Testing the new Ice-water TSLs in the Computational Benchmark BUC/Phase-VII

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I. Objectives

- Testing the new ICE-water libraries
  - JEFF-3.3T3 + IceWater Bariloche's CAB model
  - ENDF/B-VIIIb4 (IceWater EVAL-OCT16 Holmes, Zerkle)

References:

1. *Sensitivity/uncertainty Analysis Applied to the Phase VII Benchmark, O. Cabellos, B. Cabellos, N. García-Herranz, J. Sanz, P. Ortego, C. Tore. International Workshop on Advances in Applications of Burnup Credit for Spent Fuel Storage, Transport, Reprocessing, and Disposition, 27-30 October, Córdoba, Spain*
2. *Keff Sensitivity/Uncertainty Analysis of the Phase VII Burnup Credit Benchmark, O. Cabellos, B. Cabellos, N. García-Herranz, PHYSOR 2010 – Advances in Reactor Physics to Power the Nuclear Renaissance, Pittsburgh, Pennsylvania, USA, May 9-14, 2010*
3. ***UPM-CSN Agreement on Burnup Credit 2009-2013***

II. BUC Phase-VII Benchmark

"*The main objective of this benchmark, is to study the ability of relevant computer codes and associated nuclear data to predict spent fuel isotopic compositions and corresponding keff values, in a cask configuration over the time duration relevant to spent nuclear fuel disposal, up to 1 000 000 years*."

Criticality calculation

The criticality model for keff calculations is a representative cask loaded with 21 PWR-UO2 17×17 fuel assemblies.

Providing keff values for fresh fuel and isotopic compositions from the decay calculations (30 post-irradiation time steps, out to 1 000 000 years) for two cases involving:

- First set (ACT) of 11 actinides
- Second set (PFs) involving 14 actinides and 16 fission products

Set 1: Actinide-only burnup-credit nuclides (11 total)
^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, and ^{241}Am
Set 2: Actinide + fission product burnup-credit nuclides (30 total)
^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{143}Nd, ^{145}Nd, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{151}Eu, ^{153}Eu, and ^{155}Gd

PWR UO2 discharge fuel compositions for decay calculations

- 4.5-wt% 235U initial enrichment
- 50 GWd/MTU burnup

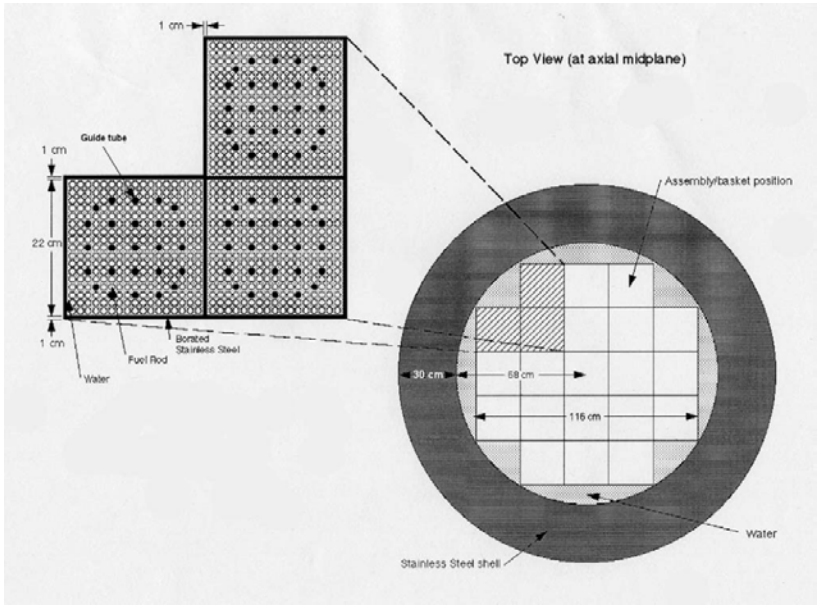


Figure. Cask model (top view)

