R&D in Nuclear Data for Reactor Physics Applications in CNL (CNL = Canadian Nuclear Laboratories)

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Improvement of TSL (Thermal Scattering *Laws*, or $S(\alpha, \beta)$ data)
New Evaluations for D_2O, H_2O, UO_2, ThO_2, …
New Models, Measurements, and Testing (Benchmarking)

D. Roubtsov, J.C. Chow, G. Bentoumi, Gang Li

Retired: K. Kozier, D. Altiparmakov, B. Wilkin, ...

Nuclear Science Division, CNL, Chalk River, Canada

From AECL to CNL

AECL is divided into:

- **CANDU Inc. (← Toronto Reactor division of old AECL)**
- **CNL (← Chalk River Labs of old AECL)**
- **AECL (or R-AECL)**

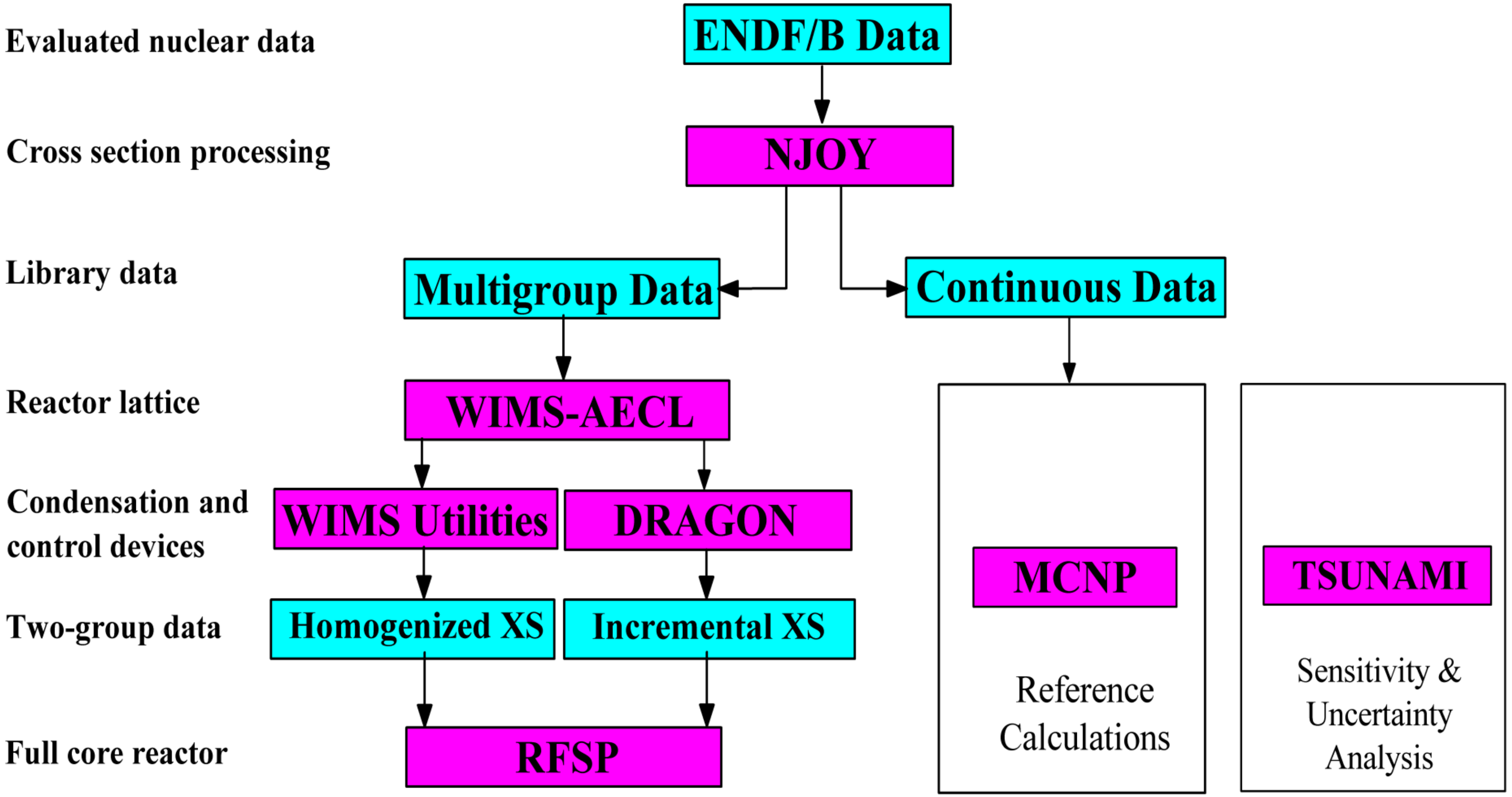
CNL will be managed following Canadian GoCo model (*GoCo* = Government-owned, Contractor-operated)

http://www.cnl.ca/en/home/about/Restructuring/default.aspx

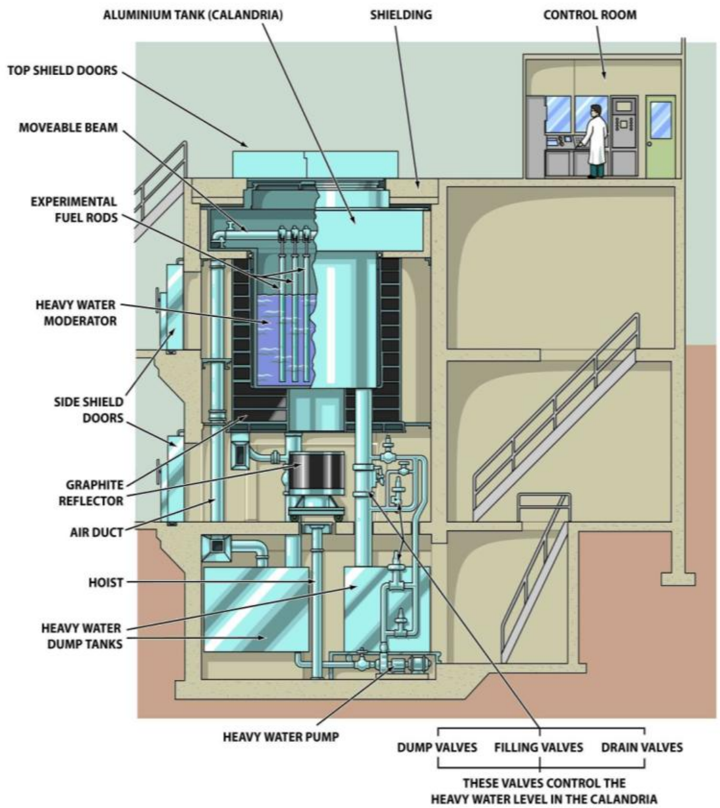
"*Restructuring of AECL's Nuclear Laboratories*"

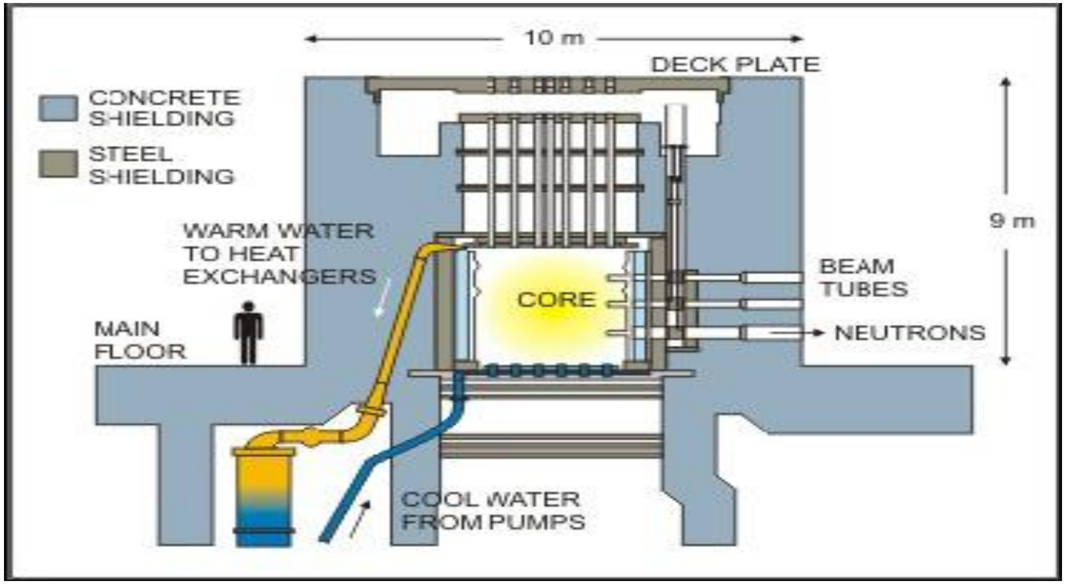
http://www.cnl.ca/en/home/about/Restructuring/NRU_decision.aspx

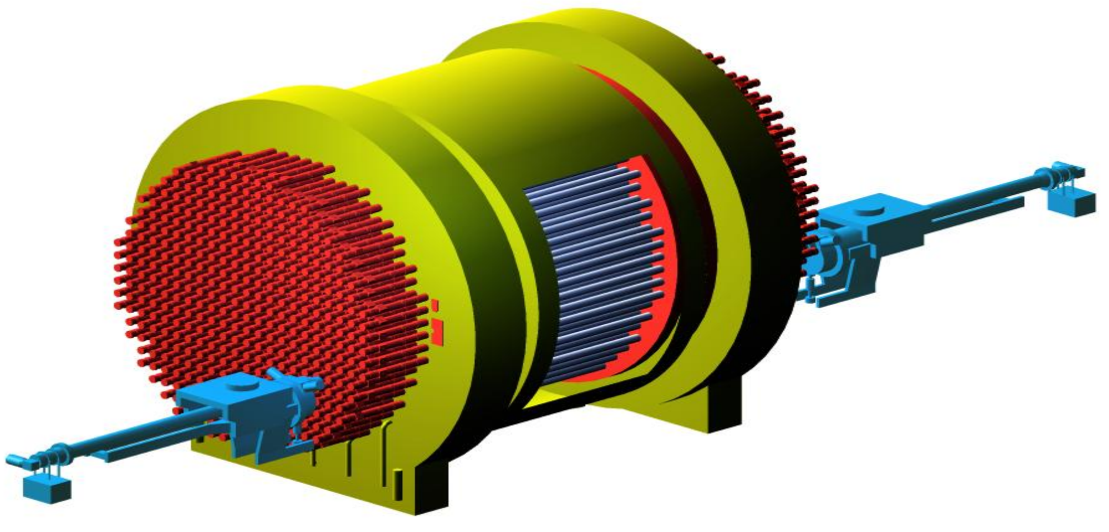
CNL (AECL) Reactor Physics Computational Scheme



