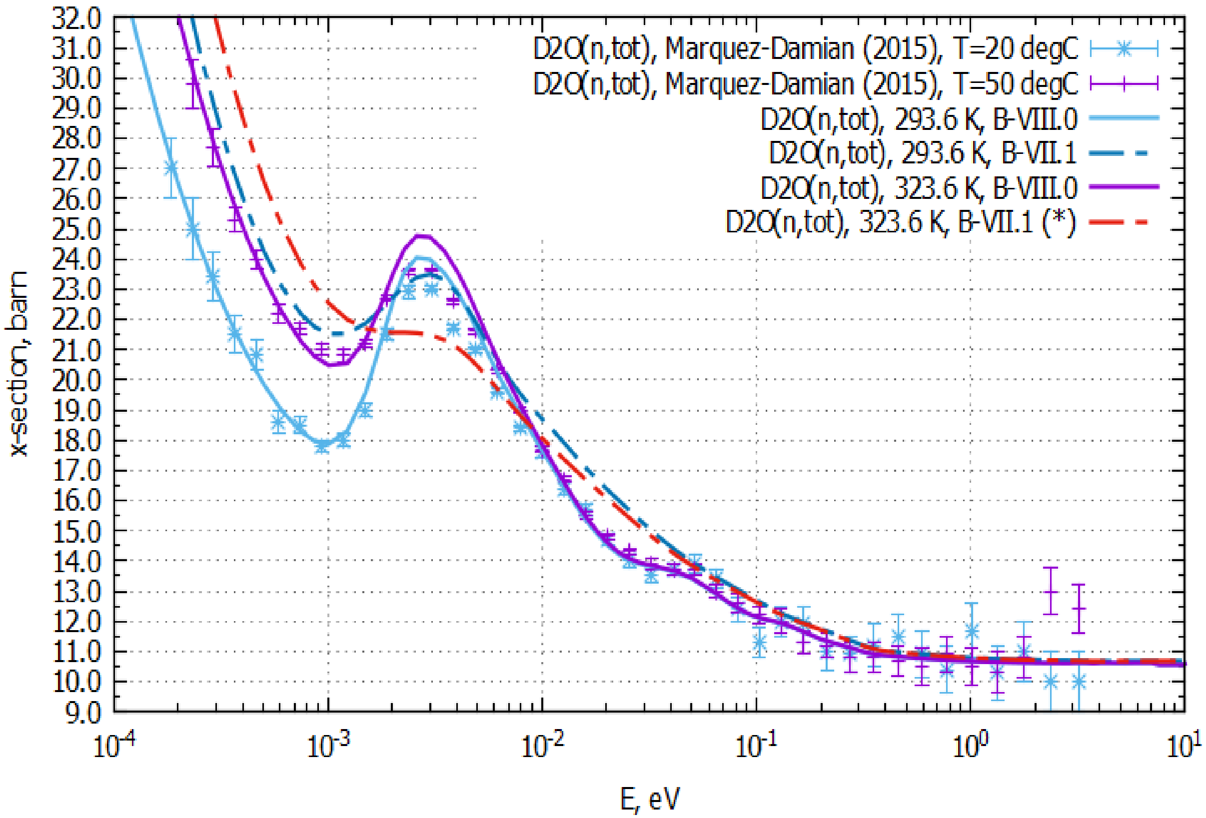


EXFOR: Marquez-Damian (2015), T = 20 and 50 °C,

Low Energy Neutron Source (LENS) at Indiana University,

http://www.indiana.edu/~lens/

TSL for D_2O : $\sigma_{tot}(E; T)$, T = 20 °C → 50 °C

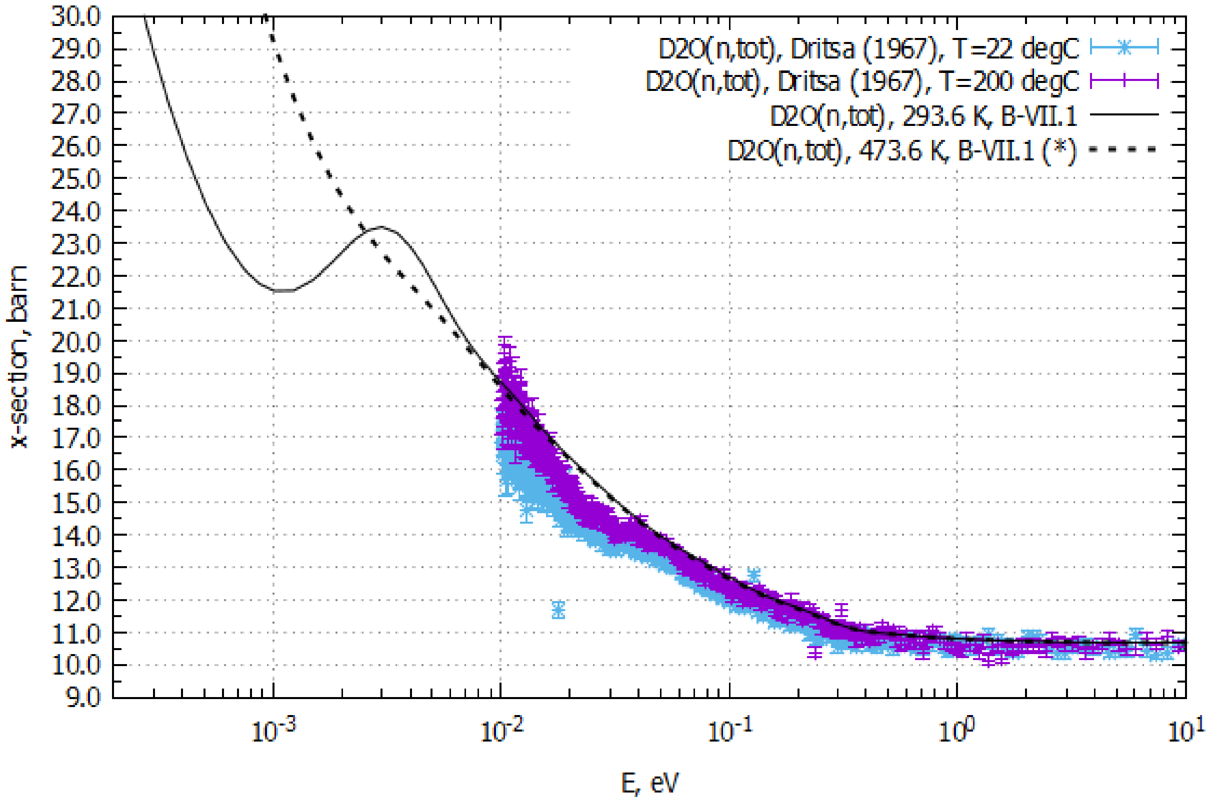


EXFOR: Marquez-Damian (2015);

TSL for D_2O in ENDF/B-VIII.0 = D-in-D_2O and O-in-D_2O (H-2 and O-16)

Model improvements → better agreement with data/measurements

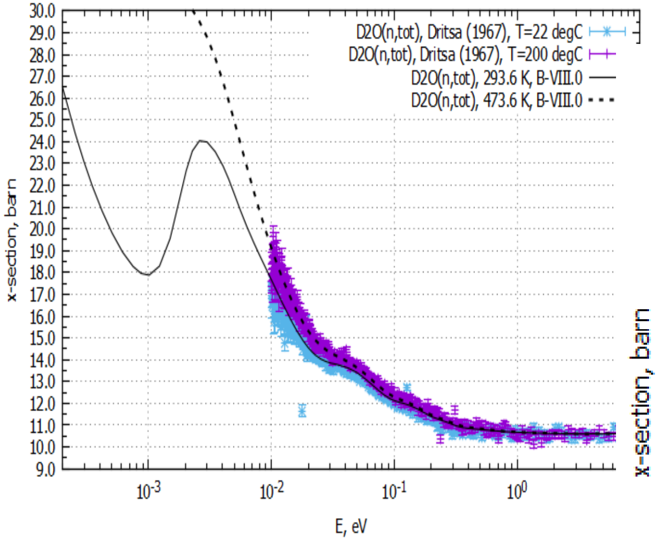
TSL for D_2O : $\sigma_{tot}(E; T)$, T = 22 °C → 200 °C

