Nuclear Data Testing at CNL (Canada) and CAB (Argentina)
Assessment of ENDF/B-VIII.0_β5

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The presented results are based on two recent publications (ZED-2 benchmarking with MCNP & ENDF/B + CIELO ^{16}O, $^{5,8}U$ and on new TSL for H_2O, D_2O)

- *Application of the CAB Evaluation of Thermal Scattering Law for Heavy Water to ZED-2 Critical Benchmarks at Room Temperature*,
  by D. Roubtsov, J.C. Chow, J.I. Márquez Damián, J.R. Granada,
  Annals of Nuclear Energy, V. **110** (2017), pp. 958-972
  DOI: http://dx.doi.org/10.1016/j.anucene.2017.07.034

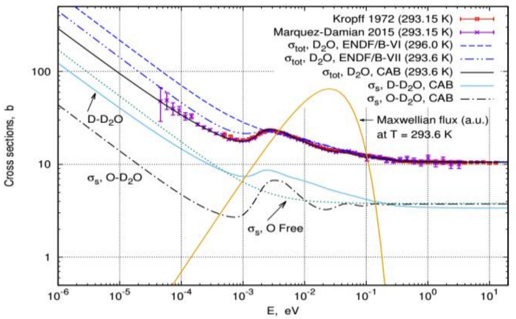


Figure 1: Total cross sections for heavy water (per molecule) at room temperature *vs.* incident neutron energy E (10^{-6} eV $< E <$ 20.0 eV). Experimental results (Kropff et al., 1974; Márquez Damián et al., 2015) are compared with calculations using the CAB model, ENDF/B-VII (IKE model), and ENDF/B-VI (GA model). The Maxwellian neutron flux for T_{eff} = 293.6 K (0.0253 eV), which would be expected for fully thermalized neutrons, is shown for reference. The differences in the evaluated σ_{tot} can be traced to the scattering cross sections of O in D_2O; compare the curves at the bottom that show the scattering cross sections of ^2H and ^{16}O.

- *New evaluation of thermal neutron scattering libraries for light and heavy water***,**
  by J.I. Marquez Damian, J.R. Granada, F. Cantargi, D. Roubtsov,
  EPJ Web of Conferences Journal, V. 46 (= Proc. of **ND2016**)
  DOI: http://dx.doi.org/10.1051/epjconf/201714613001

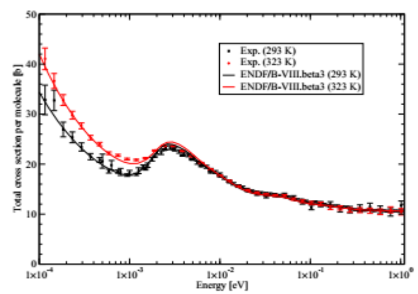
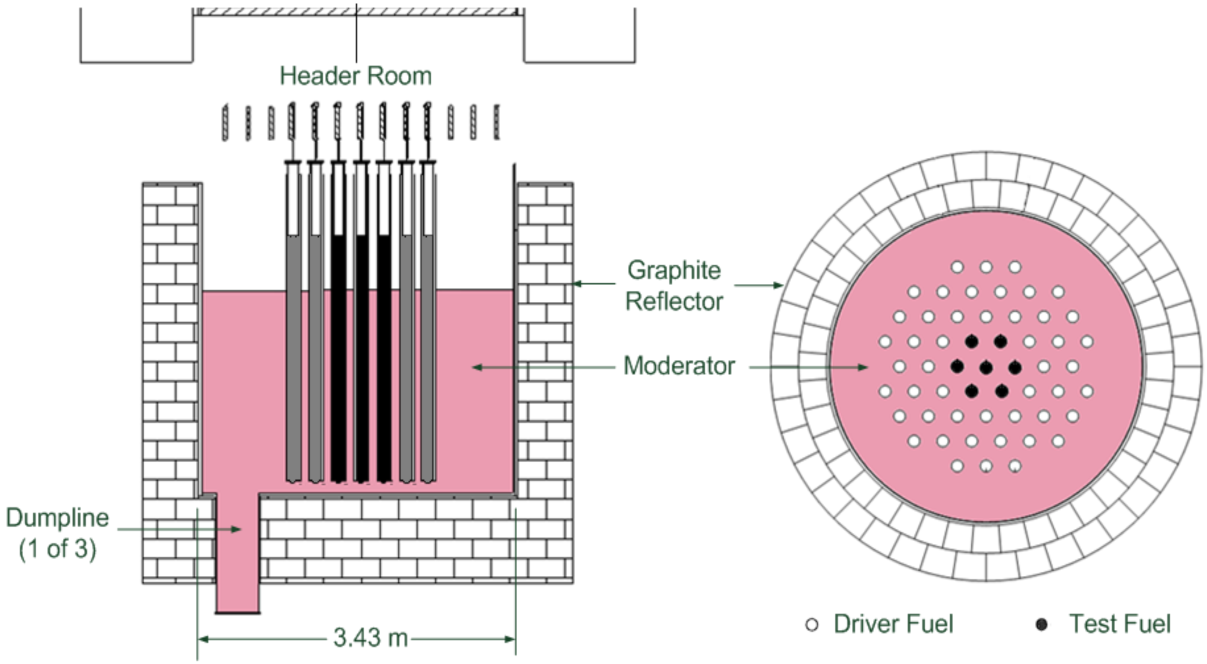


Figure 2. Total cross section for heavy water at 20 and 50 °C measured at the Low Energy Neutron Source, compared with calculations with the CAB Model.

ZED-2 reactor in CNL, Chalk River (operational)