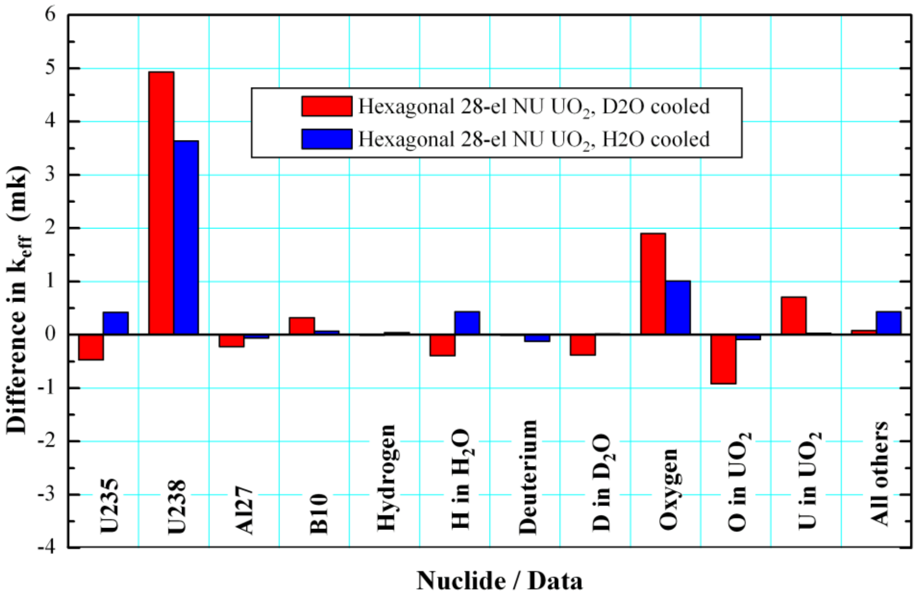
CNL libraries applied for ZED-2, NRU (Chalk River) and CANDU-type PHWRs

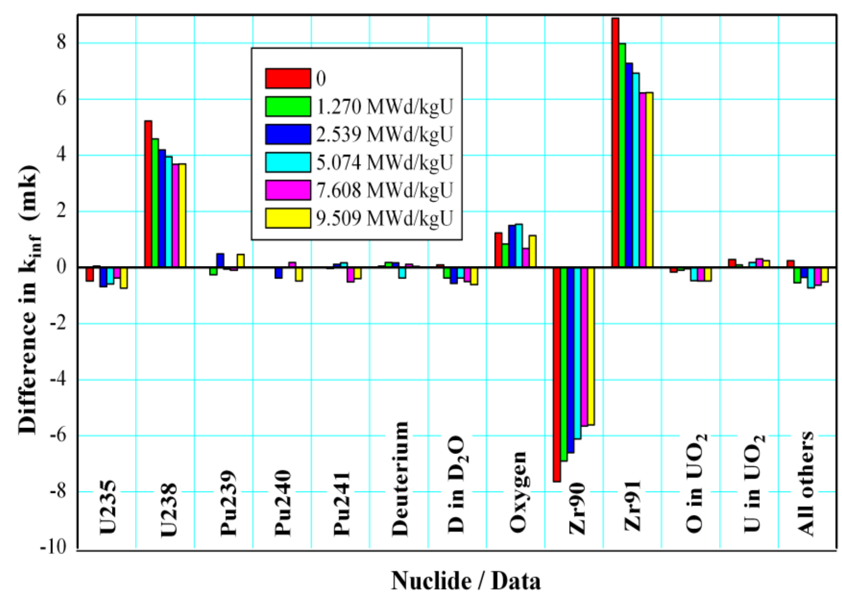






Importance of accuracy of ND and TSL: case study
(*e.g.*, in n spectra with optimal moderation by D_2O)

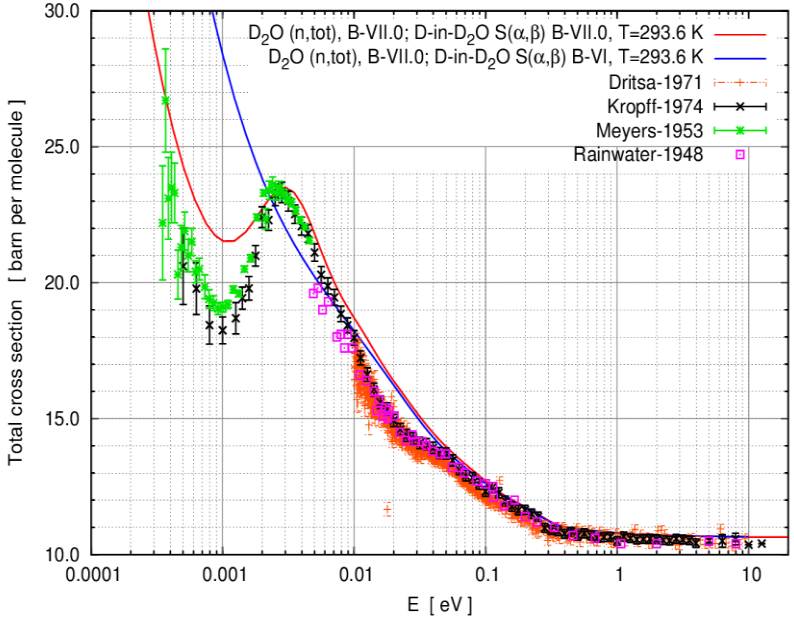


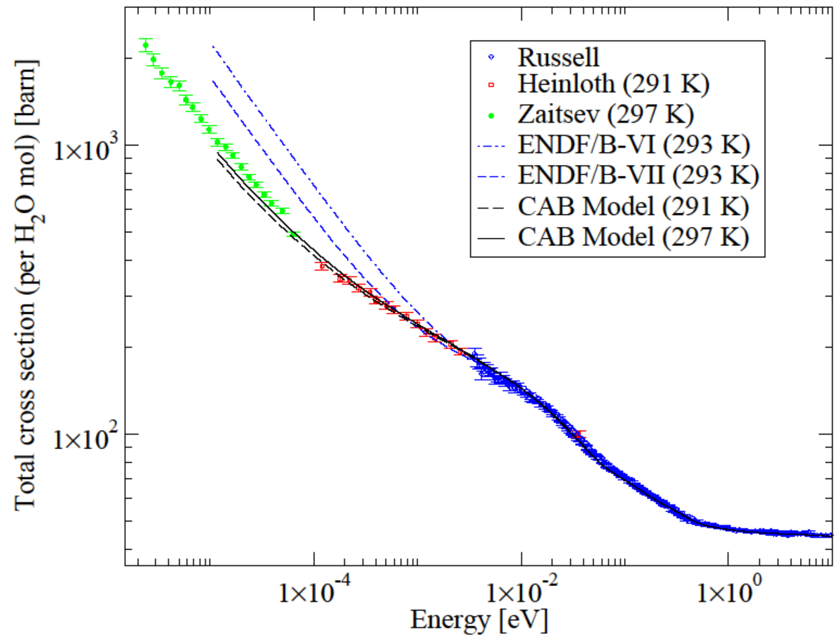


Impact of particular ENDF/B-VII.0 data on ZED-2 reactor simulation (left);
1 mk = 100 pcm
Effect of particular ENDF/B-VII.0 data on MCNP calculation of 37-element CANDU lattice cell
D. Altiparmakov, PHYSOR-2010

TSL for heavy and light water:

interaction of thermal neutrons with liquid D_2O / H_2O at different *T* and *p*



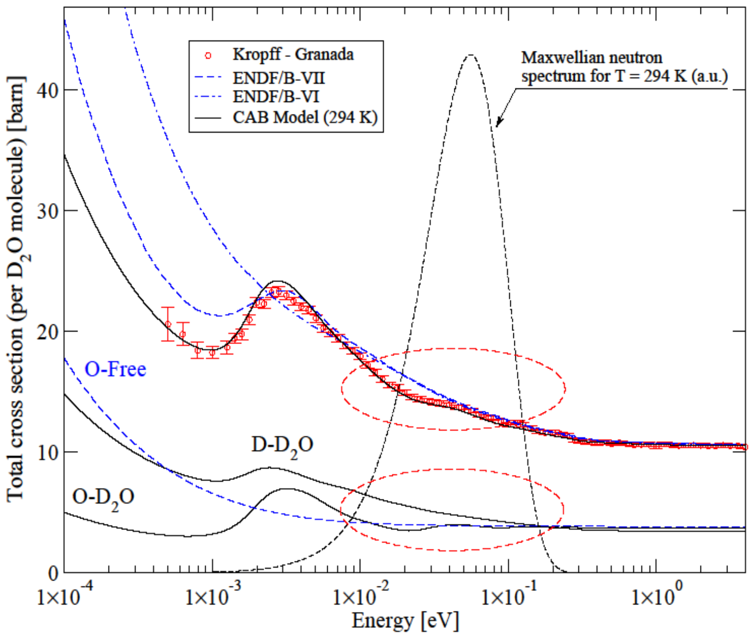


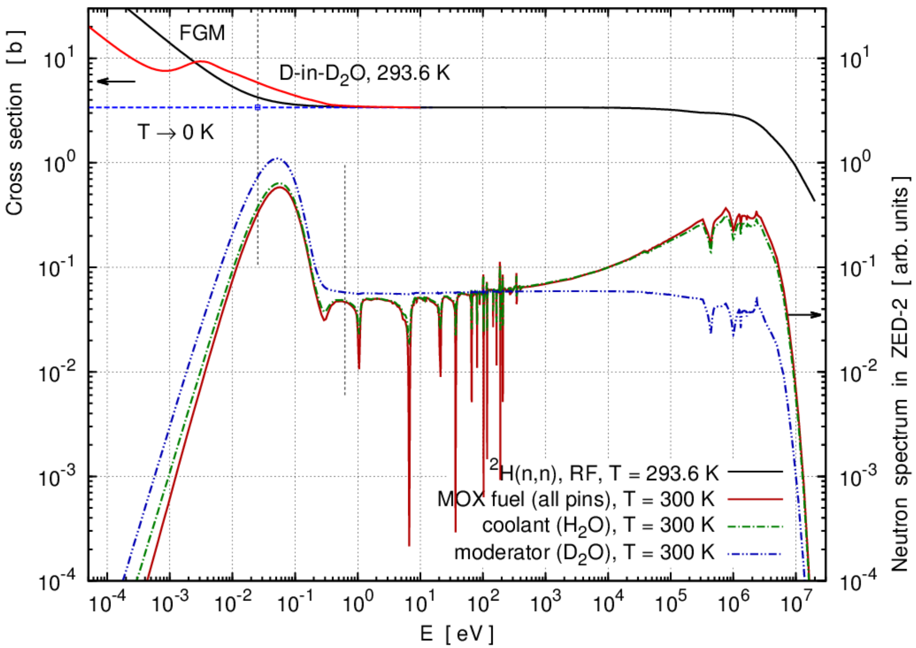
- **Discrepancy for <u>heavy water</u> in modern evaluated ND libraries: in integral values, at neutron energy *E* near E_{th} = 0.0253 eV, for liquid D_2O at room temp. *T*, we have** (*Exp*. – *Calc*.) / *Calc*. ≈ –**8.4%** (using ENDF/B-VII.0 ***S*(α,β)** for **D-in-D_2O** and Free Gas for **^{16}O**)
- What to do?