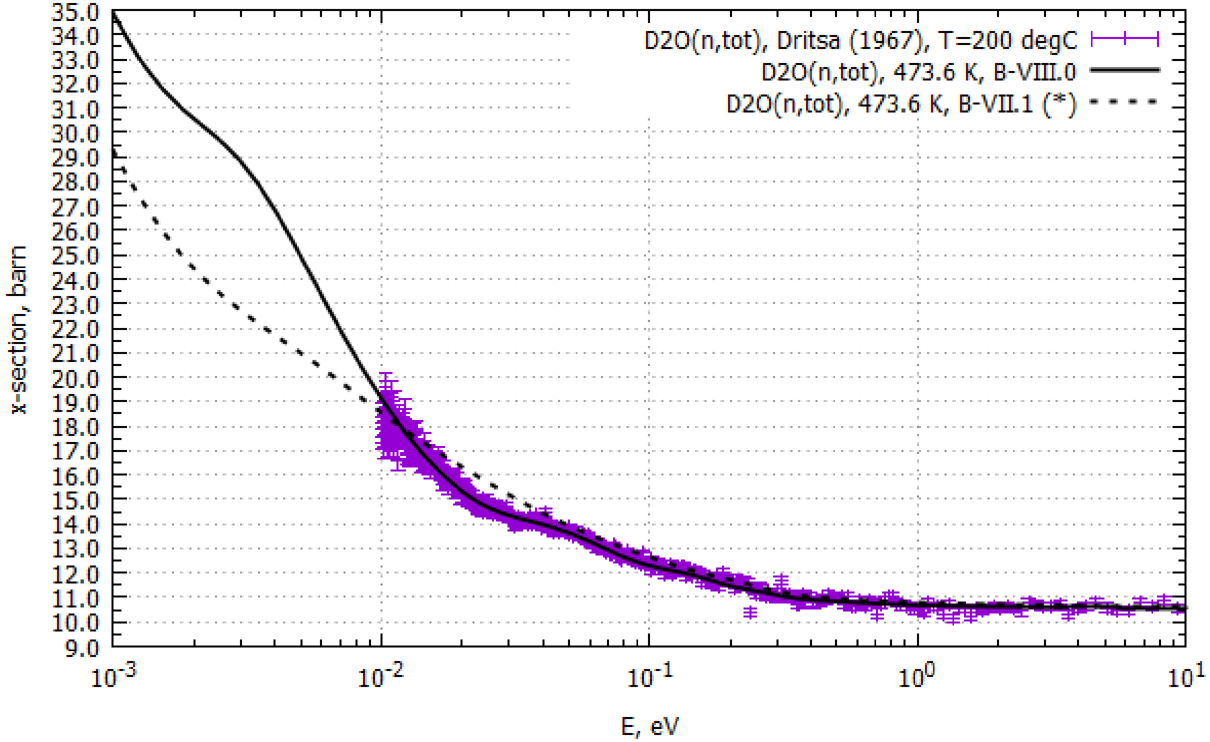


EXFOR: Dritsa (1967), T = 22 and 200 °C;

TSL for D_2O in ENDF/B-VII.0 = D-in-D_2O and O is free gas model at T

TSL for D_2O : $\sigma_{tot}(E; T)$, T = 22 °C → 200 °C



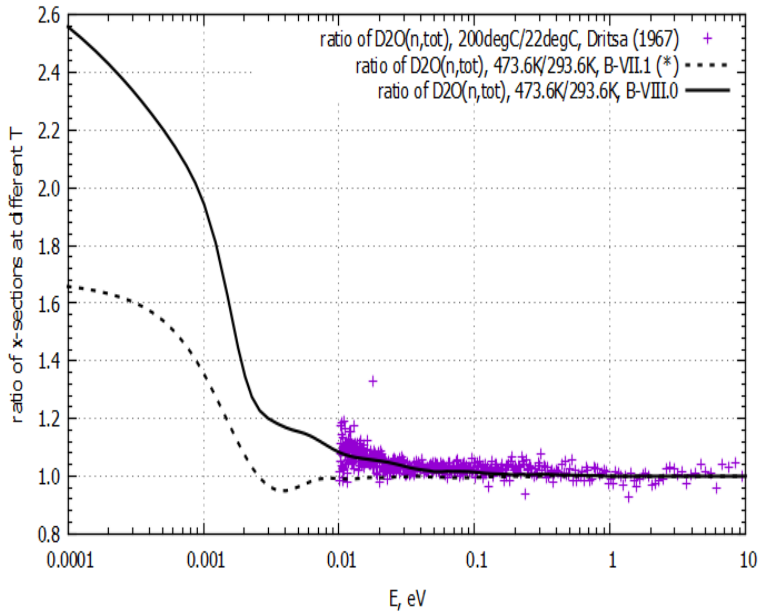


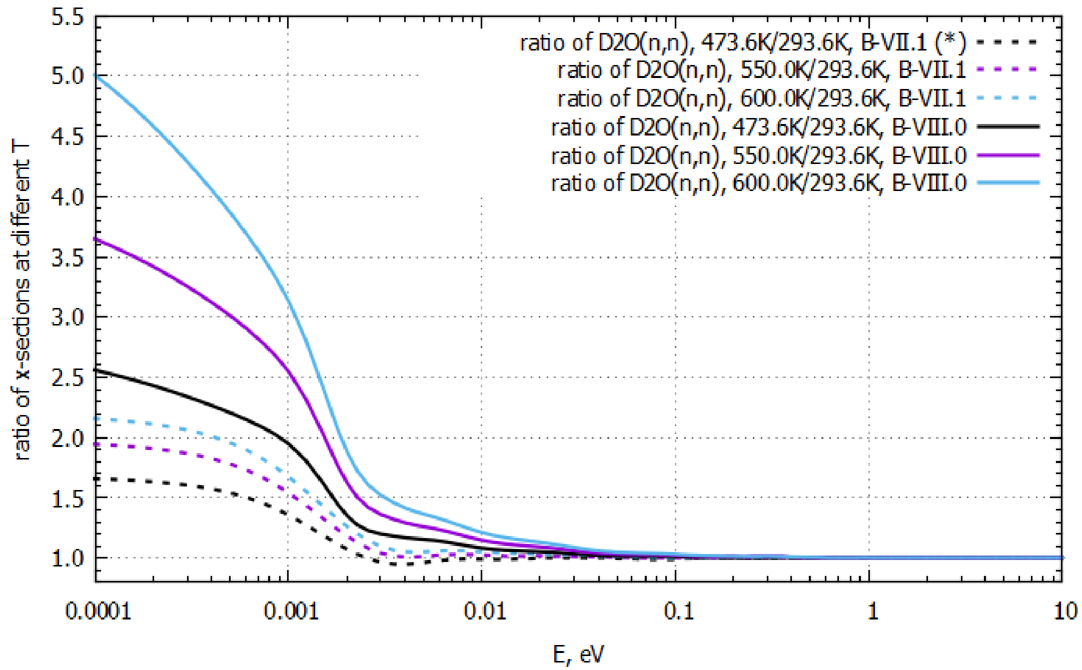
EXFOR: Dritsa (1967), T = 22 and 200 °C;

(D_2O: NEW measurements at high T , high p ?)