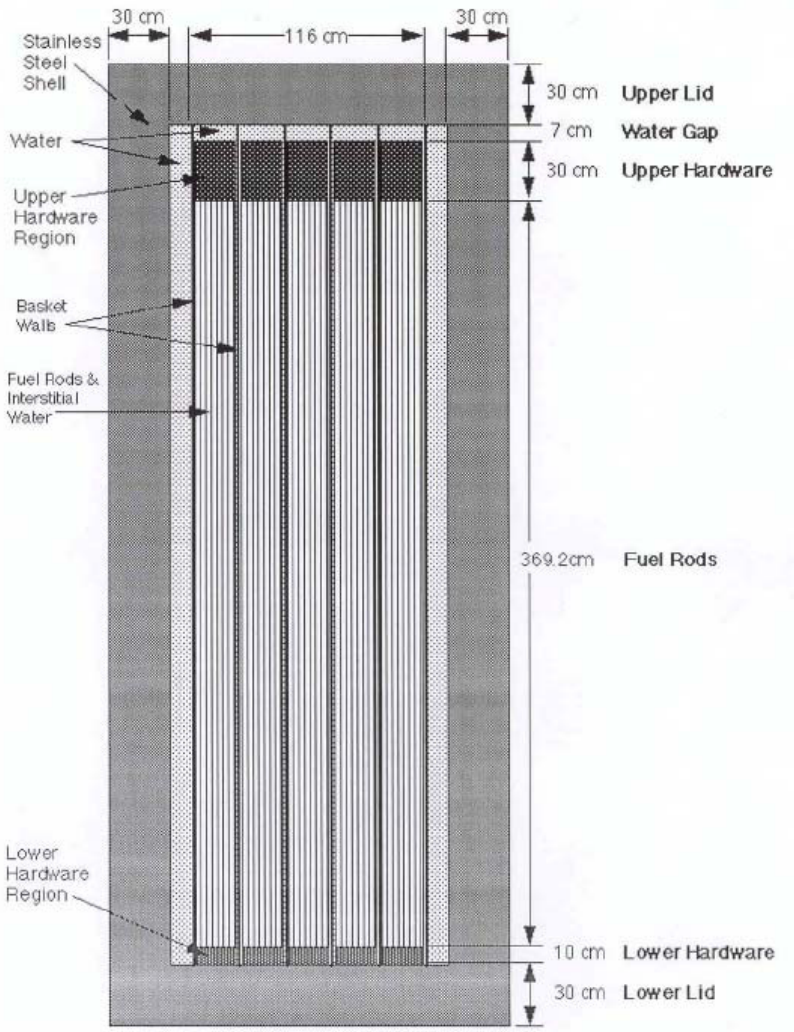
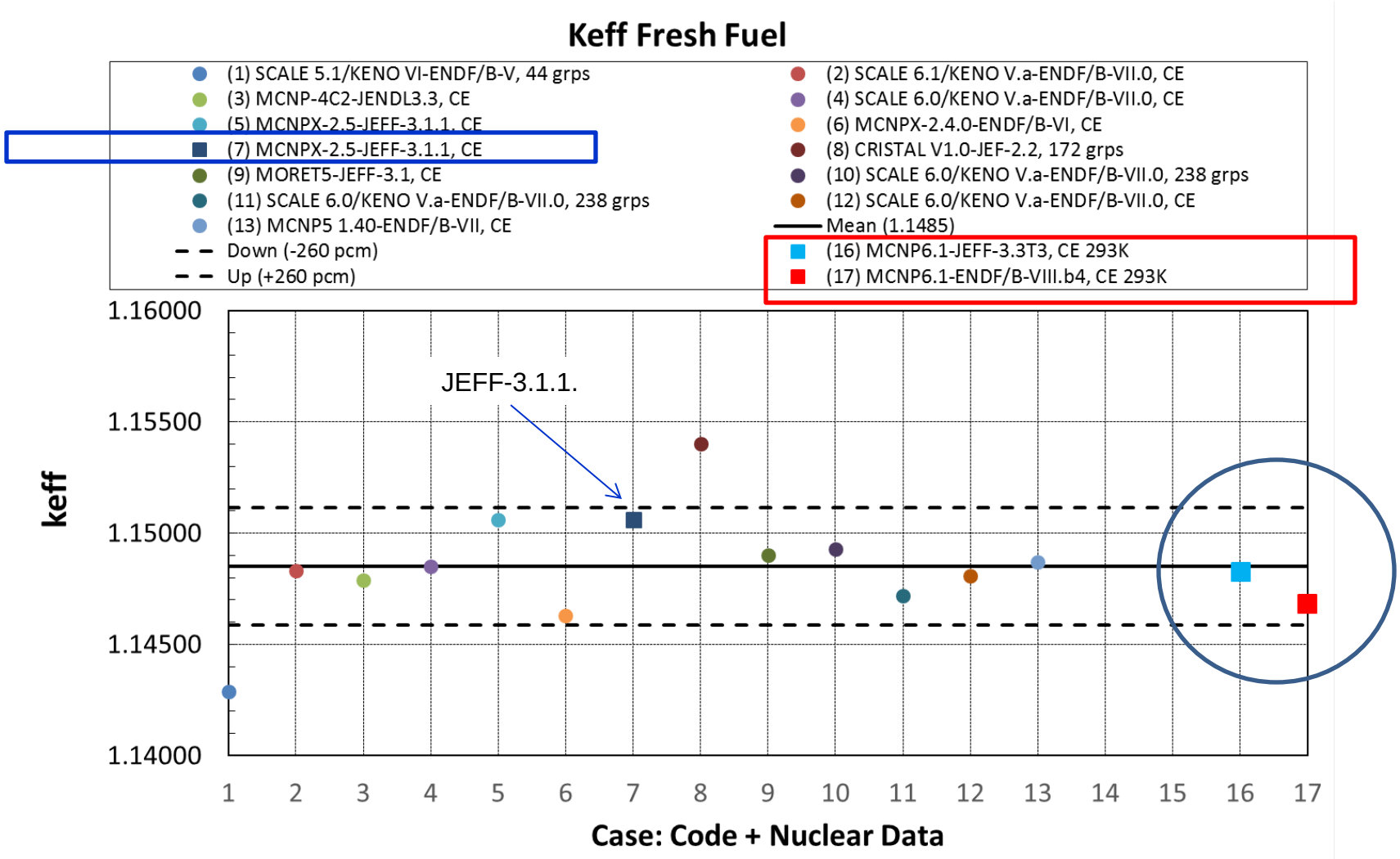