  TSL evaluation is a **model** of thermal neutron interaction with a condensed medium (liquid, solid) based on QM and Stat. Phys.; converted into dimensionless tables $S(\alpha_i, \beta_j; T_n)$ following **ENDF** format. So, improve modeling, improve numerics, …
- How to *improve* modeling ?

TSL for heavy water (FY 2014/2015)

interaction of thermal neutrons with liquid D_2O at room *T*



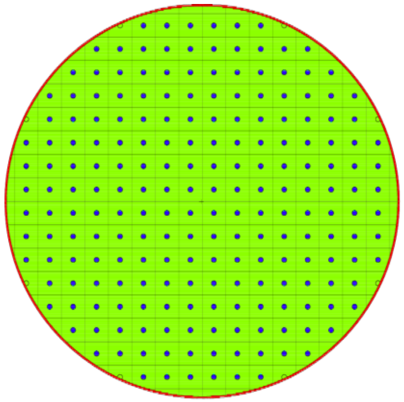


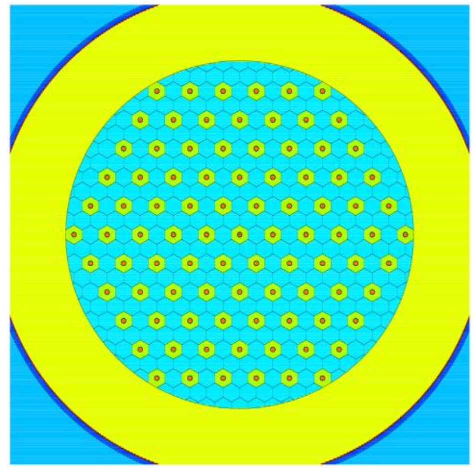
- Developing **new** TSL <u>evaluations</u> for water (**CNL**, Canada and **CAB**, Argentina): based on combining **Mol. Dynamics** (**MD**) simulations (GROMACS) and *experimental data*

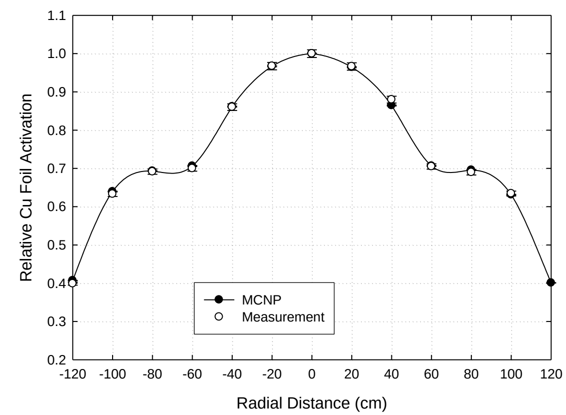
- The resulting new **models** are formulated as LEAPR input files for **LEAPR** module of **NJOY99 (up396 with additional patches)** NJOY = nuclear data post-processing code, LANL, USA

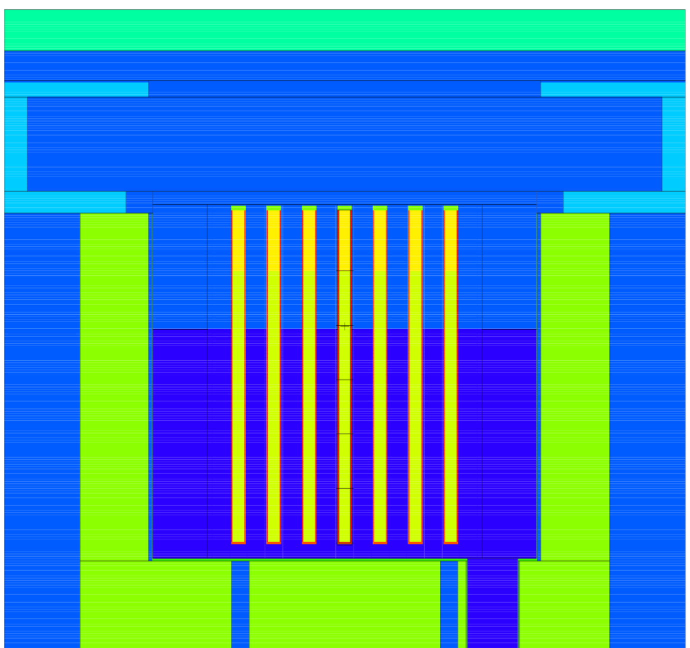
Benchmarking

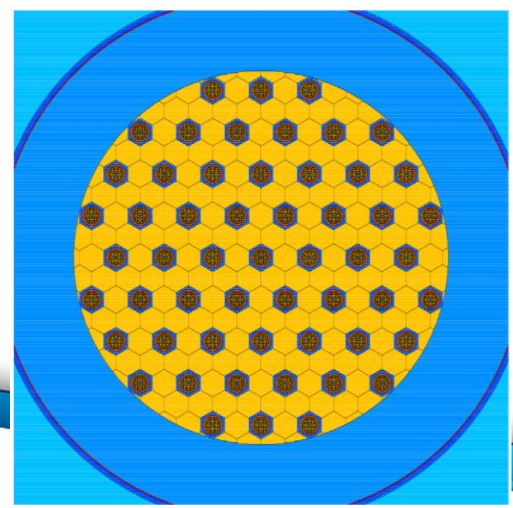
Integral experiments: k-eff, also reaction rates, spectral indices





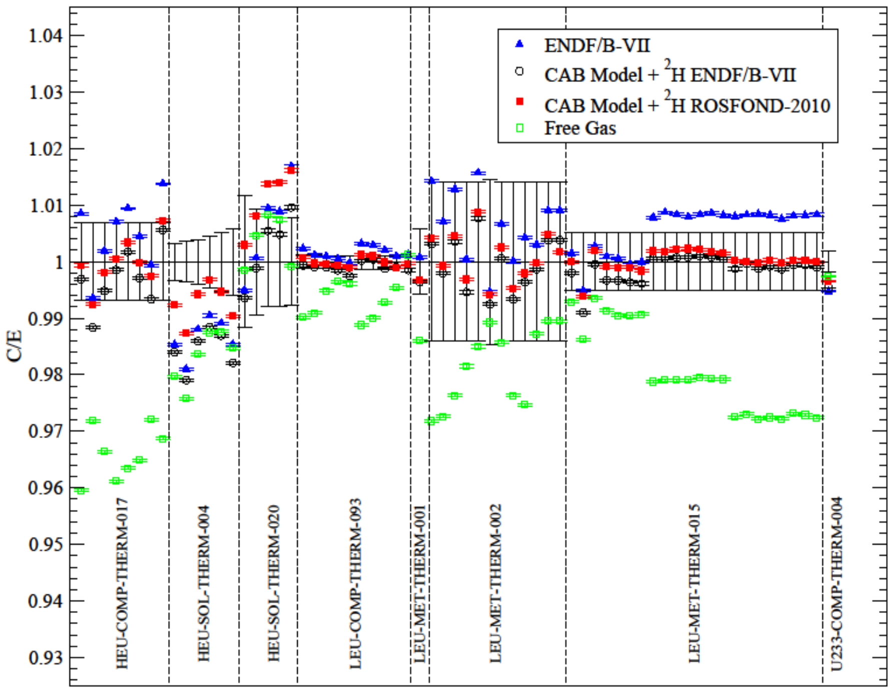


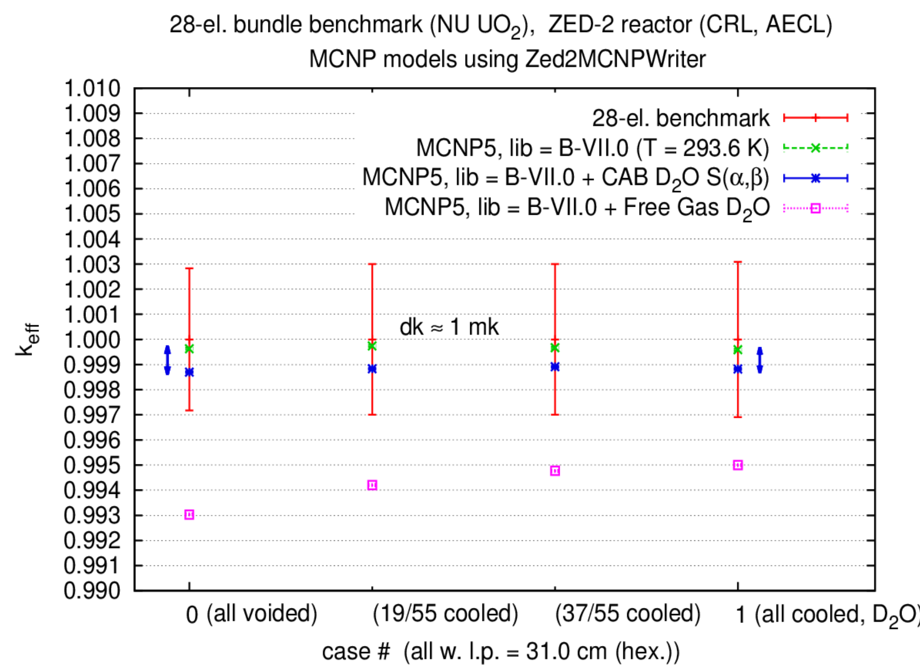




TSL for heavy water (FY 2014/2015)

interaction of thermal neutrons with liquid D_2O (at room T)