TSL for D_2O in **ENDF/B-VIII.0** = D-in-D_2O and O-in-D_2O, better agreement with Dritsa-1967 (200 °C) than ENDF/B-VII.0.

TSL for D_2O : ratio of $\sigma_{tot}(E; T)$





NEW measurements at high T ?

TSL for D_2O in ENDF/B-VIII.0 = D-in-D_2O and O-in-D_2O at the following T :

…, 523.6 K, 550.0 K, 573.6 K, 600.0 K, 623.6 K, …

V&V : ND-2019

LANL ACE Files based on ENDF/B-VIII.0

LANL **thermal** ace files, **ENDF80SaB.pdf (2018) reads :**

ENDF/B VIII.0 tsl files	B(1) total xs	B(6) Mo	THERMR natom
tsl-OinD2O.endf	7.5878	2	2

Actually, for O-in-D_2O, option "B(1) = σ_{free} = 3.794 b and B(6)=1 in MF7, MT4" with **natom = 1** in thermr [card2, natom] work as well (see slide 11).

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Discussion:

how to **choose cut-off E** (in eV) in

thermr [card4, emax] and **acer** [card8, emax] to generate thermal ace files for UO_2 (U-in-UO_2 and O-in-UO_2) with NJOY for MCNP / SERPENT .

For UO_2, the main scatterers are U-238 (U-in-UO_2) and O-16 (O-in-UO_2).

ENDF80SaB.pdf (2018) reads: emax (u-uo2) = 5.0 eV, emax (o-uo2) = 5.0 eV

TSL → ACE for materials with U (UO_2, UN, …): be careful and check the result …

LANL ACE Files based on ENDF/B-VIII.0

tsl-UinUO2.endf :

…

```
1.480000+2 2.360058+2          0          1                    0          0          48 7  4
0.000000+0 0.000000+0          0          0                    6          0          48 7  4
9.283302+0 1.976285+2 2.360058+2 5.000001+0 0.000000+0 1.000000+0  48 7  4    [ B(1) B(2) B(3) …]
```

…

For U-in-UO_2, B(2) = 197.628 (dimensionless), B(4) = 5.0 eV [MF7, MT4 of mat=48]

This is β_{max} (= B(2)) → E* (= B(4)). MF7, MT4 was generated by NJOY. Therefore, see

leapr , **subroutine endout** :

…

!--write inelastic part

…

scr(7) = npr∗spr *! This is B(1) = natom ∗* σ_{free}

scr(8) = beta(nbeta) *! This is B(2) =* β_{max}

scr(10) = sigfig(therm ∗ beta(nbeta), 7, 0) *! This is B(4) = 0.0253 ∗* β_{max}

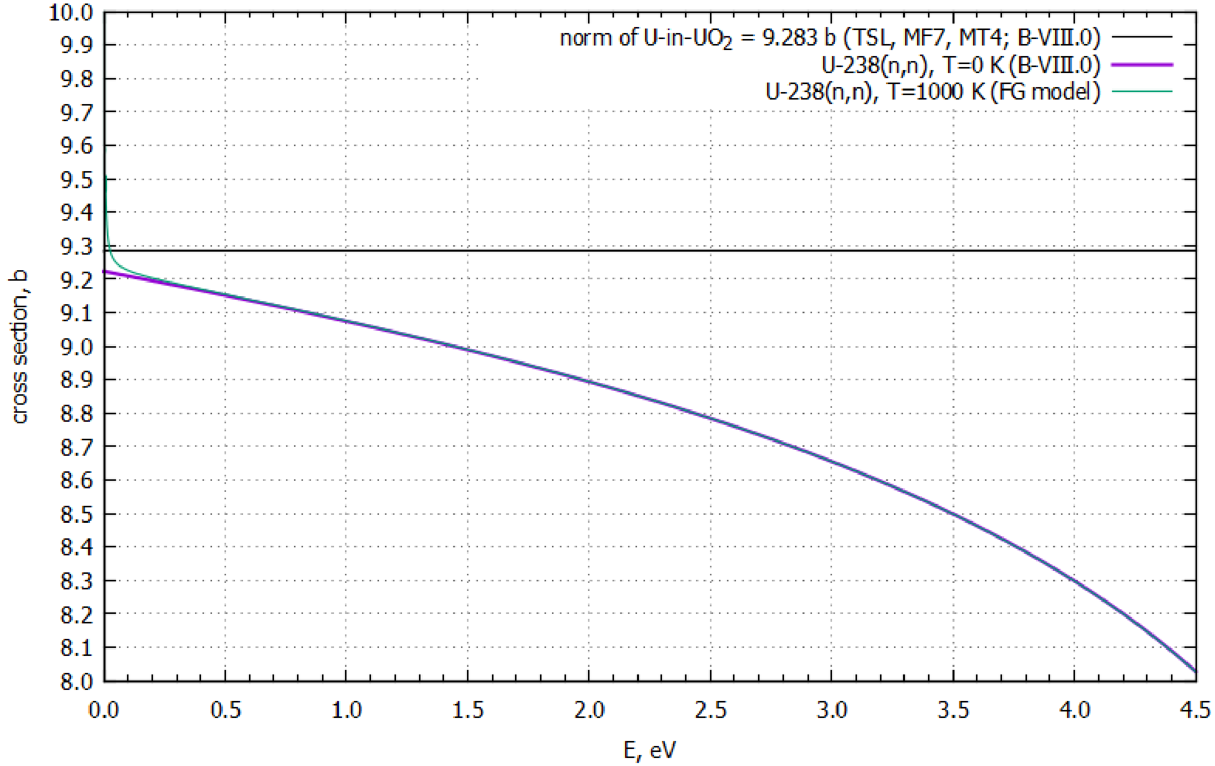
…

Although the current ENDF-6 **Manual** interprets B(4) as "upper limit for constant σ_{free}" (see pp. 161,162), **subroutine endout** assigns it as B(4) = 0.0253 ∗ β_{max} eV.

For example, for Al-met, B(2)= 90 & B(4) = 2.277 eV (< 5.0 eV) ;

for H-H_2O, B(2)= 395.26 & B(4) = 10.0 eV (> 5.0 eV) .

cut-off *E*: from TSL of UO_2 to thermal ACE files (1)