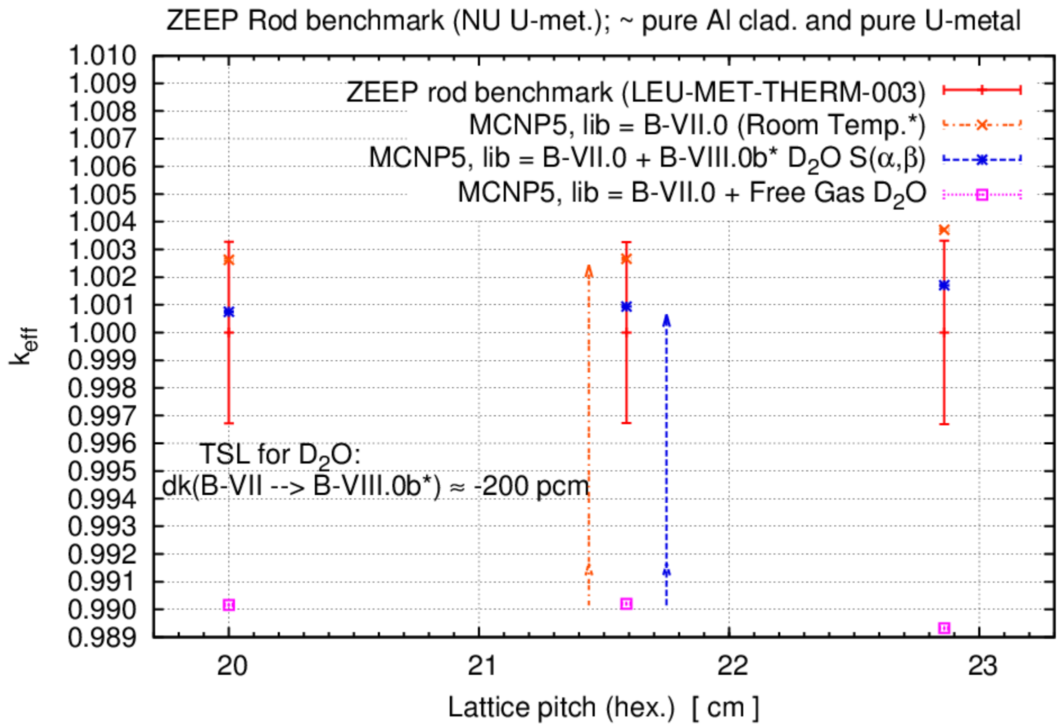
ZED-2 is a reactor of the calandria vessel type. It is a cylindrical tank made from **Al** with a sidewall thickness of 0.64 cm.

The calandria has a 3.36-m diameter and 3.30-m depth.

It is surrounded by **graphite blocks** arranged with an average thickness of 60 cm radially and 90 cm below the tank (ρ = 1.63 g/cm^3)

Fuel assemblies are hung vertically from beams located above the calandria.

ZEEP rod benchmark (LEU-MET-THERM-003) 0



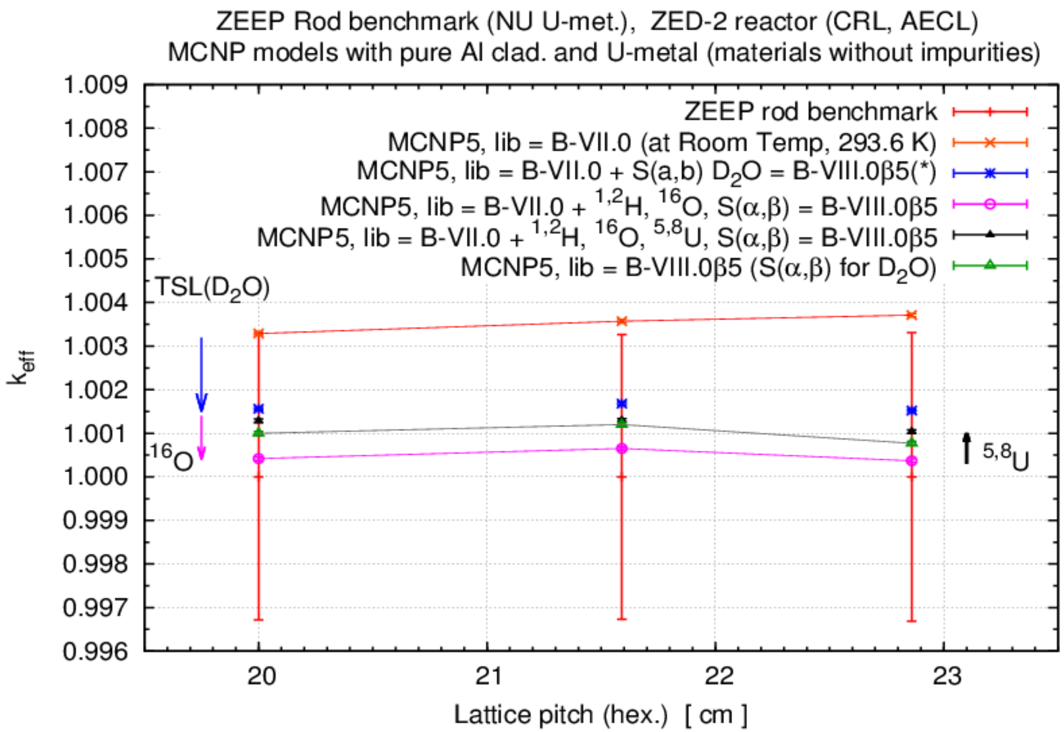
Benchmark k : k_{eff} = 1.000 ± 0.003 ; Fuel rods = U-metal (NU) in Al clad ;

All cases at "room T" (and can use ND libraries at T=293.6 K for testing);

D_2O TSL worth is ~ 1000 pcm ; |TSL worth| > Δk_benchmark ; so we need it ;

Then changed TSL for D_2O, B-VII.0 → B-VIII.0β* : k_{eff} decreased by ≈ 200 pcm

ZEEP rod benchmark (LEU-MET-THERM-003) 1



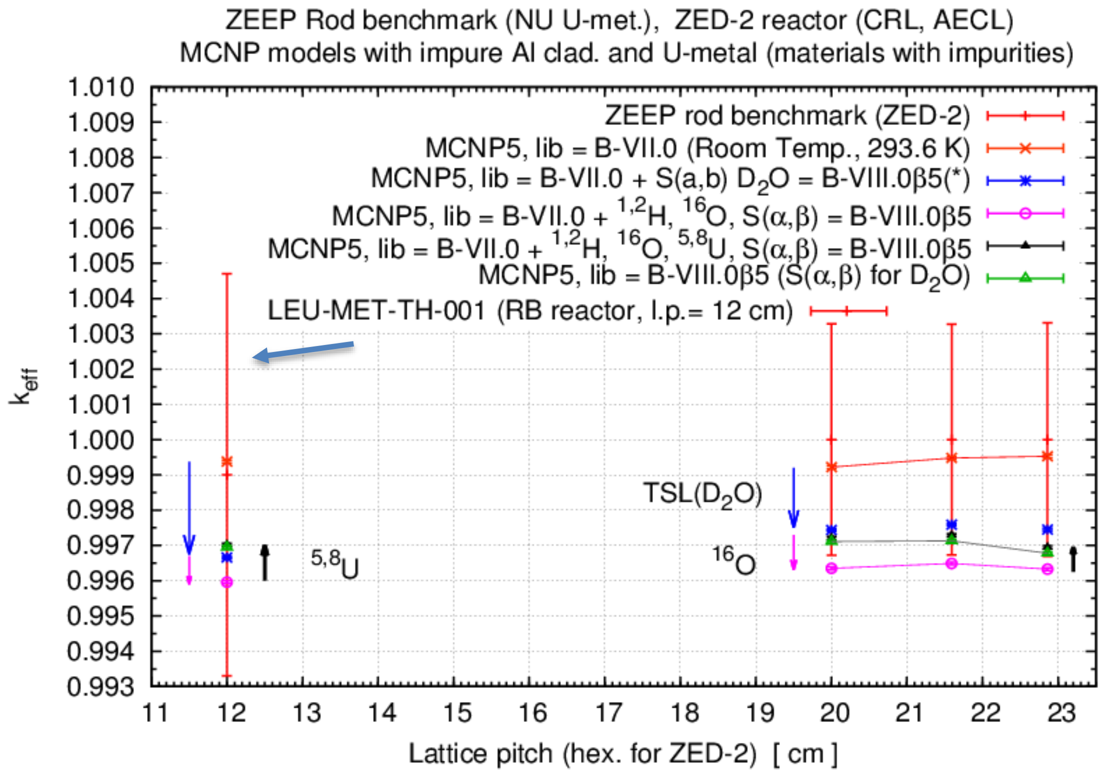
Benchmark k : k_{eff} = 1.000 ± 0.003 ; Fuel rods = U-metal (NU) in Al clad ;