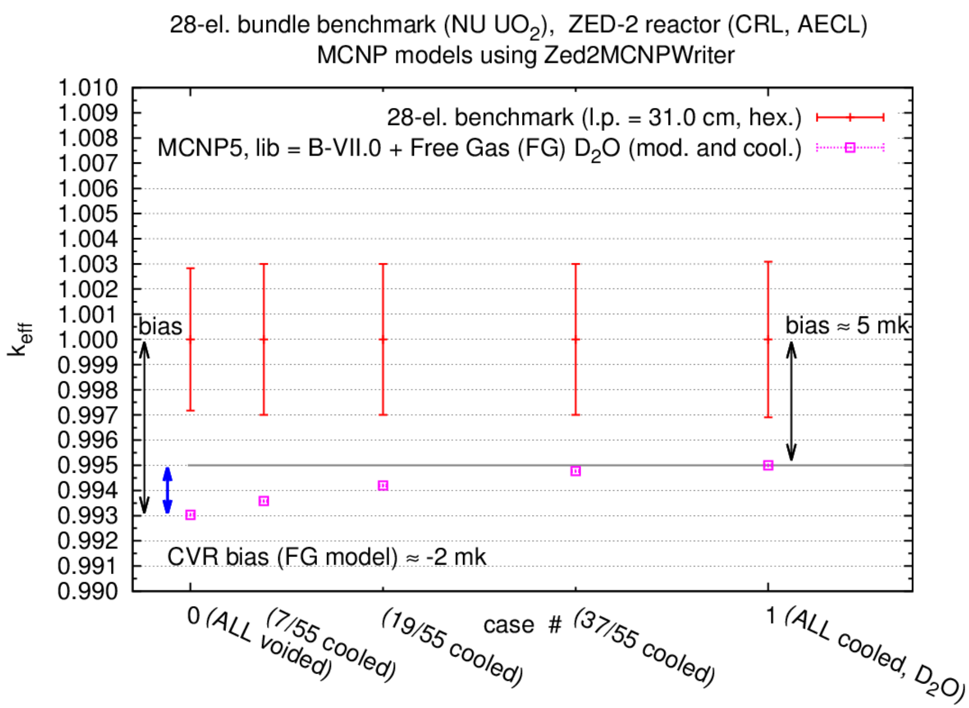


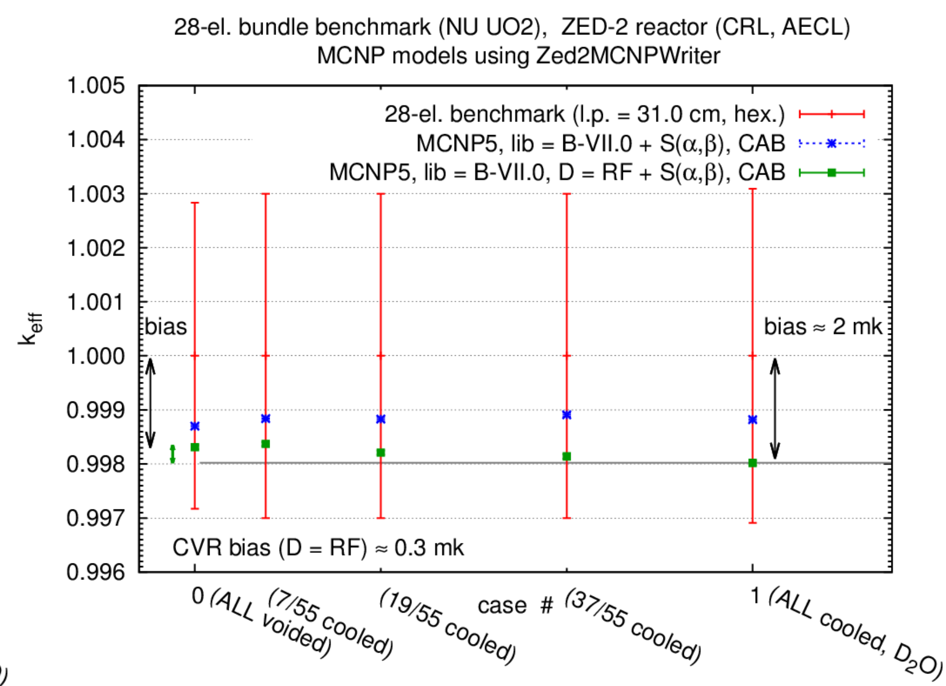
- **Testing**: using Crit. Safety **Benchmarks** with D_2O, overall, it is an improvement in k_{eff} **C/E** **if** ENDF/**B-VII.0** D_2O $S(\alpha,\beta) \rightarrow$ **new** D_2O $S(\alpha,\beta)$ (we call it CAB models)
- We expect that k_{eff} (**CAB** D_2O) **<** k_{eff} (**B-VII.0** D_2O), but what is the difference dk = k_{eff} (B-VII.0 D_2O) – k_{eff} (CAB D_2O) = **? ; cases with** dk **>** Δk_{Bench} **of special interests**

answer for ZED-2 reactor: **dk ≈ 100 pcm , dk <** Δk_{Bench} **, ZED2-HWR-EXP-00**1 benchmark **(28-element NU UO_2 bundles, at room T, evaluator = J. Atfield, CNL)**

TSL for heavy water (FY 2014/2015)

interaction of thermal neutrons with liquid D_2O (at room T)





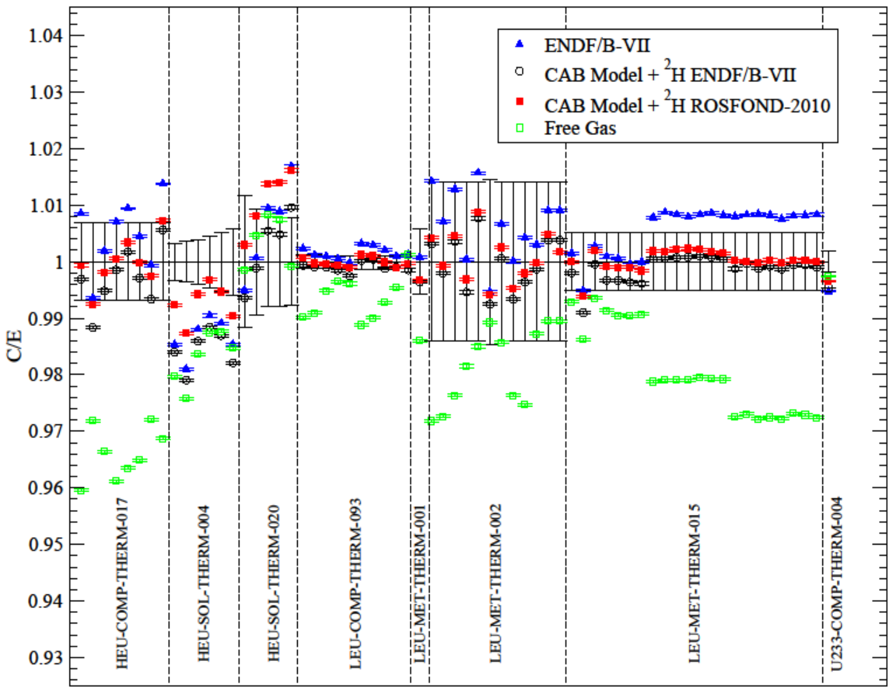
Discuss: how accurately do we model criticality (critical zero-power assemblies), *i.e.*, k_{eff} = **?**
k_{eff} = 1.0, in theory. In practice (i.e., in modeling), …..

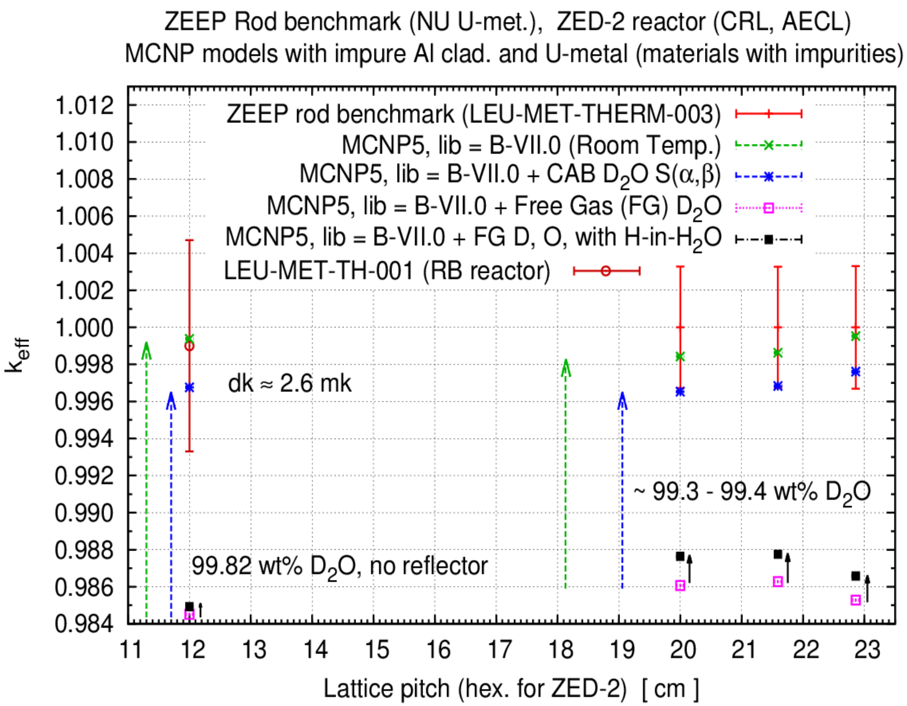
- we have a **Bias** (in k_{eff})
- **CVR bias: assume we have cooled and voided <u>critical</u> cases, then :**

Is any dependency / trend of k_{eff} bias upon voiding of the coolant in a crit. assembly ?
Is it possibly to decrease the experimental (benchmark) uncertainty by factor of … (3-5) ?