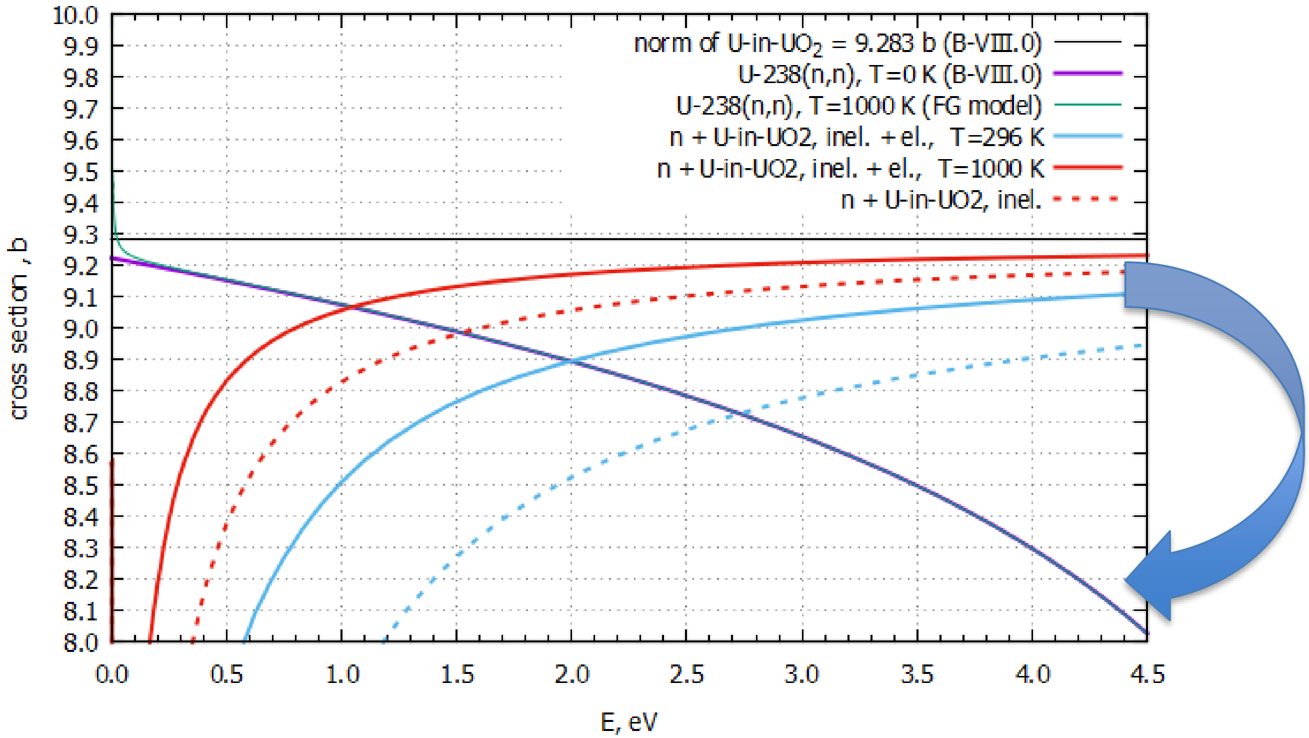
ENDF/B-VIII.0, U-238

Plot $\sigma_s(E)$ for U-238(n,n) at T = 0 K, and, say, T = 1000 K (T_{max} = 1200 K for UO_2 TSL), and $B(1) = \sigma_{free}$ from MF7, MT4 (natom = 1 for U-in-UO_2).

NOTE: use lin-lin scale ;

$\sigma_s(E) \rightarrow 9.224$ b as $E \rightarrow 0$ (T = 0 K) ; σ_{free} = 9.238 b .

cut-off *E*: from TSL of UO_2 to thermal ACE (2)



Plot $\sigma_s(E)$ for **U-238**(n,n) at T = 0 K, and, say, T = 1000 K (T_{max} = 1200 K for UO_2 TSL),

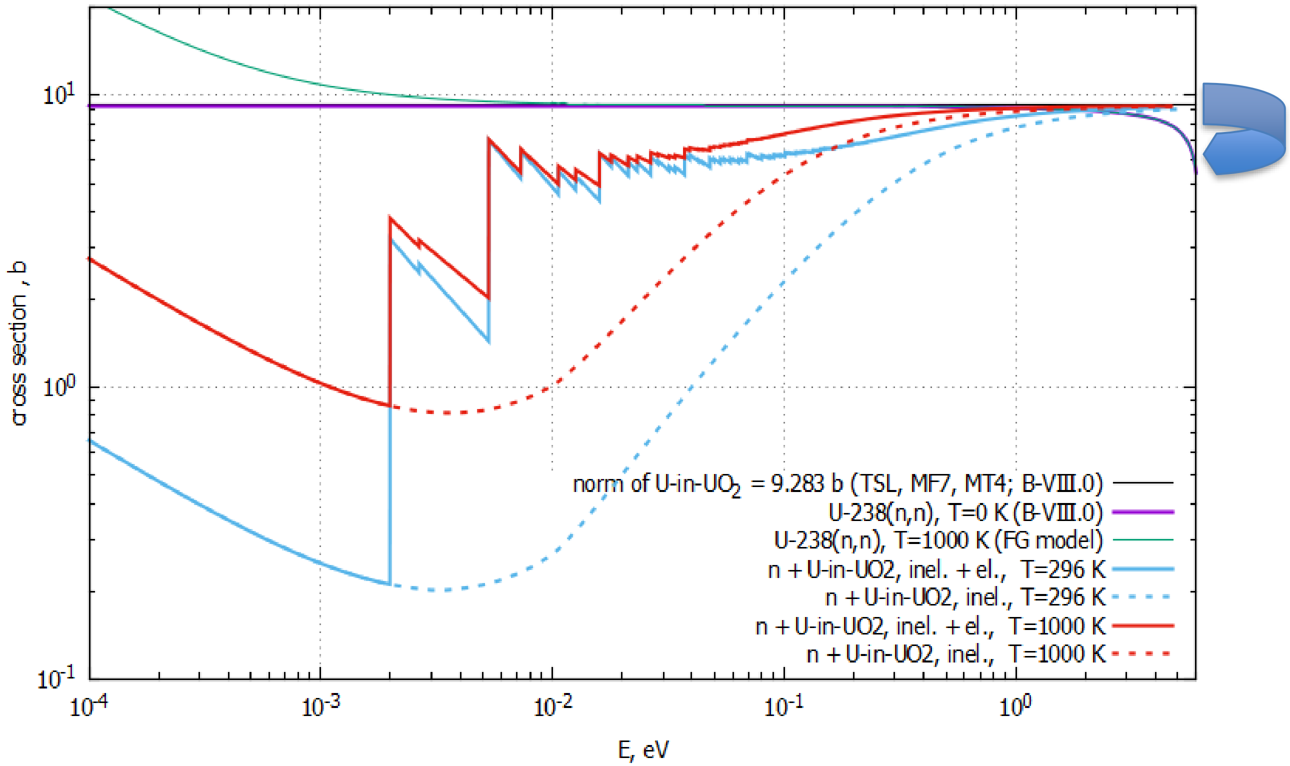
and B(1) = σ_{free} from MF7, MT4 (natom = 1 for U-in-UO_2);

Add thermal scattering cross sections, n + **U-in-UO_2** : σ_{inel} (E;T) + σ_{el} (E; T), ENDF/B-VIII.0.

If E (cut-off) ~ 4.0 eV, mismatch between σ_s (E; T) fee-gas and σ_{inel} (E;T) + σ_{el} (E; T) : ~ 10 % .