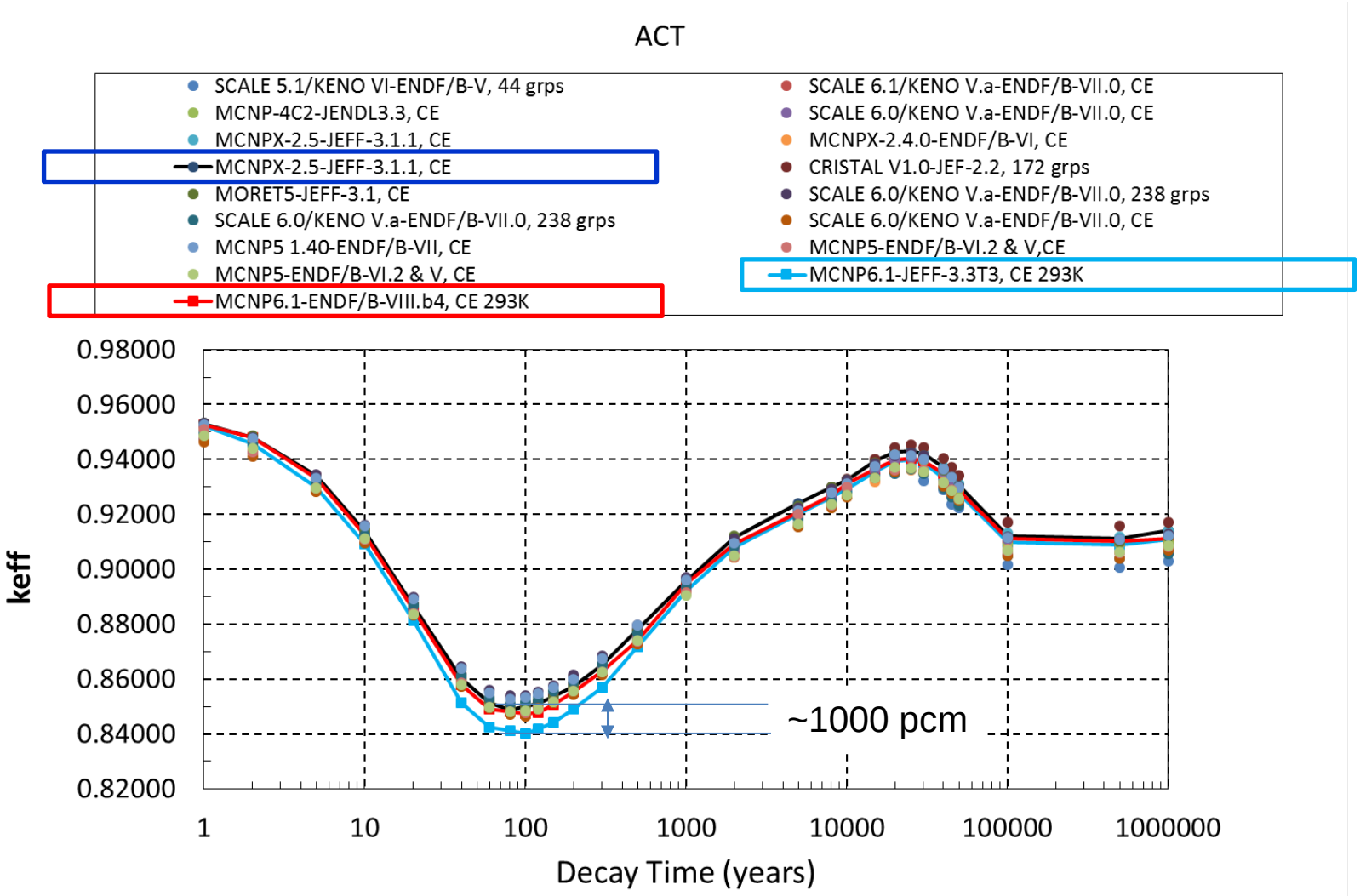
Figure. Cask model (side view)