TSL for heavy water (FY 2014/2015)

interaction of thermal neutrons with liquid D_2O (at room T)





- **Testing**: using Crit. Safety **Benchmarks** with D_2O, overall, it is an <u>improvement</u> in k_{eff} C/E
  if ENDF/**B-VII.0** D_2O $S(\alpha,\beta)$ → **CAB** D_2O $S(\alpha,\beta)$
- We expect that k_{eff} (**CAB** D_2O) **<** k_{eff} (**B-VII.0** D_2O), but what is the difference
  dk = k_{eff} (B-VII.0 D_2O) – k_{eff} (CAB D_2O) = **?, and check:** dk **< or >** Δk_{Bench} **?**

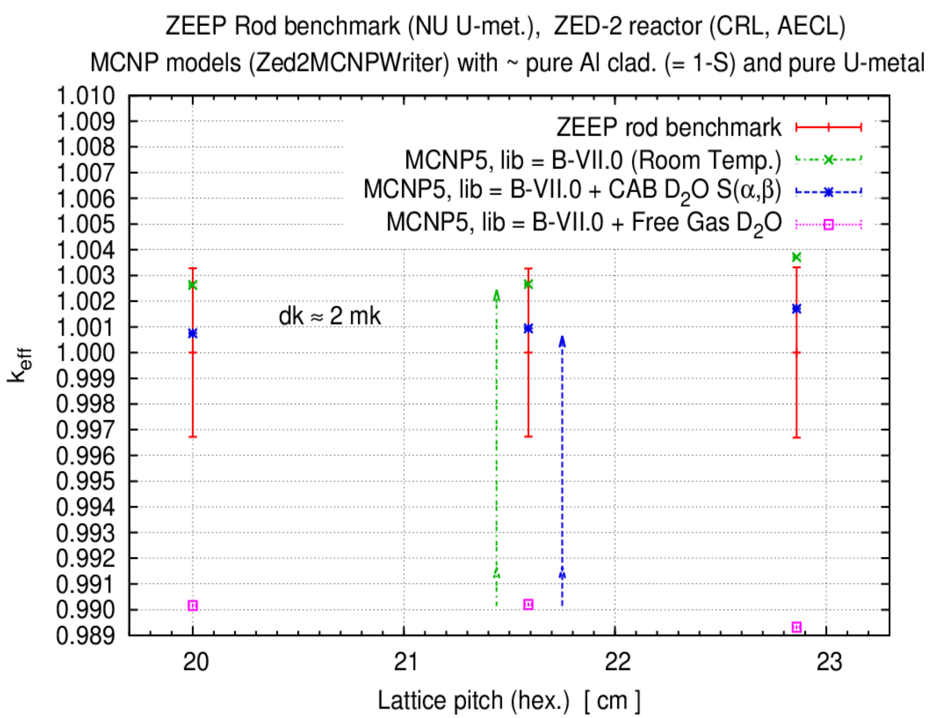
answer for ZED-2 reactor critical core (CNL, Chalk River) **:**

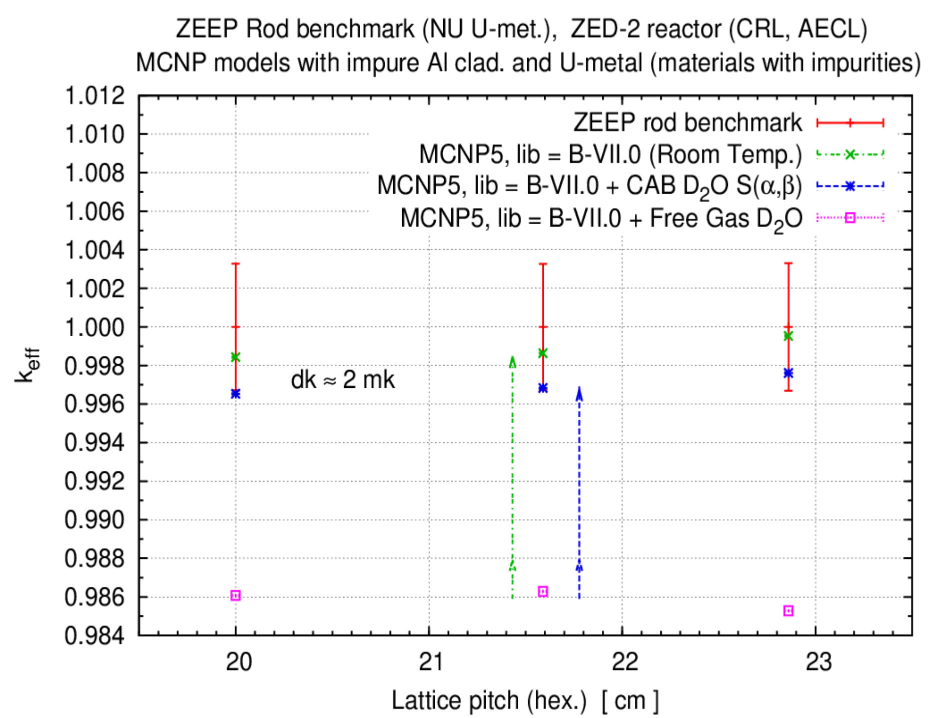
dk ~ 100 pcm using **LEW-MET-THERM-003** benchmark, note H-in-H_2O for r.gr. heavy wat

This is NU U metal in Al cladding, at room T, evaluator = J. Atfield (CNL)

TSL for heavy water (FY 2014/2015)

interaction of thermal neutrons with liquid D_2O (at room *T*)





LEW-MET-THERM-003: ZEEP rods in ZED-2 reactor in CNL, Chalk River**:**

art of modeling materials (J. Atfield): conversion of mass-spec data into MCNP data

Example:

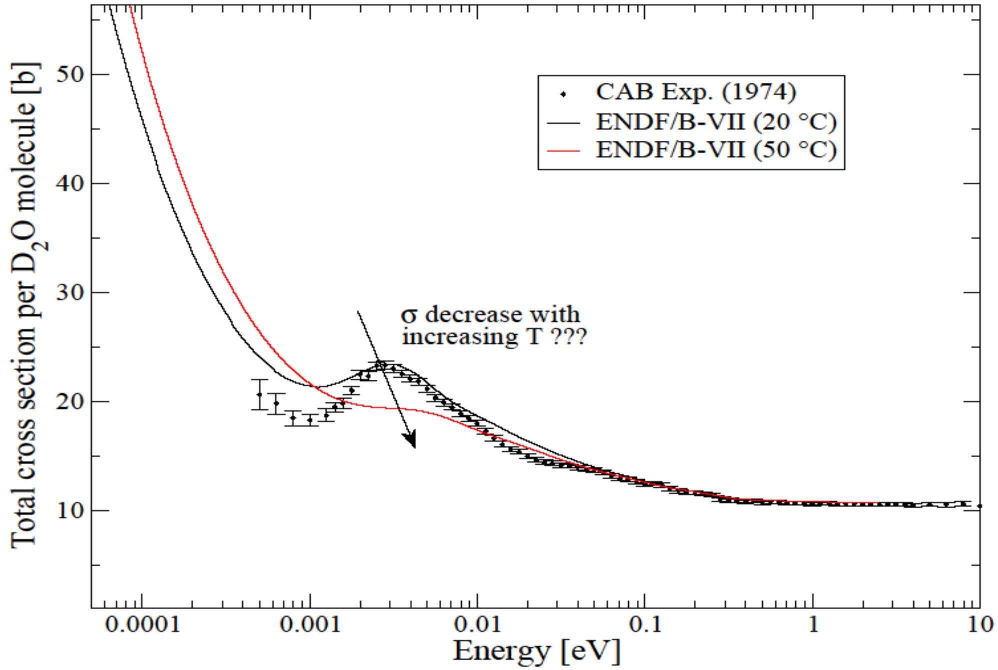
benchmark k_{eff} **= 1.0000** ± **0.0033**

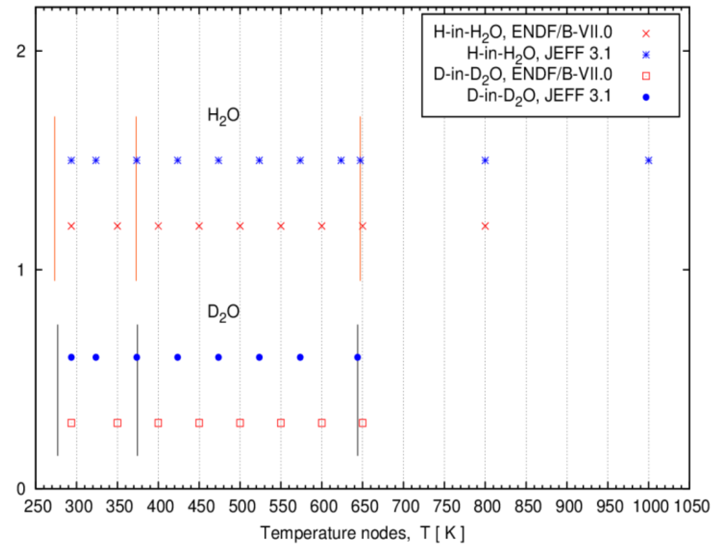
impurity worth ≈ **4 mk** (*e.g.*, 1.00371 - 0.99953 ≈ 4.2 mk , std. dev [k_{eff}] = ± 0.00004 **)**

compare with *S*(α,β) sensitivity: dk (CAB *vs.* B-VII.0) ≈ -**1.9** mk **(= 0.99761 - 0.99953)**

TSL for heavy water (2014/2015, 2015/2016)