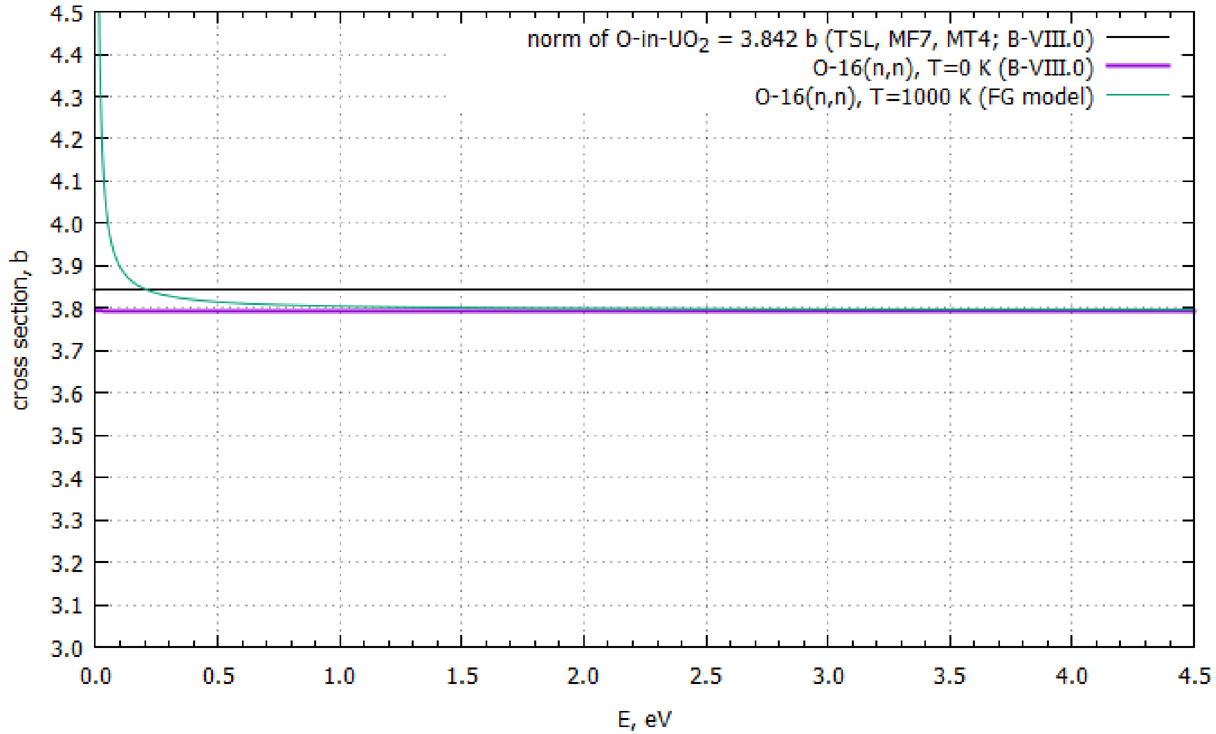
(acceptable ?)

cut-off *E*: from TSL of UO_2 to thermal ACE (3)



Plot $\sigma_s(E)$ for **U-238**(n,n) at T = 0 K, and, say, T = 1000 K (T_{max} = 1200 K for UO_2 TSL),
and $B(1) = \sigma_{free}$ from MF7, MT4 (natom = 1 for U-in-UO_2);
add thermal scattering cross sections, n + **U-in-UO_2**, σ_{inel} (E;T) + σ_{el} (E; T), ENDF/B-VIII.0.
Here, we use log – log scale (otherwise the same data sets are shown in slide 23), E < 5 - 6 eV .
So, for **U-in-UO_2**, E (cut-off) ~ 2.0 eV (?)

cut-off *E*: from TSL of UO_2 to thermal ACE (4)



ENDF/B-VIII.0, O-16

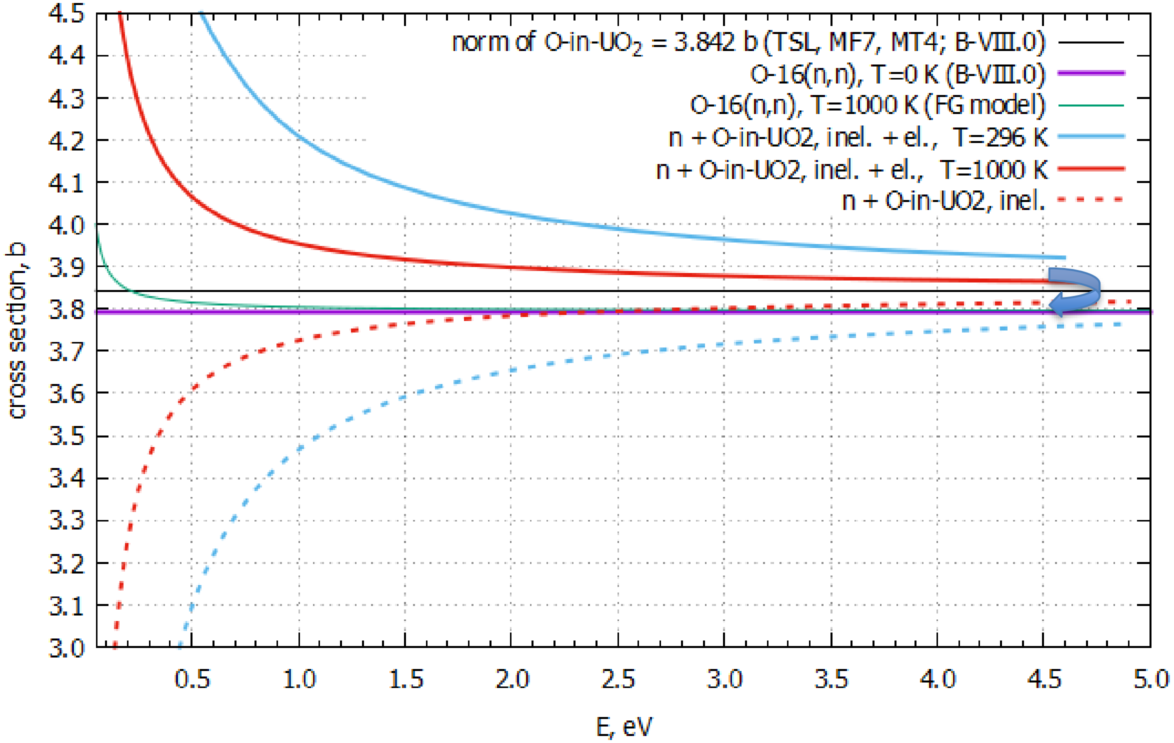
Plot $\sigma_s(E)$ for **O-16**(n,n) at T = 0 K, and, say, T = 1000 K (T_{max} = 1200 K for UO_2 TSL),

and B(1) = σ_{free} from MF7, MT4 (natom = 1 for O-in-UO_2).

$\sigma_s(E) \rightarrow$ 3.794 b as $E \rightarrow 0$ (T = 0 K) ; σ_{free} = 3.842 b .

Then, add thermal scattering cross sections, n + **O-in-UO_2** : σ_{inel} (E;T) + σ_{el} (E; T), ENDF/B-VIII.0;

cut-off *E*: from TSL of UO_2 to thermal ACE (5)



Plot $\sigma_s(E)$ for **O-16**(n,n) at T = 0 K, and, say, T = 1000 K (T_{max} = 1200 K for UO_2 TSL),

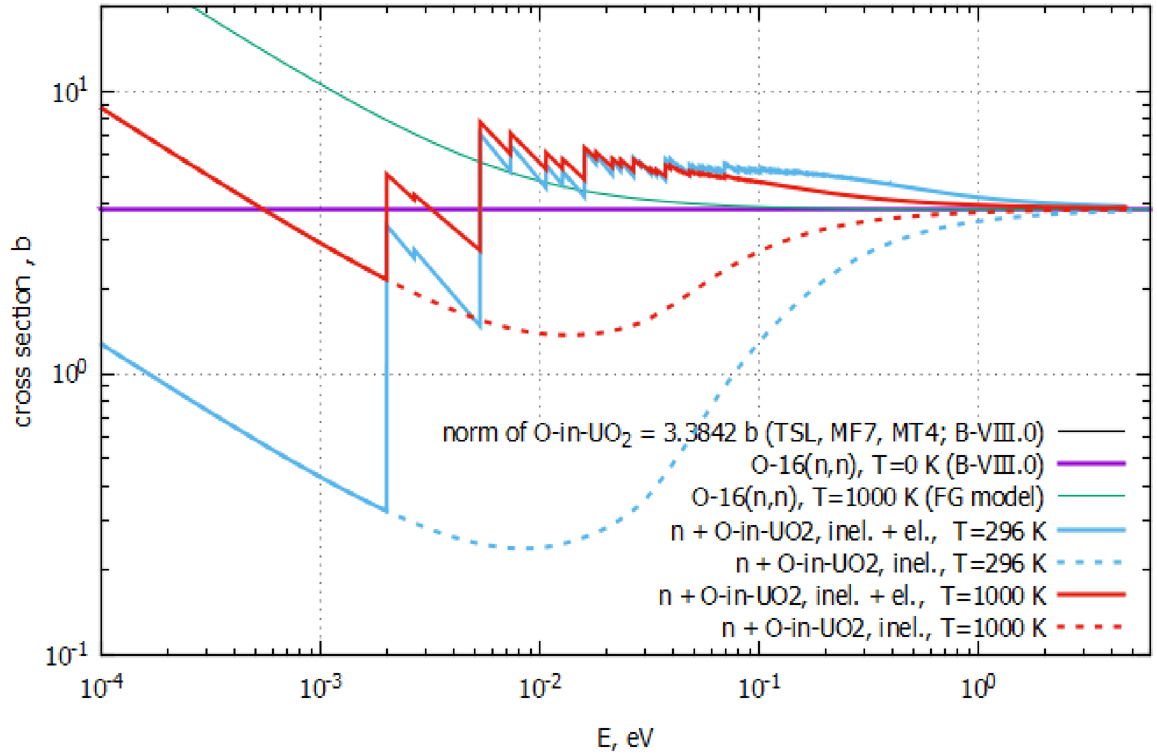
and B(1) = σ_{free} from MF7, MT4 (natom = 1 for O-in-UO_2);