Reference: *John C. Wagner and Georgeta Radulescu, Specification for Phase VII Benchmark UO2 Fuel: Study of spent fuel compositions for long-term disposal, NEA Expert Group on Burn-up Credit, November, 2008*

II. Keff values – mean value and std.



II Keff as a function of decay time for Actinide-only in fuel



```
moder / Extract thermal Scattering Law
1 61
' H-H2O    from Bariloche, CAB model'/
60 10
0/
moder / Extract/convert neutron evaluated data
1 21
'1-H-1 from JEFF-3.3T3'/
20 125
0/
reconr / Reconstruct XS for neutrons
21 22
'1-H-1 PENDF from JEFF-3.3T3'/
125 2/
0.001 0.0 / err tempr errmax (default = err*10)
'Reconstructed 1-H-1 PENDF from JEFF-3.3T3'/
'Processed with NJOY2012.050, at NEA 2017-03-20'/
0/
broadr / Doppler broaden XS
21 22 23
125 1 0 0 0./
0.001 / errthn thnmax errmax
233.0
0/
unresr
21 23 24
 125 1 1  1 /
233.0 /
1.E10 /
0/
thermr / Add thermal scattering data (free gas)
0 24 62
0  125 32 1 1    0       2 221 1 / Add free-gas model(mt=221)
233.0 /
0.001 10.0 / tolerance emax (max energy for thermal treatment in eV)
thermr / Add thermal scattering data (bound)
 61 62 27
10 125 32 1  4    0      2 222 1 /
233.0 /
0.001 10.0 /
acer / Prepare ACE files
21 27 0 28 29
2 0 1 .33/
'H-H2O   233.0 K from (JEFF-3.3T3) NJOY2012.50, NEA_MARCH2017'/
125 233.0 'lw14  ' /
 1001    0  0 /
 222 128  223  1  1 10.0 0/
acer / Check ACE files
0 28 0 71 81
7 1 1 -1/
/
stop
```

III. Processing TSL for ice light water

- o IceWater Bariloche's CAB model
  Processed with NJOY99.396 (only)