interaction of thermal neutrons with liquid D_2O at different *T* and *p*

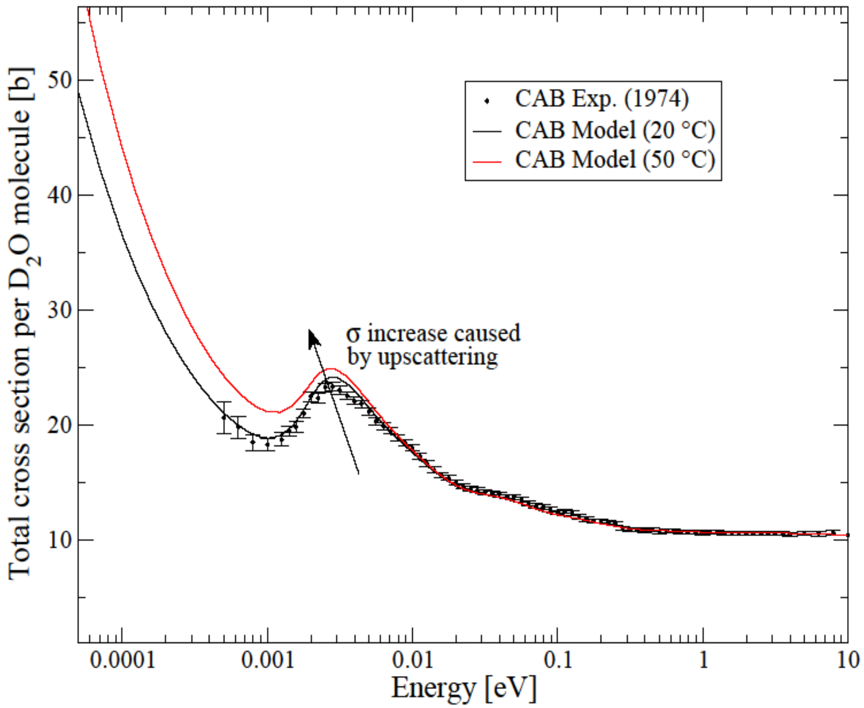


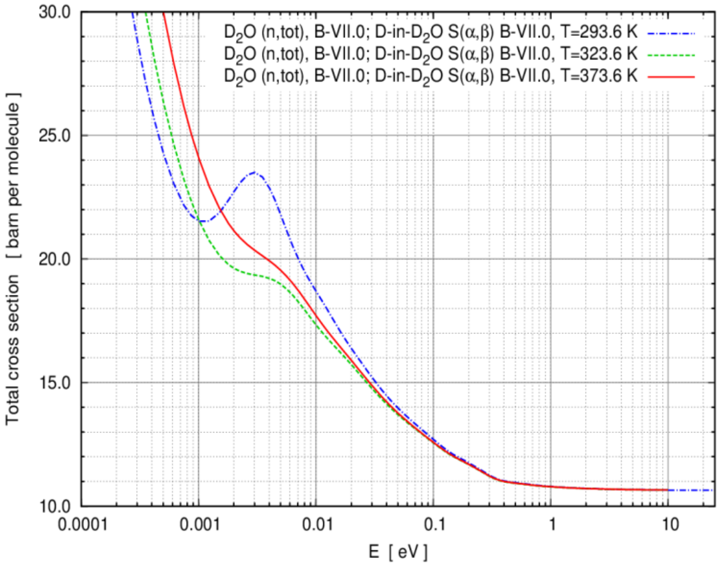


- **Inconsistency for <u>heavy water</u> TSL in modern evaluated ND libraries:**
  if $\boldsymbol{T > T_{room}}$ (p = 1 atm), what happens with $\sigma_s(E; T)$?
- D_2O moderator T in CANDU-6: ≈ 68 deg. C (≈ 341 K)
- D_2O moderator T in some ZED-2 experiments up to ~ 50-60 deg C. **What for ?**
  Moder. T coefficient of reactivity is an important parameter in CANDU reactor physics analysis

TSL for heavy water (2014/2015, 2015/2016)

interaction of thermal neutrons with liquid D_2O at different *T* and *p*





- **Inconsistency (?) for <u>heavy water</u> in modern evaluated ND libraries:**
  if 100 C **>** ***T*** **>** $\boldsymbol{T_{room}}$ (p = 1 atm), what happens with $\sigma_s(E; T)$?
- New experimental results at 50 deg. C (~ 323 K) : J.I. Márquez Damián and D. Baxter
- What can we do to improve $S(\alpha,\beta)$ for D_2O at **100** C **>** ***T*** **> 10** C (at p = 1 atm) ?
- New (improved) **models** → **NJOY** (LEAPR) → ACE files & testing (benchmarking) using MCNP,
  migrate to GROMACS 5.0, NJOY99 → NJOY2012, MCNP5 → MCNP6 & SERPENT (student-friendly MC)

TSL for heavy water: new & improved models → new evaluation

New **evaluation** (in **ENDF** format) can be based on combining
molecular dynamics (**MD**) simulations and reliable *experimental data*,
and the resulting new **models** can be implemented in / have to be compatible with /
LEAPR module of **NJOY** (nuclear data post-processing code, LANL, latest is **NJOY 2012**)

The **key points** for building new $S(\alpha,\beta)$ **models** are:

1. use of molecular **(self)diffusion** for translational motion of liquid H_2O / D_2O
(instead of free gas approximation (FG) used in **all** evaluated ND libraries);

2. continuous **vibrational spectra** computed from molecular dynamics (**MD**) simulation
at a given thermodynamic state of the liquid, (p, T) and density $\rho(p, T)$,
(instead of derived / adjusted spectra from neutron scattering experiments);

3. a more precise description of **the structure of liquid:** e.g., models for D **and** O in D_2O based
on **experimental results** (instead of using the incoherent approximation in ENDF/B-VI
or the Lennard-Jones **model** for D-D structure in JEFF 3.1 and ENDF/B-VII.0 → ENDF/B-VII.1)

4. better **numerics** (*e.g.*, extended grid(s), α_i , β_j , T_n , and NJOY data processing options revisited,
and we need NJOY patches in leapr and thermr ;)

5. **ACE files** to be generated for **testing/benchmarking** with MCNP5, MCNP**6**, and SERPENT

The resulting scattering kernels & cross sections will be an improvement over existing evaluations:
they are compared with measurements of double differential scattering cross sections,
quasi-elastic neutron scattering measurements, angular distributions of out-scattered neutrons,
average cosine of the scattering angle (mu-bar), and total cross sections;

Need to do all this at different (*p, T*)

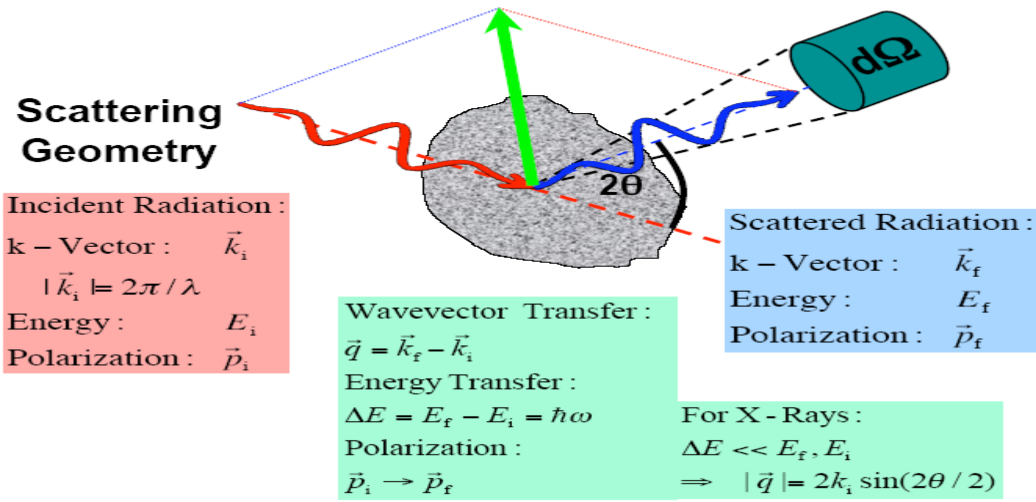
New TSL for heavy water and benchmarking: References

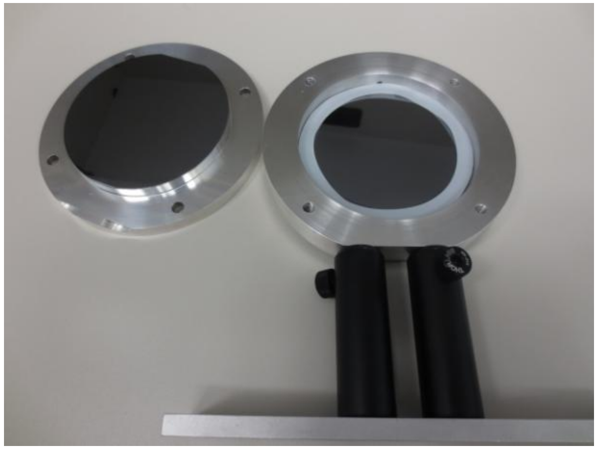
- J.I. Márquez Dámian, J.R. Granada, D.C. Malaspina,
  "*CAB models for water: A new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format*,"
  Annals of Nuclear Energy, Vol. **65**, pp. 280-289, **2014** (March); doi:10.1016/j.anucene.2013.11.014
  http://www.sciencedirect.com/science/article/pii/S0306454913005987

- J.I. Márquez Dámian, J.R. Granada, D. Roubtsov,
  "*Improvement on the calculation of D_2O moderated critical systems with new thermal neutron scattering libraries*,"
  Annals of Nuclear Energy, Vol. **71**, pp. 206-210, **2014** (September); doi:10.1016/j.anucene.2014.03.024
  http://www.sciencedirect.com/science/article/pii/S0306454914001467

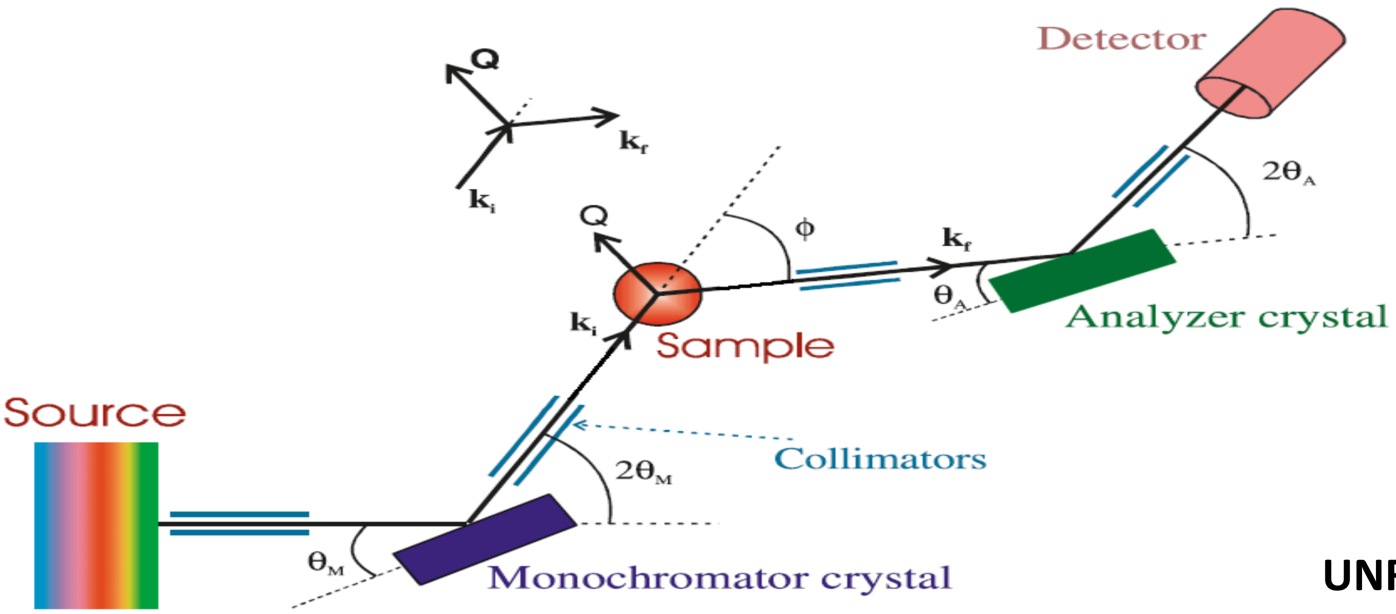
- J.I. Márquez Damián, J.R. Granada, D. Roubtsov, J.C. Chow,
  "*From Molecular Dynamics to Reactor Physics: Improvement on the Calculation of D_2O Moderated Critical Systems with New Thermal Neutron Scattering Libraries*",
  in Proceedings of XXI Congress of Numerical Methods and Their Applications (**ENIEF 2014**), Bariloche, September 2014, Argentina;
  http://www.cimec.org.ar/ojs/index.php/mc/article/view/4899