added thermal scattering cross sections, n + **O-in-UO_2**, σ_{inel} (E;T) + σ_{el} (E; T), ENDF/B-VIII.0;

If E (cut-off) ~ 4 - 5 eV, mismatch between σ_s (E; T) fee-gas and σ_{inel} (E;T) + σ_{el} (E; T) : ~ 2-4 %

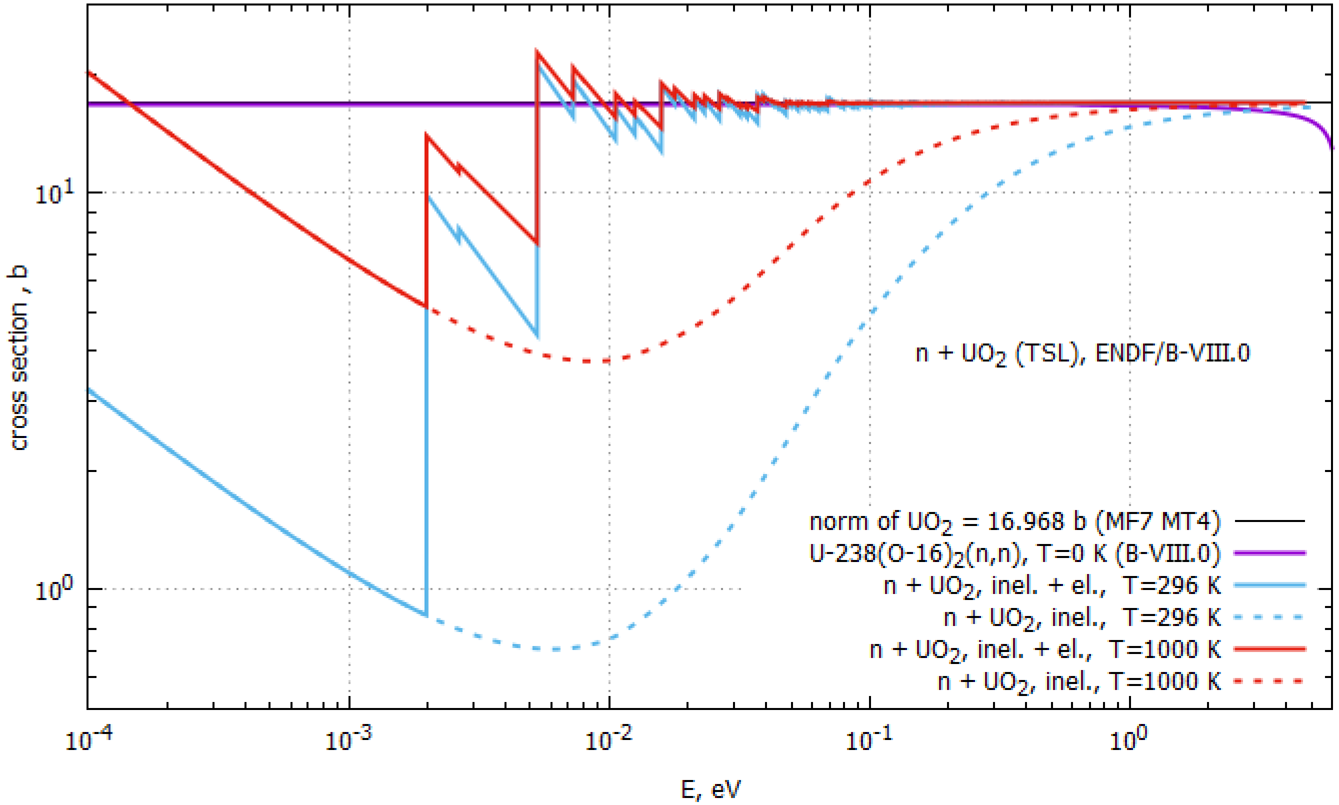
(acceptable ?)

cut-off *E*: from TSL of UO_2 to thermal ACE (6)



Plot $\sigma_s(E)$ for O-16(n,n) at T = 0 K, and, say, T = 1000 K (T_{max} = 1200 K for UO_2 TSL),
and B(1) = σ_{free} from MF7, MT4 (natom = 1 for O-in-UO_2).
Add thermal scattering cross sections, n + **O-in-UO_2**, σ_{inel} (E;T) + σ_{el} (E; T), **ENDF/B-VIII.0.**
If E (cut-off) ~ 4.5 eV, mismatch between σ_s (E; T) fee-gas and σ_{inel} (E;T) + σ_{el} (E; T) : ~ 2-4 %;
it can not be seen in log-log scale.

TSL of UO_2, ENDF/B-VIII.0 (1)



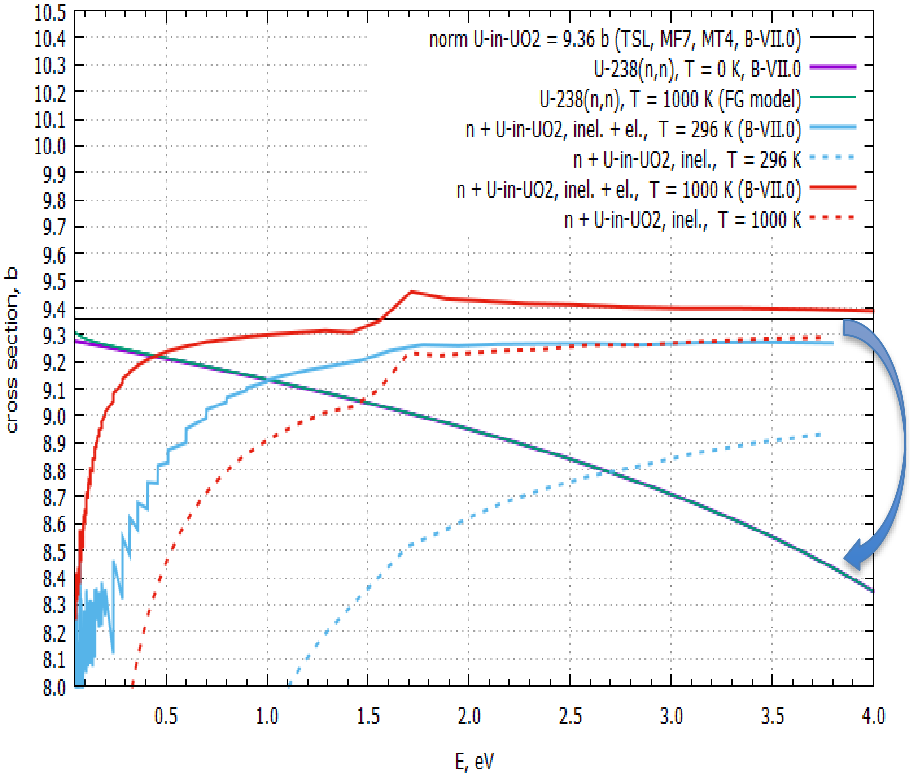
Now we can discuss applications of TSL model, *e.g.*, V&V (benchmarking, *etc.*).