All cases at "room T" (and can use ND libraries at T=293.6 K for testing);

Changed TSL for D_2O; **changed H-2 and O-16** ; changed ^{235}U and ^{238}U in U (NU)

Result: k_{eff} (ENDF/B-VIII.0_**β5**) ≈ 1.001 (modeling with MCNP, ±4 pcm)

ZEEP rod benchmark (LEU-MET-THERM-003) 2



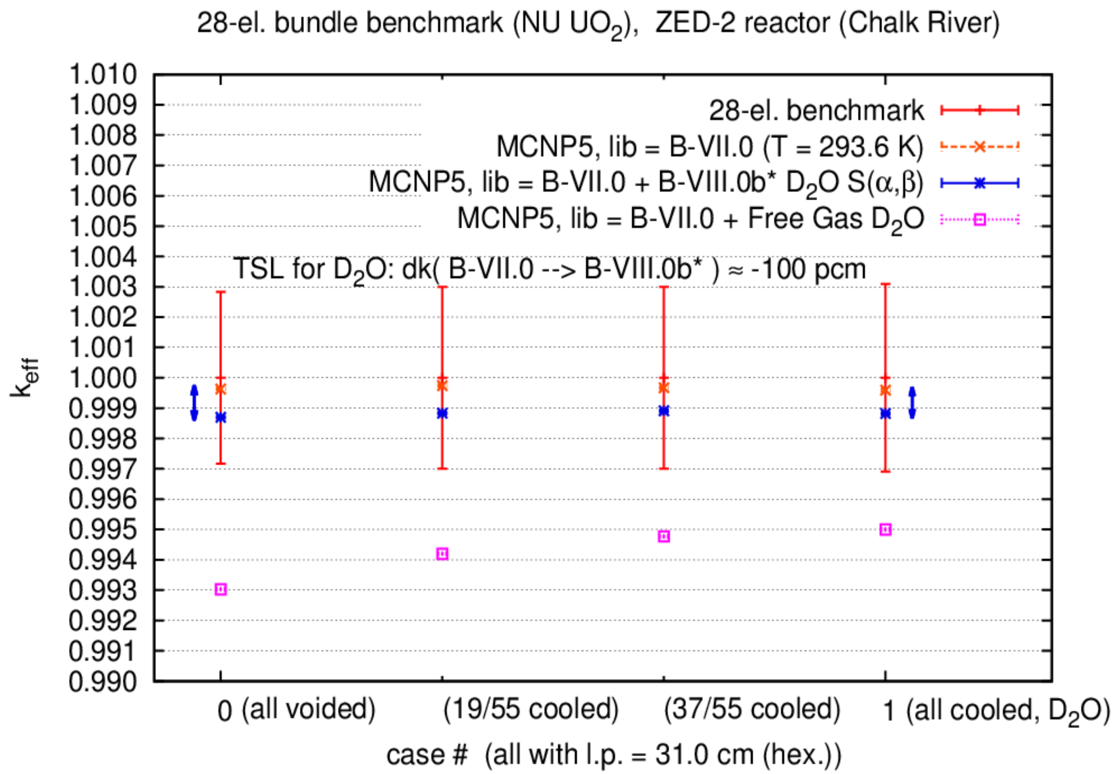
Fuel = U-metal and Clad = Al **with impurities** taken from mass-spec. measur.

Changed TSL for D_2O; changed H-2 and **O-16** ; changed U-235 and U-238 ;

Result: k_{eff} (ENDF/B-VIII.0_**β5**) ≈ 0.997 (modeling with MCNP, ±4 pcm); biased (?)

Question: any bias in k_{eff} with *l.p.* in rod-type (heavy water) benchmarks ?

28-el. bundle benchmark (ZED2-HWR-EXP-001)