Neutron Scattering on Water using triple axis spectrometer at NRU reactor n beam at CNL (Chalk River)





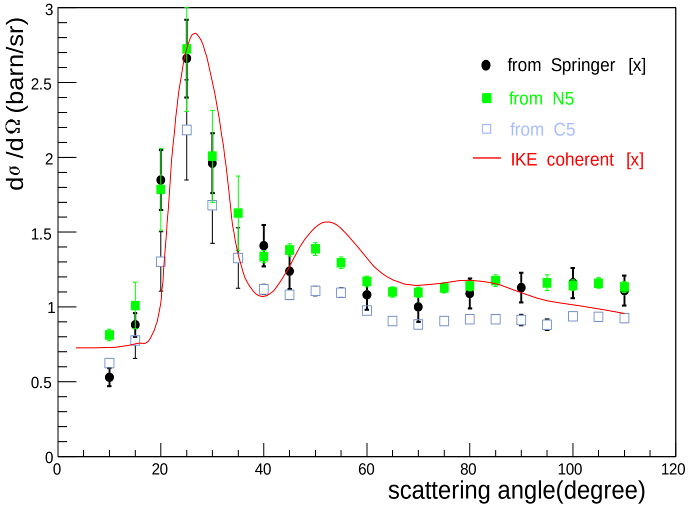
Sample sizes:
0.1 mm to 3 mm



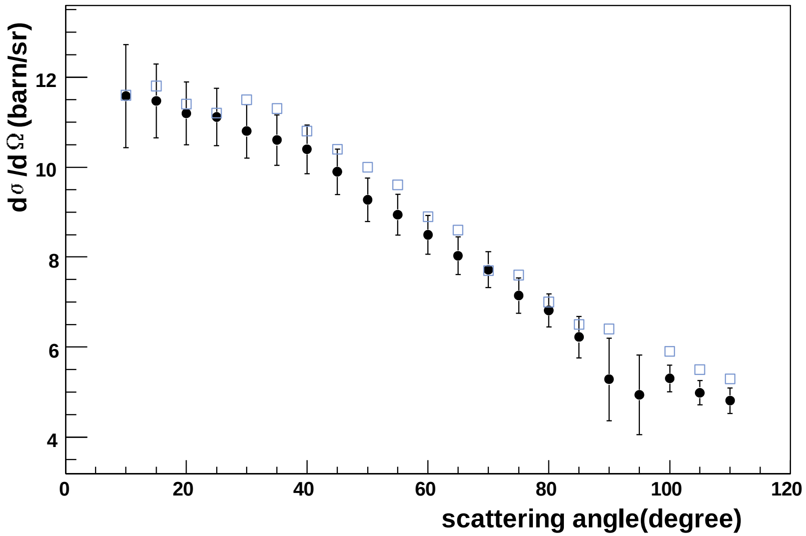
Triple axis spectrometer

UNRESTRICTED / ILLIMITÉ

New Measurements at NRU to reduce ND uncertainties to improve Reactor Safety



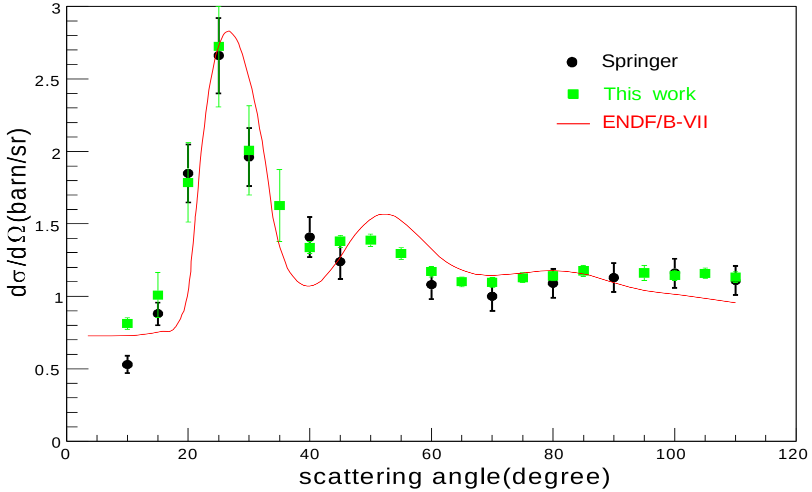
Differential scattering cross section of D_2O.
Beam energy is 44 meV
(except for that the result from C5 is at E_0 = 41.44 meV).

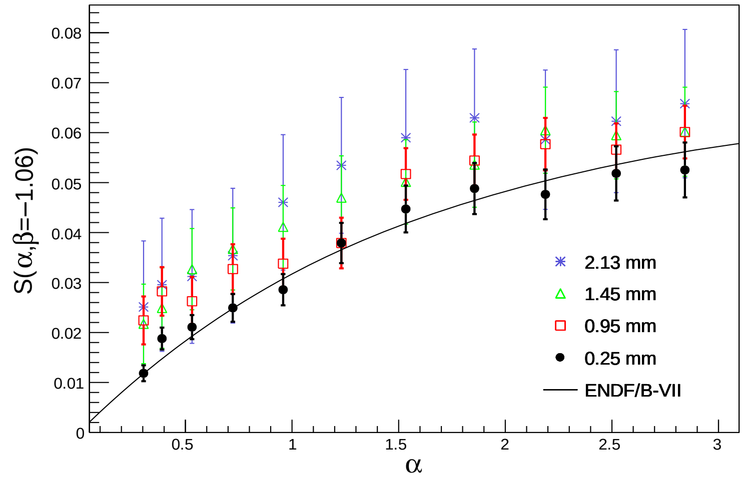


Absolute differential cross section
(in barn/sr)
for Light water, at E_0 = 41 meV,
Beyster's data: ±5%.

- G. Bentoumi, G. Li, B. Sur, and Z. Tun (Canadian Neutron Beam Centre)

New Measurements at NRU to reduce ND uncertainties to improve Reactor Safety





NRU measured differential cross sections of D_2O (Beam energy is 44 meV)
and *S*(α,β) functions of H_2O (using samples with different widths), after multiple-scattering corrections, all at room T

Importance:

- Safety and operating margins for nuclear reactors are crucially dependant on the availability and accuracy of nuclear data that are used for modeling, in particular for **safety analysis** and **licensing applications**

Objectives:

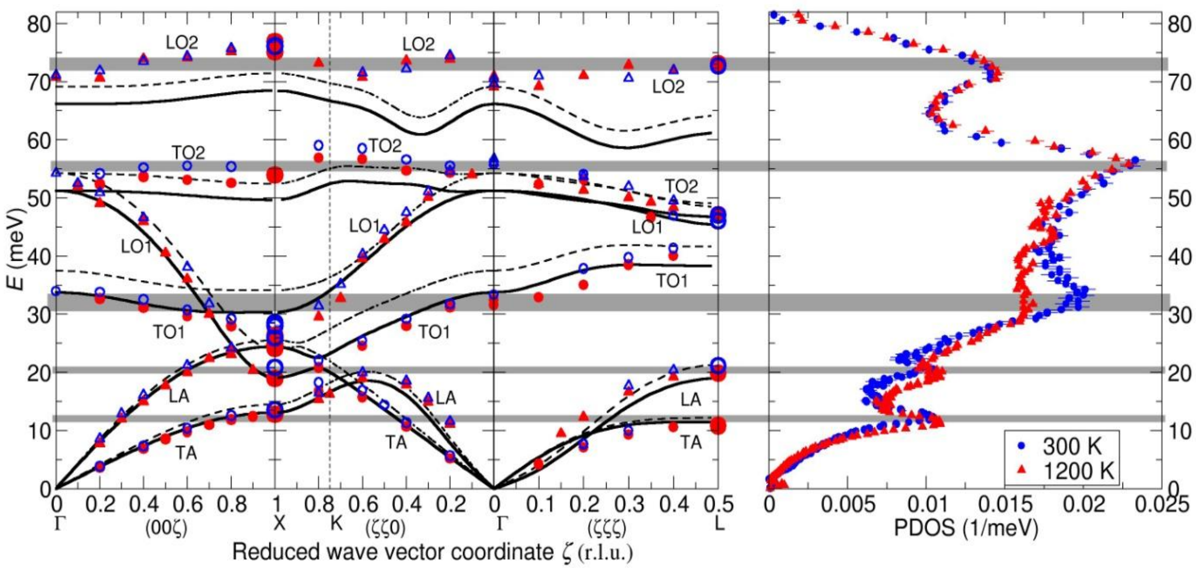
1. Carry-out new experiments at neutron beam facilities, such as NRU and (?) SNS (ORNL), and also at ZED-2 (CRL), to accurately measure the relevant nuclear data parameters
2. Investigate the discrepancy between the information obtained experimentally and existing nuclear data evaluations
3. **Compare new experimental results with predictions based on new models**

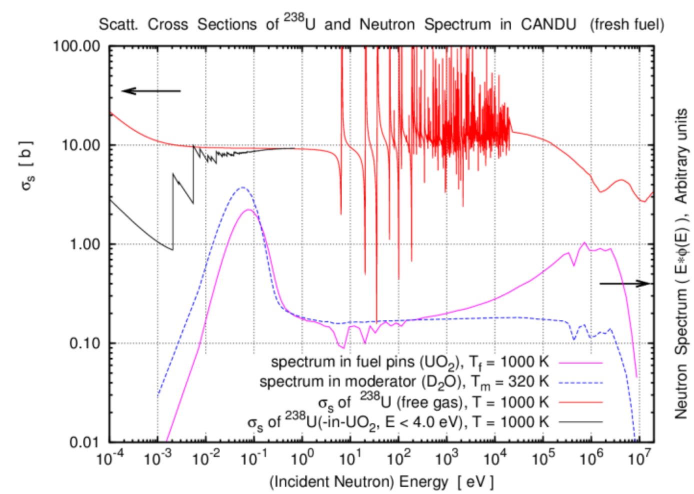
TSL for UO_2: phonon PDOS + coh. elastic

Phonons in actinides: active area of research,

Judy Pang *et al.*, Phonon density of states and anharmonicity of UO_2 ,

PHYSICAL REVIEW B 89, 115132 (2014)