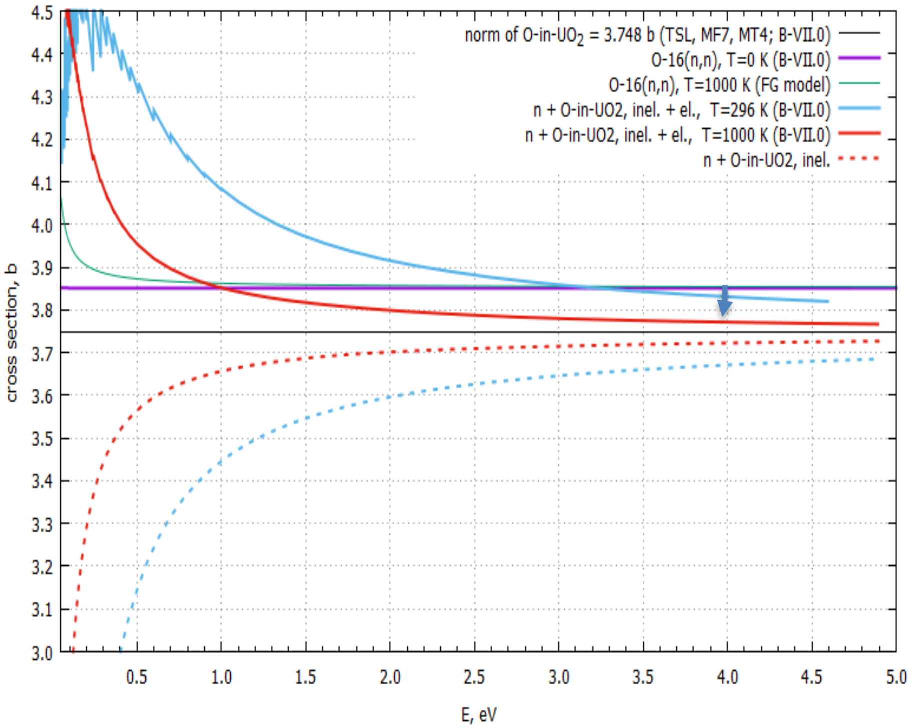
Note: one can add U and O into UO_2 (*i.e.*, use normalization per UO_2).

Then, we have some physical meaning of σ_{el} (E; T) for UO_2.

Work in progress …

cut-off *E*: from TSL of UO_2 to thermal ACE (7)





To compare performance of UO_2 TSL, **ENDF/B-VIII.0** *vs.* ENDF/B-VII, (MCNP/SEREPNT), first, consistency check for TSL → ACE processing options with NJOY (NJOY2016).

ENDF/B-VII : if E(cut-off) ~ 4 eV for U-238-in-UO2, mismatch ~ 10% (acceptable ?) ;
if E(cut-off) ~ 4 eV for O-16-in-UO2, mismatch <~ 1% (acceptable ?) .

New ND library for MCNP5 / SERPENT

We converted ENDF/B-VIII.0 library created by LANL for MCNP6,
https://nucleardata.lanl.gov
for MCNP5 and SERPENT applications.

ACE files created by LANL are for MCNP6 applications.
LANL **fast** ace files are in ACE-2 format (see ace file headers; we converted them to ACE).
LANL **thermal** ace files were generated with **iwt=2** option (NJOY, acer, card9);
we re-created (most important) thermal ace files with iwt=0 (default iwt),

and LANL/CNL library nodes are

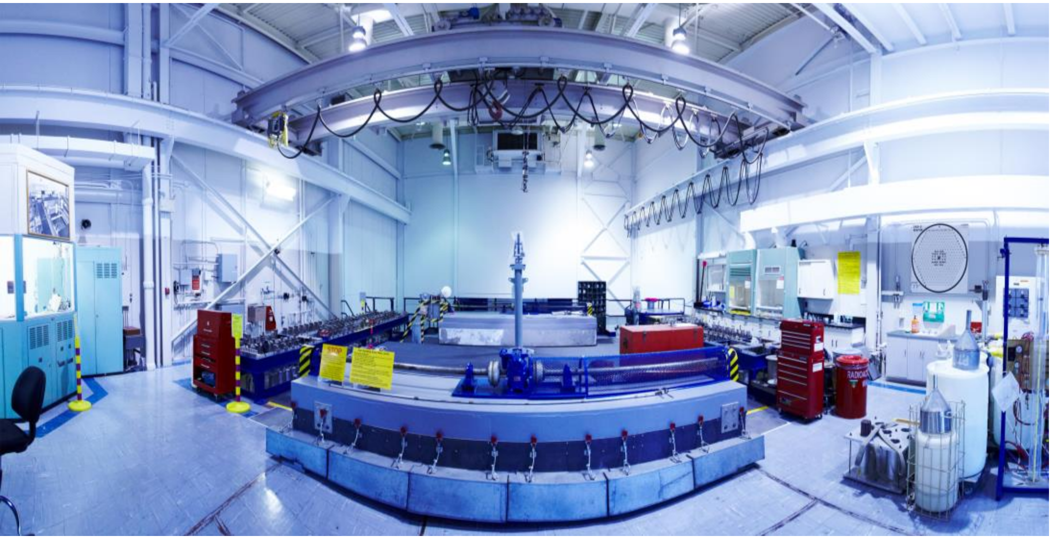
*.01c T = 0.1 K
*.02c T = 250.0 K
*.03c T = 293.6 K
*.06c T = 600.0 K
*.09c T = 900.0 K
*.12c T = 1200.0 K
*.25c T = 2500.0 K