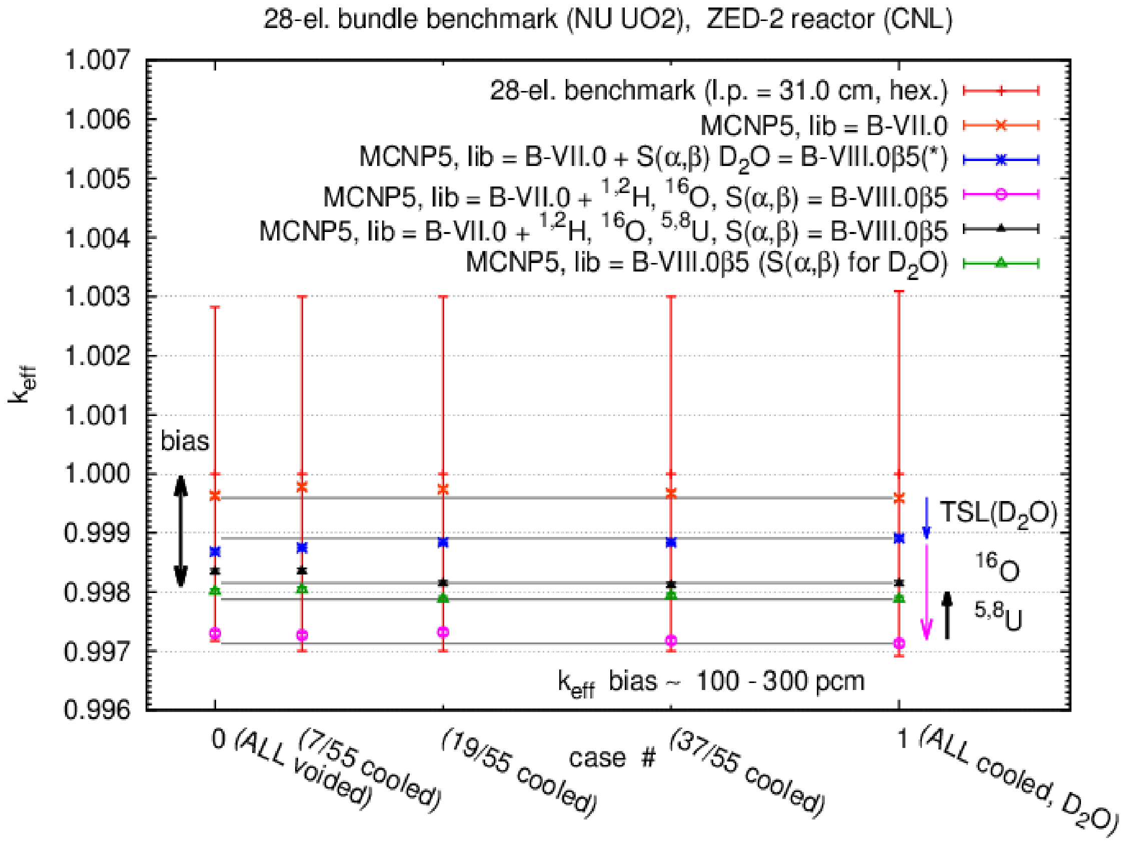


Benchmark: k_{eff} = 1.000 ± 0.003; Fuel = UO_2 (NU) and Clad = Zr alloy ; room T;

D_2O TSL worth is ~ 500 - 700 pcm ; |TSL worth| > Δk_benchmark ; we need it ;

Then changed TSL for D_2O, B-VII.0 → B-VIII.0β* : k_{eff} decreased by ≈ 100 pcm

28-el. bundle benchmark (ZED2-HWR-EXP-001)



Benchmark: k_{eff} = 1.000 ± 0.003; Fuel = UO_2 (NU) and Clad = Zr alloy ; room T;

Changed TSL for D_2O ; **changed H-2 and O-16** ; changed U-235 and U-238 in U

Result: k_{eff} (ENDF/B-VIII.0_β5) ≈ 0.998 (modeling with MCNP, ±4 pcm)

CVR bias (= k_{eff}(voided) – k_{eff}(cooled)) with B-VIII.0_β5 (?) **no evidence …**

ZED-2 reactor benchmarks: a lot of Graphite [*reflectror*] and Al (*calandria*, …)

LEU-MET-THERM-003, k_{eff} = 1.000 ± 0.003

k_{eff} (ENDF/B-VIII.0_**β5**) ≈ 1.001 (±4 pcm)

k_{eff} (ENDF/B-VIII.0_**β5**) ≈ 0.997 (±4 pcm) [with impurities in U-met and Al clad]

ZED2-HWR-EXP-001, k_{eff} = 1.000 ± 0.003

k_{eff} (ENDF/B-VIII.0_**β5**) ≈ 0.998 (±4 pcm), for all cases

These are the results with TSL applied to (reactor-grade) **D_2O** (^{1}H, ^{2}H, ^{16}O) ;

TEST : Graphite (Free Gas model for all nuclides) → Graphite TSL for Carbon (**6000.00c**)

Al (Free Gas model for all nuclides) → Al metal TSL for Al-27 (**13027.00c**)

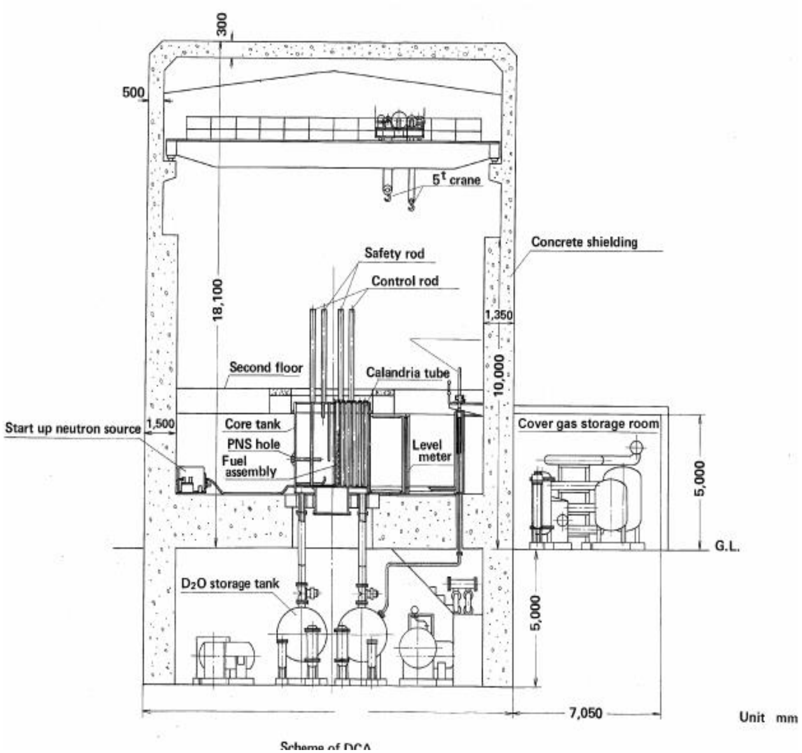
Essentially, we obtain **the same results for k_{eff}**, and | Graphite / Al TSL worth | < Δ*k*_benchmark ;

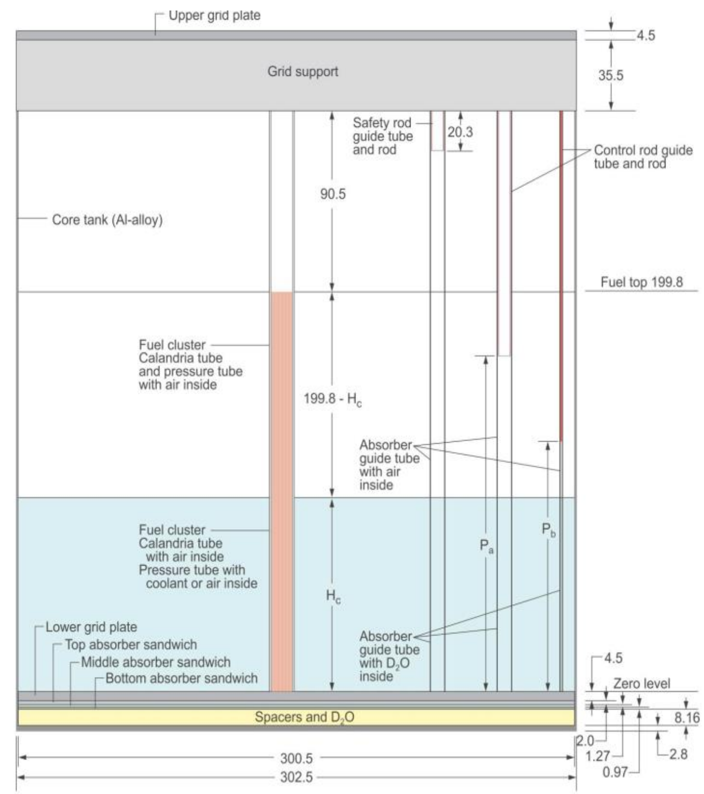
TSL worth of **Graphite TSL** and Al metal TSL is ~ **10 pcm** in these benchmarks ;