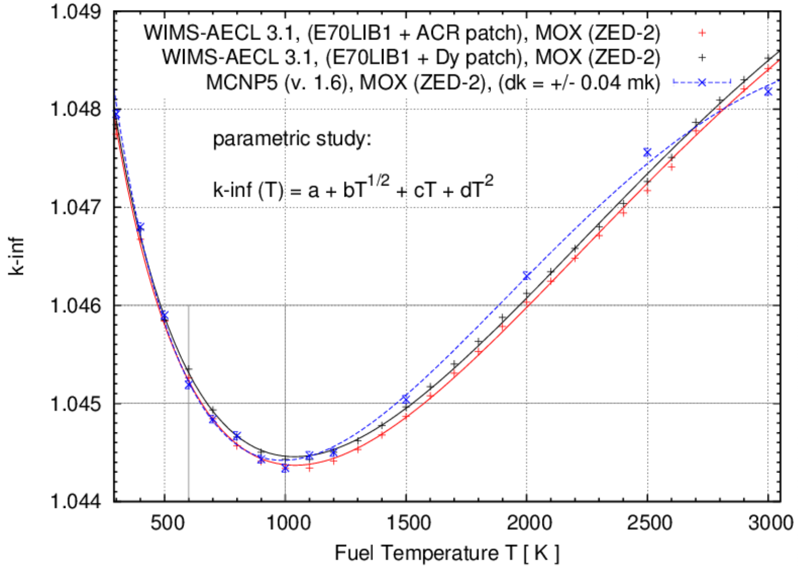


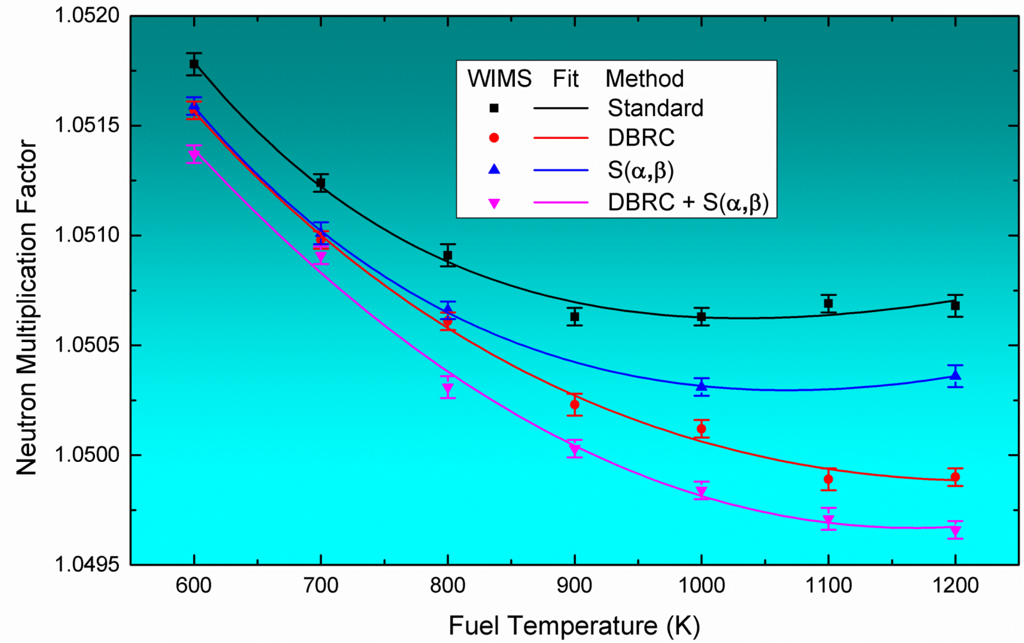


In reactor physics, for safety and licensing application:

fuel temperature coefficient of reactivity (FTC); T can go ~ 2000 K

MCNP Results: Criticality Calculations, k-inf *vs.* T_f





PHWR typical fuel bundle with UO_2 fuel near the middle of burn-up

D. Altiparmakov and D.R.

CNL Collaborations in Nuclear Data R&D

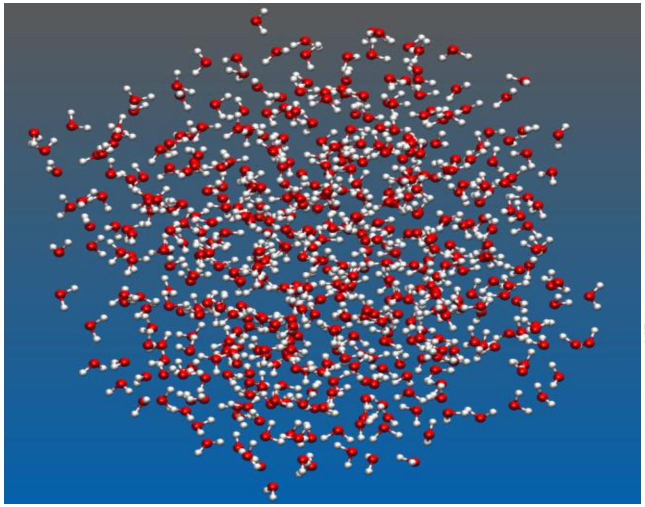
- Member of **CSEWG**, **USA**
  CSEWG = Cross Section Evaluation Working Group
  (responsible for the U.S. Evaluated ND Files ENDF/B, latest = ENDF/B-**VII.1**, 2011)
  https://www.nndc.bnl.gov/csewg/

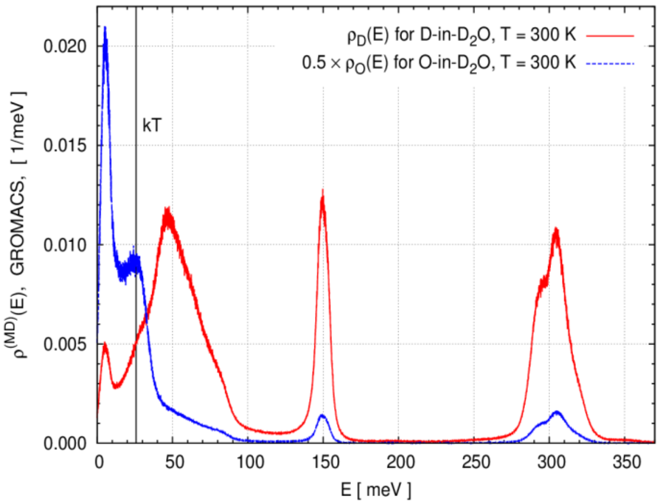
- Participation in **WPEC** sub-group activity under **OECD/NEA** (**EU**)
  WPEC = Working Party on International Nuclear Data Evaluation Co-operation,
  https://www.oecd-nea.org/science/wpec/
  e.g., **sub-group 40**:
  The CIELO Collaboration: Neutron Reactions on ^{1}H, ^{16}O, ^{56}Fe, ^{235,238}U, and ^{239}Pu, https://www.oecd-nea.org/science/wpec/sg40-cielo/

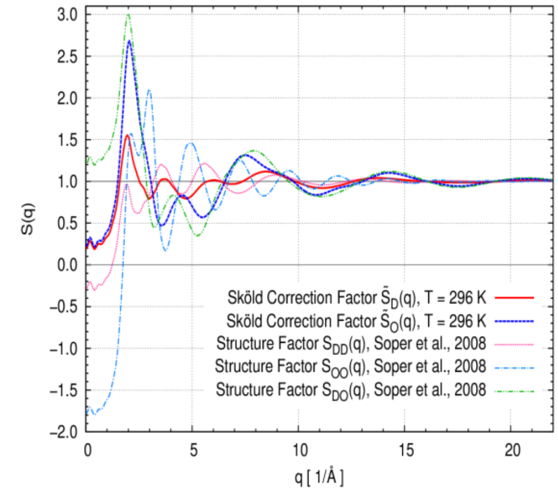
- Continue our collaboration with scientists from Neutron Physics Department,
  Centro Atómico Bariloche (**CAB**), **Argentina**: New TSL evaluations for **D_2O**, **H_2O** and testing them using International Benchmarks (Crit. Saf. and Reactor Phys.)

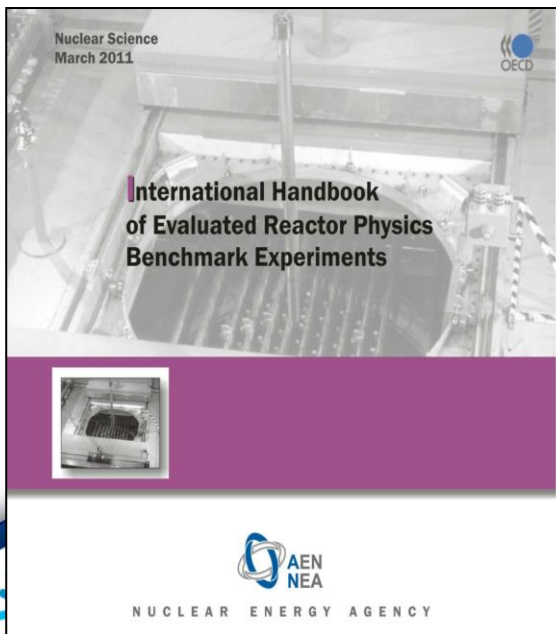
- INERI USA-Canada R&D Collaboration, **2015 - ... :**
  new collaborations with US scientists (ORNL, LANL, ..., academia): **?**

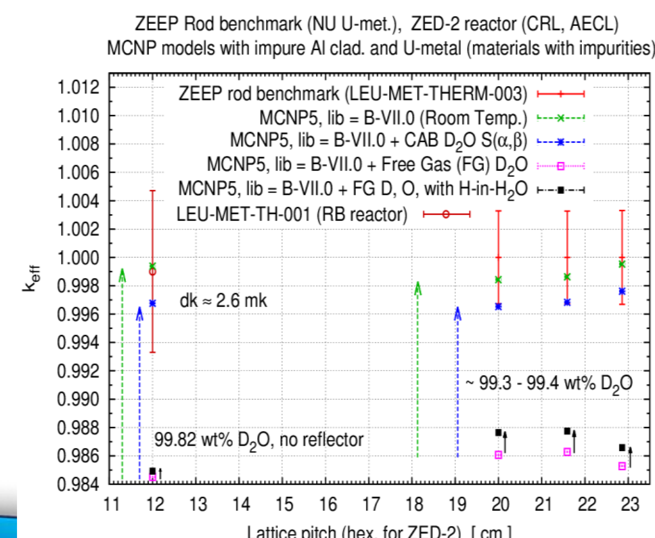
TSL ($S(\alpha,\beta;\ T)$) of water in a nutshell: from MD to RP











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