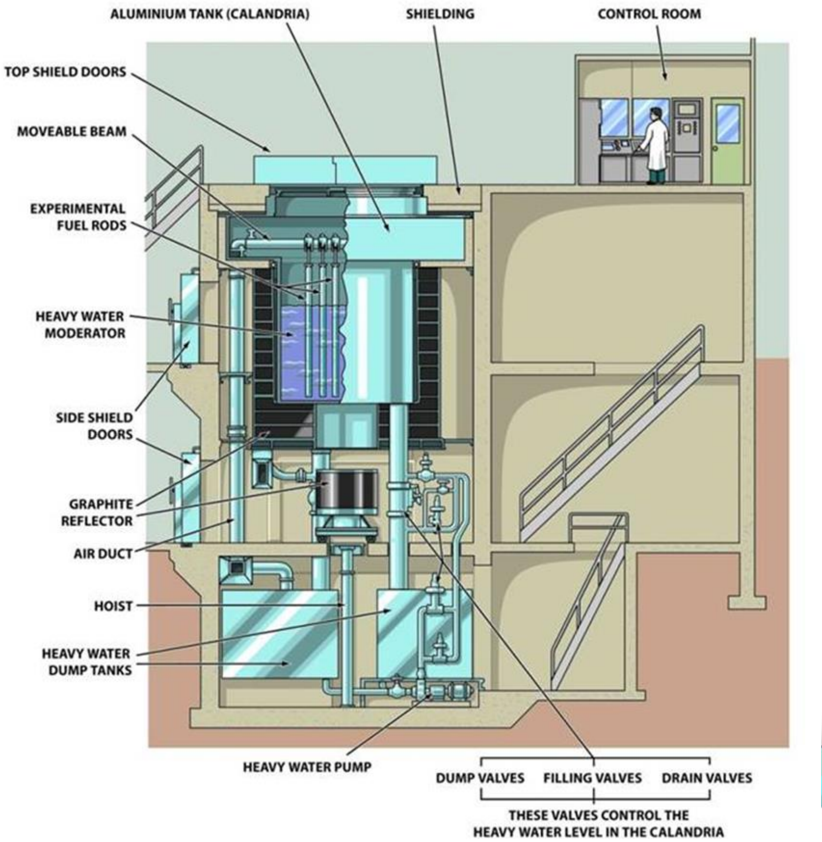
SERPENT

set acelib "/scratch/lib80xs/e80ace.xsdata"
set declib "/scratch/lib80xs/sss_endfb80.dec"
set nfylib "/scratch/lib80xs/sss_endfb80.nfy"
set sfylib "/scratch/lib80xs/sss_endfb80.sfy"

http://serpent.vtt.fi/mediawiki/index.php/Input_syntax_manual

ZED-2 reactor in CRL: experiments and modeling to be continued





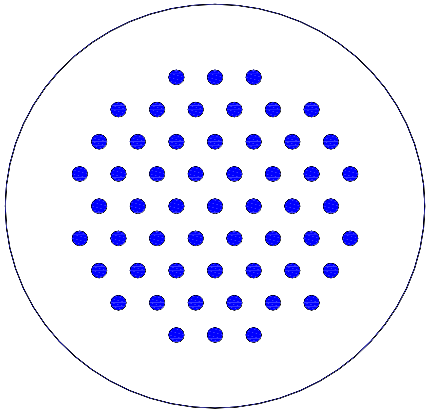
First criticality: 7 September 1960

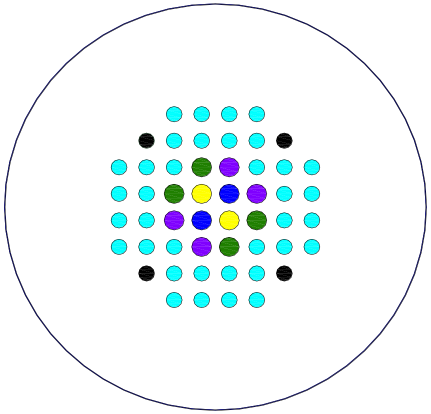
Tank type:
reactor control via moderator (D_2O) level

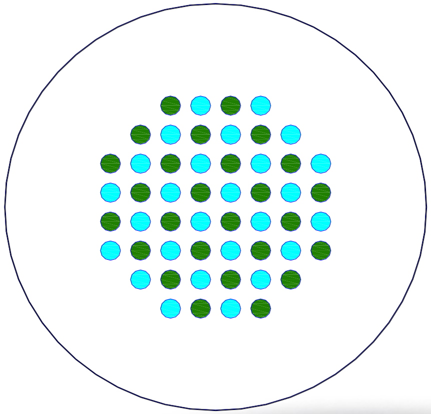
Integral part of the reactor physics design of **all Canadian power reactors**

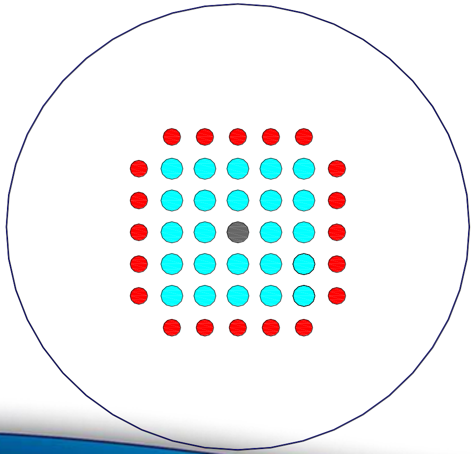
ZED-2 reactor in CRL: 2521 cores built

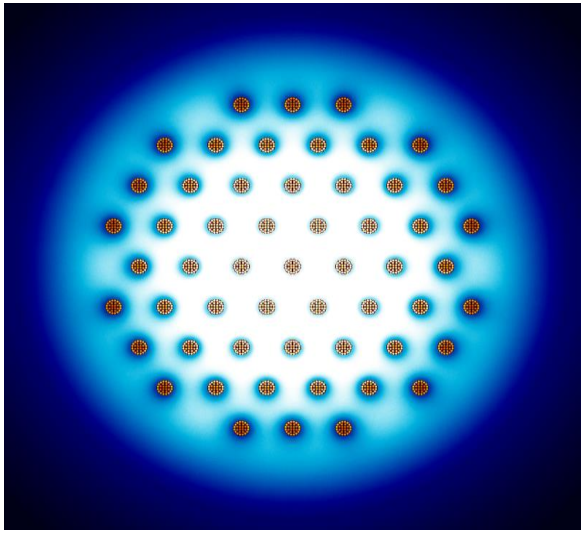
Fuel Lattices

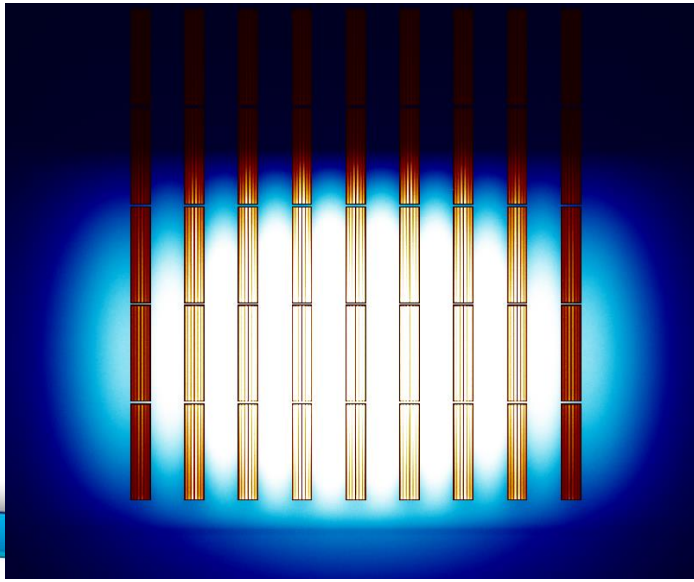












ZED-2 capabilities for benchmarking

In summary, ZED-2 measures critical configurations using its

- Large test region (3.36 m in diameter, 3.35 m in height)
- Variable lattice pitch (from 20 to 40 cm)
- Variable driver fuel
- Zero power (up to ~ 200 W (thermal))
  - negligible activation

Practically, this lets us

- Measure reactor physics phenomena (*e.g.*, fuel/coolant temperature coefficient of reactivity, absorber worth, kinetics parameters)
- Validate reactor physics codes (MCNP, KENO, SERPENT, …)
- **Validate nuclear data, including TSL at different T .**

Conclusion

New measurements of TSL for H_2O, D_2O at different T :
progress with H_2O,
but more effort is necessary, especially in high (T, p) domain +
EXFOR entries ?

Left for future studies:

- **high-temperature benchmarks sensitive to TSL (H_2O, D_2O, …)**
- **selection of and studying ZED-2 high-temperature configurations to be analysed with ENDF/B-VIII, JEFF, etc.;**
- **MCNP and SERPENT : consistent models for ZED-2 benchmarks using ZED2MCNP and ZED2Serpent generator**

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