Example: case 1 (ZED2-HWR-EXP-001 **),** TSL Graph1,2 + Al, **B-VIII.0**_β5 ↓

k_{eff} = 0.998*01* (4) → **0.998*24*** (4) [TSL Graph(B-VII.0) + Al-met(B-VIII.0β)] ; 0.998*35* (4) ; 0.998*69* (4)

DCA benchmark (DCA-HWR-EXP-001) 1



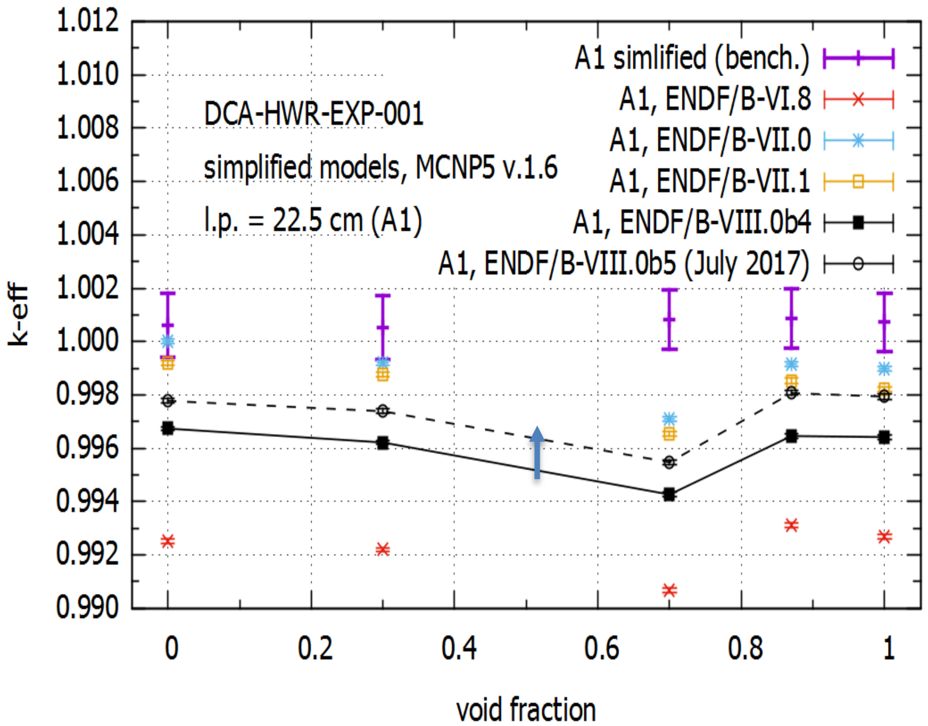


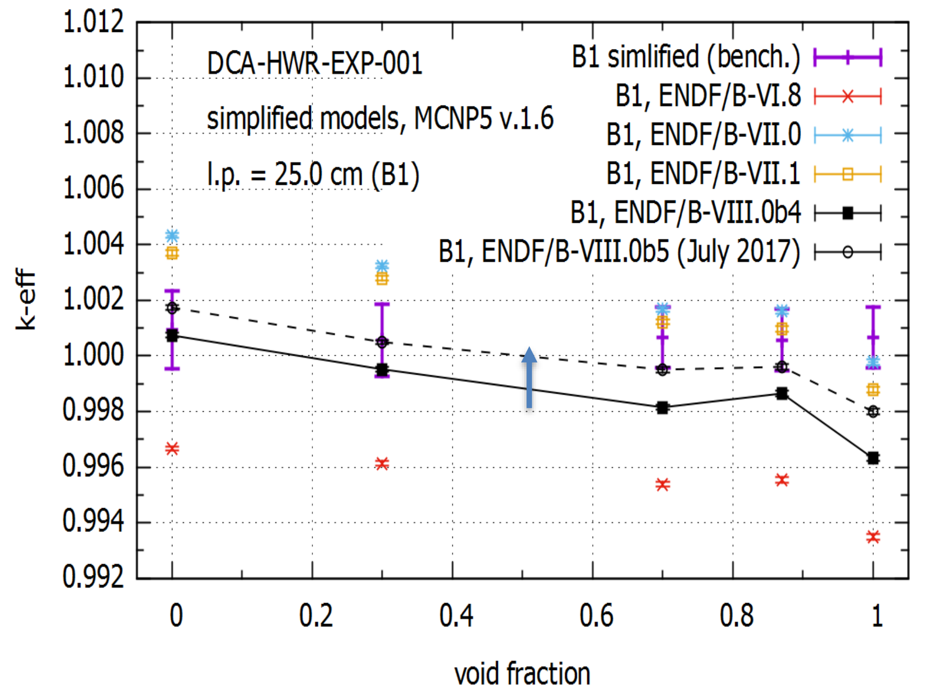
DCA is Deuterium Critical Assembly, Japan

DCA-HWR-EXP-001 (available from NEA/OECD **IRPhE Project**)

There is some interest in this benchmark in the context of **CVR bias** .

DCA benchmark (DCA-HWR-EXP-001) 2





DCA is Deuterium Critical Assembly, Japan

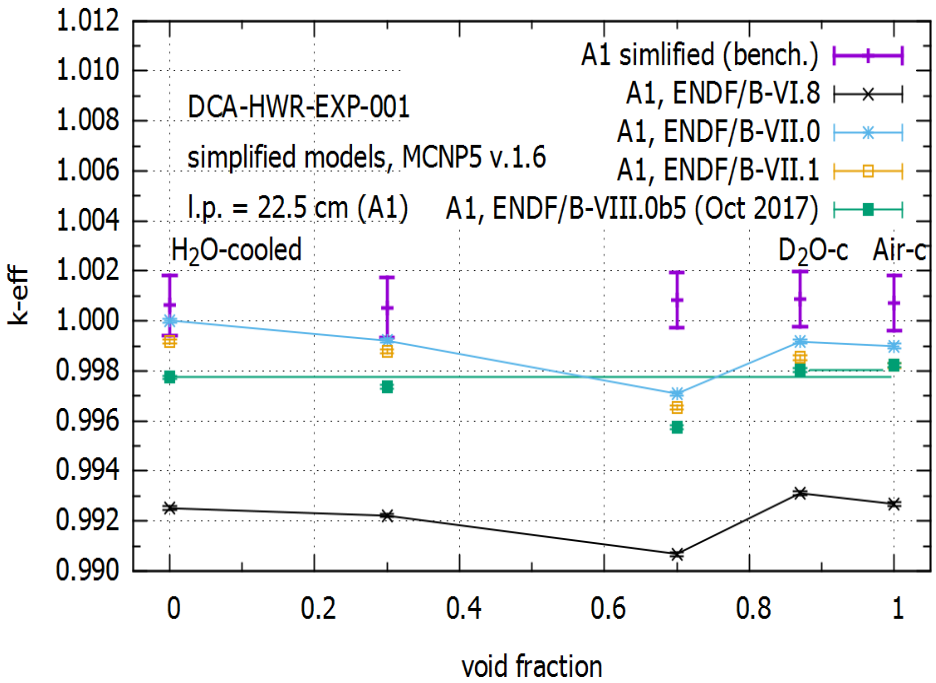
[Heavy water moderated crit. cores with 28-el. fuel bundles, sim. to ZED-2]

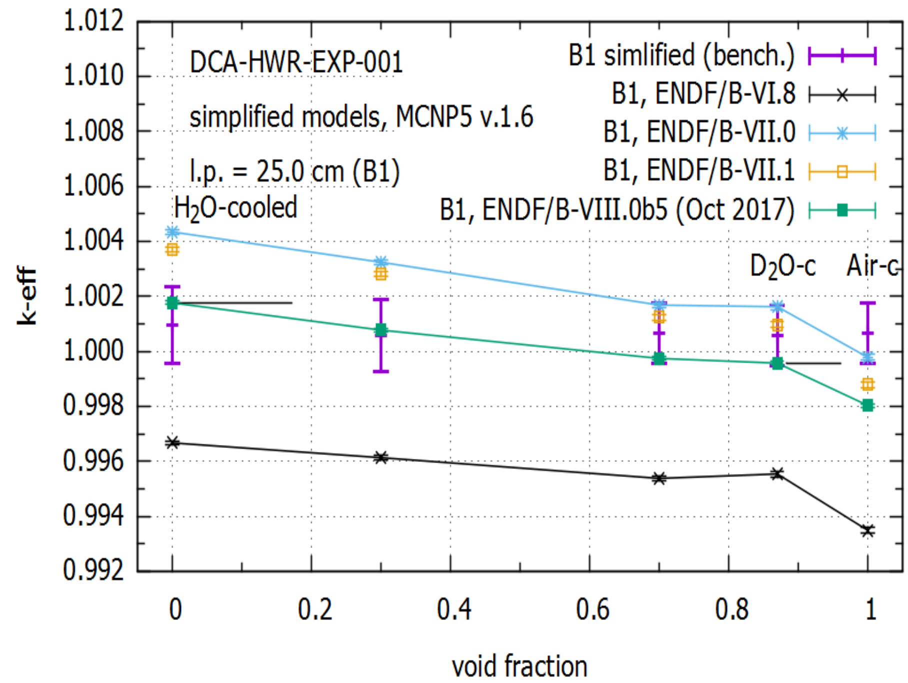
Fuel = LEU UO_2 (1.2%), in Al clad; **simplified benchmark models** were used ;

Simplified benchmarks: k_{eff} = 1.000 + ε ± 0.001 (ε ~ 50-80 pcm); all at room T ;

Note: results changed from **β4** to **β5** (modified evaluation of ^{2}H in **β5** improves k_{eff})

DCA benchmark (DCA-HWR-EXP-001) 3





Fuel = LEU UO_2 (1.2%), in Al clad; **simplified benchmark models** were used

For simplified benchmarks, k_{eff} = 1.000 + ε ± 0.001 (ε ~ 50-80 pcm)

For lattice pitch = 22.5 cm (left), **CVR bias** is insignificant (in B-VIII.0_**β5**) ;

For lattice pitch = **25.0 cm** (right), D_2O-cooled *vs*. air-cooled case: ~ 150 - 160 pcm, H_2O-cooled *vs*. air-cooled case: ~ 370 - 380 pcm ; better than in B-VII.0, VII.1

HEU-COMP-THERM-016, case 4 (T = 27 °C) 1

IGA reactor: U-Graphite blocks reflected by Graphite

Benchmark k_{eff} = 1.000 , with **±1.1%** uncertainty ;

Graphite: ρ = 1.71 g/cm^3 (core) ; ρ = 1.65 g/cm^3 (reflector) ;

Modeling: Lib = ENDF/B-VII.0 ; MCNP with CNL lib. at T = 293.6 K (20.4 °C)

	k_{eff} (MCNP)	
Free gas model for all nucl.:	1.03299 (7)	
Free gas model for all but H-1:	1.03465 (7)	[H-H_2O]
Free gas model for all but H-1, C-Graph (B-VII.0)	1.00862 (7)	
Free gas model for all but H-1, C-Graph (IKE-2005)	1.00926 (7)	

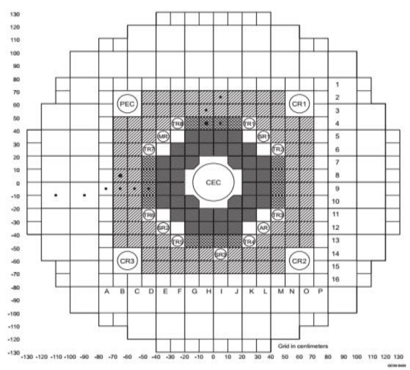
Graphite TSL worth ~ 2000 - 3000 pcm, > Δk_benchmark ;

This is **thermal** benchmark:

average neutron lethargy causing fission ~ 0.06 eV ;

thermal fission fraction: ~ 93% ;

above thermal leakage fraction: ~ 9.6% ;



HEU-COMP-THERM-016 (Graphite benchmark) 2

case 4 (T = 27 °C)

Lib = ENDF/B-VIII.0_β5 (at 293.6 K), with MCNP

Benchmark k_{eff} = 1.000 , with ±1.1% uncertainty

	k_{eff} (MCNP)	
Free gas model for all nucl.:	1.02694 (7)	
Free gas model for all but H-1:	1.02827 (7)	[H-H_2O]

different versions / models of Graphite TSL ↓

Free gas model for all but H-1, C-Graph (B-VII.0)	1.00336 (7)	
Free gas model for all but H-1, C-Graph (IKE-2005)	1.00389 (7)	

B-VIII.0 : Graph1 = crystalline graphite ; Graph2 = reactor graphite

Free gas model for all but H-1, C-Graph1 (B-VIII.0β4)	0.99720 (7)	
Free gas model for all but H-1, C-Graph2 (B-VIII.0β4)	1.03728 (7)	(> 1.02827)
Free gas model for all but H-1, C-Graph1 (B-VIII.0β5)	1.00901 (7)	
Free gas model for all but H-1, C-Graph2 (B-VIII.0β5)	1.01959 (7)	

HEU-COMP-THERM-016 (Graphite benchmark) 3

case 4 ; with ^{12}C and ^{13}C : similar results !

Lib = ENDF/B-VIII.0_β5 (at 293.6 K), **6000.*c → 6012.*c and 6013.*c**

Benchmark k_{eff} = 1.000 , with ±1.1% uncertainty

	k_{eff} (MCNP)	
Free gas model (w. C-nat)	1.02848 (20)	[H-H_2O]
Free gas model (w. ^{12}C, ^{13}C)	1.02967 (20)	[H-H_2O]

different versions of Graphite TSL

From B-VIII.0_β4 → β5 , Graph1 = crystalline graphite ; Graph2 = reactor graphite

	β4		β5
C-Graph1 (w. C-nat)	0.99722	→	1.00890 (20)
C-Graph2 (w. C-nat)	1.03747	→	1.01937 (20)
C-Graph1 (w. ^{12}C), ^{13}C free gas	0.99901	→	1.01046 (20)
C-Graph2 (w. ^{12}C), ^{13}C free gas	1.03797	→	1.02099 (20)
C-Graph1 (w. ^{12}C & ^{13}C)	0.99704	→	1.00965 (20)
C-Graph2 (w. ^{12}C & ^{13}C)	1.03760	→	1.02008 (20)

Conclusion and Future Outlook

ENDF/B-VIII.0_β5 performs very well for selected heavy water critical benchmarks (at room temperature),
namely, modeling ZED-2 reactor (Canada) and DCA (Japan).

We checked for possible biases in k_{eff} with changing lattice pitch and also for CVR bias (when applicable).

Left for future study:

- **selection and studying ZED-2 high-temperature benchmarks with ENDF/B-VIII.0_β5 ;**
- **extended study of DCA configurations (with Dr. I. Attieh, CANDU Inc.);**
- **more tests with TSL's from ENDF/B-VIII.0_β5 collection:**
  H_2O, D_2O, and Graphite, metals, and UO_2 , …
- **MCNP and SERPENT : consistent models for ZED-2 benchmarks using ZED2MCNP and ZED2Serpent generator**

Acknowledgement

Thanks to our CNL colleagues:
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CANDU Inc. (*SNC-Lavalin*) :
I. Attieh

CAB
F. Cantargi, J.R. Granada
==

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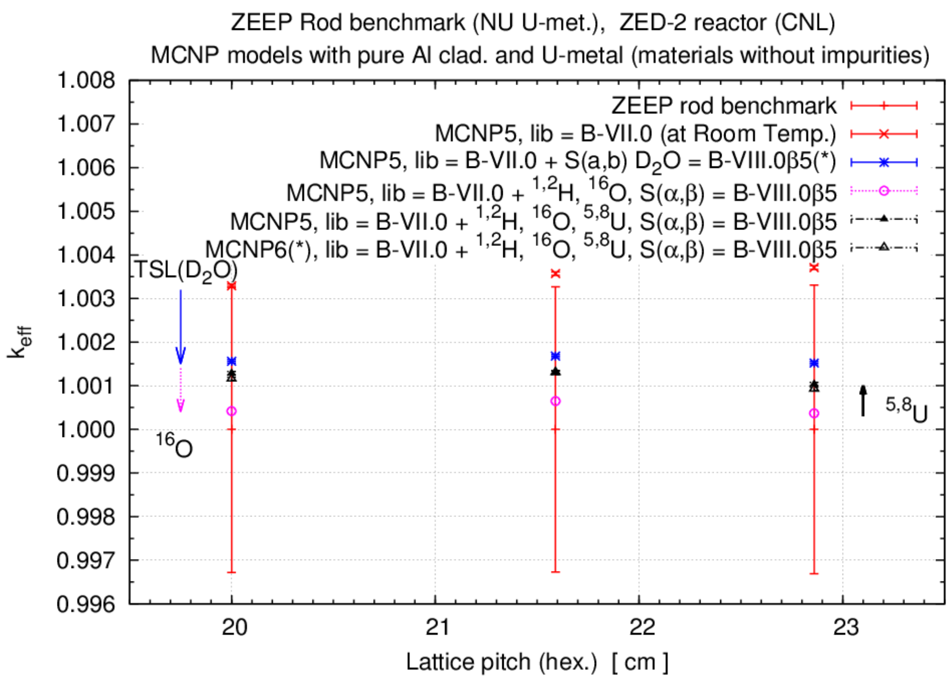
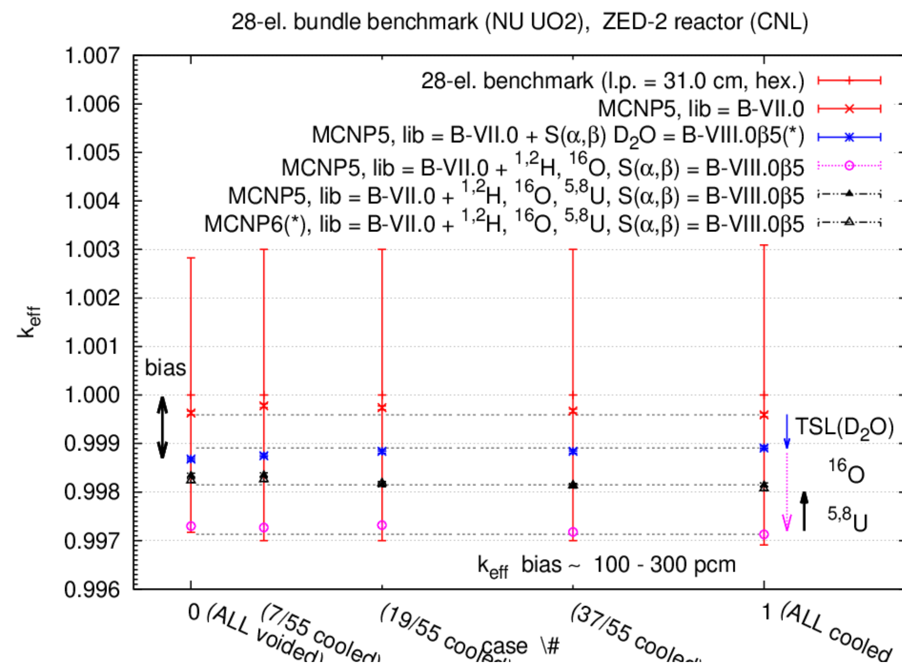
http://www.cnl.ca/en/home/default.aspx

Technical details for NJOY and MCNP users 1





Thermal ACE files for **MCNP6** :

Generated with **NJOY**, with iwt = **0** or iwt = **2** option in **ACER** (**both versions can be used**)

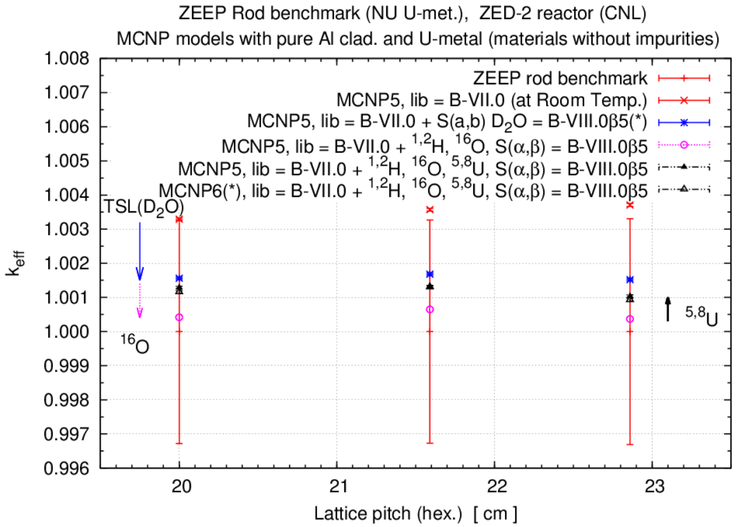
Difference in k_{eff} ? (yes, but expected to be insignificant)

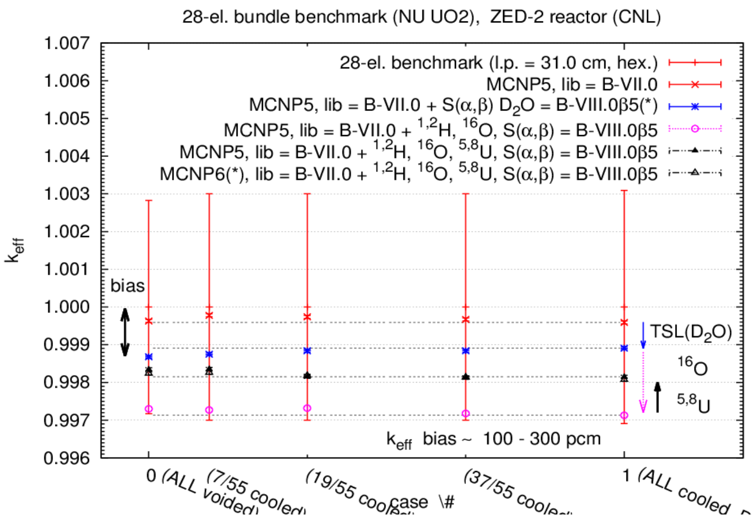
In heavy water benchmarks, ACE (iwt=**0**) *vs.* ACE (iwt=**2**) : <~ 10 pcm << Δ*k*_benchmark ;

Another important parameter for thermal ACE : nbin (# of equi-probable angles) in **THERMR**;

For many practical applications, **nbin = 32** is adequate (but **test it**, *e.g.*, 20 *vs.* 32 *vs.* 64 , ≤ **64**)

Technical details for NJOY and MCNP users   2





Thermal ACE files for **MCNP6** :

what to do **IF** you use MCNP6 with thermal ACE (**iwt=2**) and got "bad trouble" like this

```
Expire parameter is
cosine =          NaN
bad trouble in subroutine rotas of mcrun
```

However, there are **no NaN's** among scatt. cosines μ_j written in a thermal ACE file that upsets MCNP6 : **??**

Solution 1: have **two versions** of thermal ACE files (with the same **nbin**); switch to ACE (**iwt=0**), **re-run.**

Solution 2: check nbin ; decrease nbin in thermr (*e.g.*, is nbin = **32** O.K. for **iwt= 0/2** ?);
generate **two versions** of thermal ACE files **(iwt= 0/2);**
run the same case with both versions (if yes/yes , are the results ~ the same?).

Solution 3 : this is a rare event ; include "**RAND GEN=2**", try different rand. num. generators (=1 , =2 , =3) ;

Technical details for NJOY and MCNP users 3

NJOY processing, from TSL (MF=7) to thermal ACE:

thermr : can fix scattering cosines μ to +1.0 / -1.0 if they are outside (-1.0, +1.0) due to numerical issues. For example, you can see warnings like :

---message from calcem---1cos= 1.0068, set to 1. enow, e' = 8.19720E-02 1.18594E-04
---message from calcem---1cos= 1.0100, set to 1. enow, e' = 3.57681E-01 1.17171E-04

Note: when **thermr** finished, we expect that **all** scattering cosines μ_j **satisfy** $-1.0 \leq \mu_j \leq +1.0$

acer : can also fix scattering cosines, but it was implemented as a double protection layer [in aceth.f90, we opened *cosine warning messages* commented out in the official versions]

acer with **iwt = 0** : is expected to finish without warnings from aceth, **and so it does**.

acer with **iwt = 2** : surprise (**!**), got ***warnings*** like these

---warning from acesix--- cosine 1.09000303 outside [-1,1] range for e_in = 2.800000E-02
---warning from acesix--- cosine 1.14882338 outside [-1,1] range for e_in = 1.844370E-01

These cosines are too far outside **(-1.0, +1.0) to be just a numeric issue, so suspected a bug …**
… We found one flaw in the logic for processing with **iwt = 2 option,** and fixed it .

Technical details for NJOY and MCNP users 4

acer with **iwt = 2** : surprise (**!**), got ***warnings for "suspicious" cosines:***

---warning from acesix--- cosine 1.09000303 outside [-1,1] range for e_in = 2.800000E-02
---warning from acesix--- cosine 1.09625987 outside [-1,1] range for e_in = 1.720000E-01
---warning from acesix--- cosine 1.14882338 outside [-1,1] range for e_in = 1.844370E-01

Some cosines are too far outside **(-1.0, +1.0) to be just a numeric issue, so suspected a bug .**
We found one flaw in the logic for processing with **iwt = 2 option,** and fixed it .

acer with **iwt = 2**

In **aceth.f90 , we opened *cosine warning messages* commented out in the official versions**
and fixed one bug found in subroutine acesix [aceth_dan2a.f90]
Then, acer with **iwt = 2** finished **without any** "---warning from acesix--- cosine" .

Does it help with "bad trouble" (cosine = NaN) **?**

In some cases, yes it does, but not always …

We have to think about MC sampling algorithms that are used in MCNP6 for thermal ACE (iwt = 2).

We suspect that, if nbin > 30, for some scattering events $E \rightarrow E'$, P(μ), the arrays(s) of equi-probable cosines like μ_j = (..., 0.999, 1.000, 1.000) or μ_j = (..., 0.999, 1.000, 1.000, 1.000), j = 1, ... , nbin,
[fixed in **thermr** for some μ_j > 1.0] can upset MCNP6 sampling of μ **(iwt = 2).**