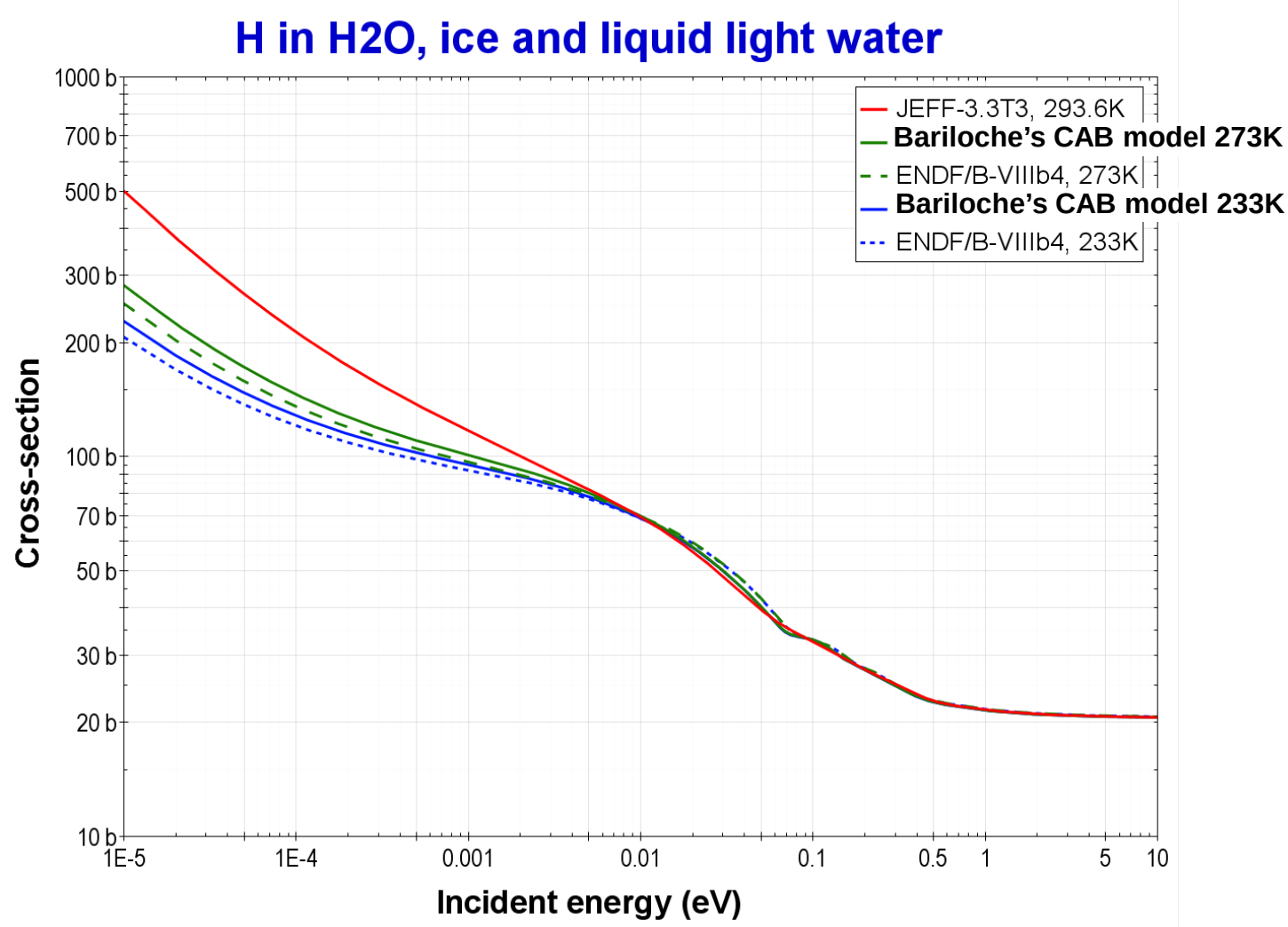
- o ENDF/B-VIIIb4 (EVAL-OCT16 Holmes, Zerkle)
  Processed with NJOY2012.82

Caution in ENDF/B-VIIIb4 !!!

```
thermr / Add thermal scattering data (bound)
 61 62 27
10 125 16 1  2    0 0     1 222 1 /
233.15 /
0.001 10.0 /
acer / Prepare ACE files
21 27 0 28 29
2 0 1 .08/
'H-H2O   233.15 K from (ENDFB8b4) NJOY2012.82, NEA_MARCH2017'/
125 233.15 'lw10  ' /
 1001    0  0 /
 222 64  223  1  1 10.0 0/
acer / Check ACE files
0 28 30 71 81
7 1 1 -1/
/
stop
```

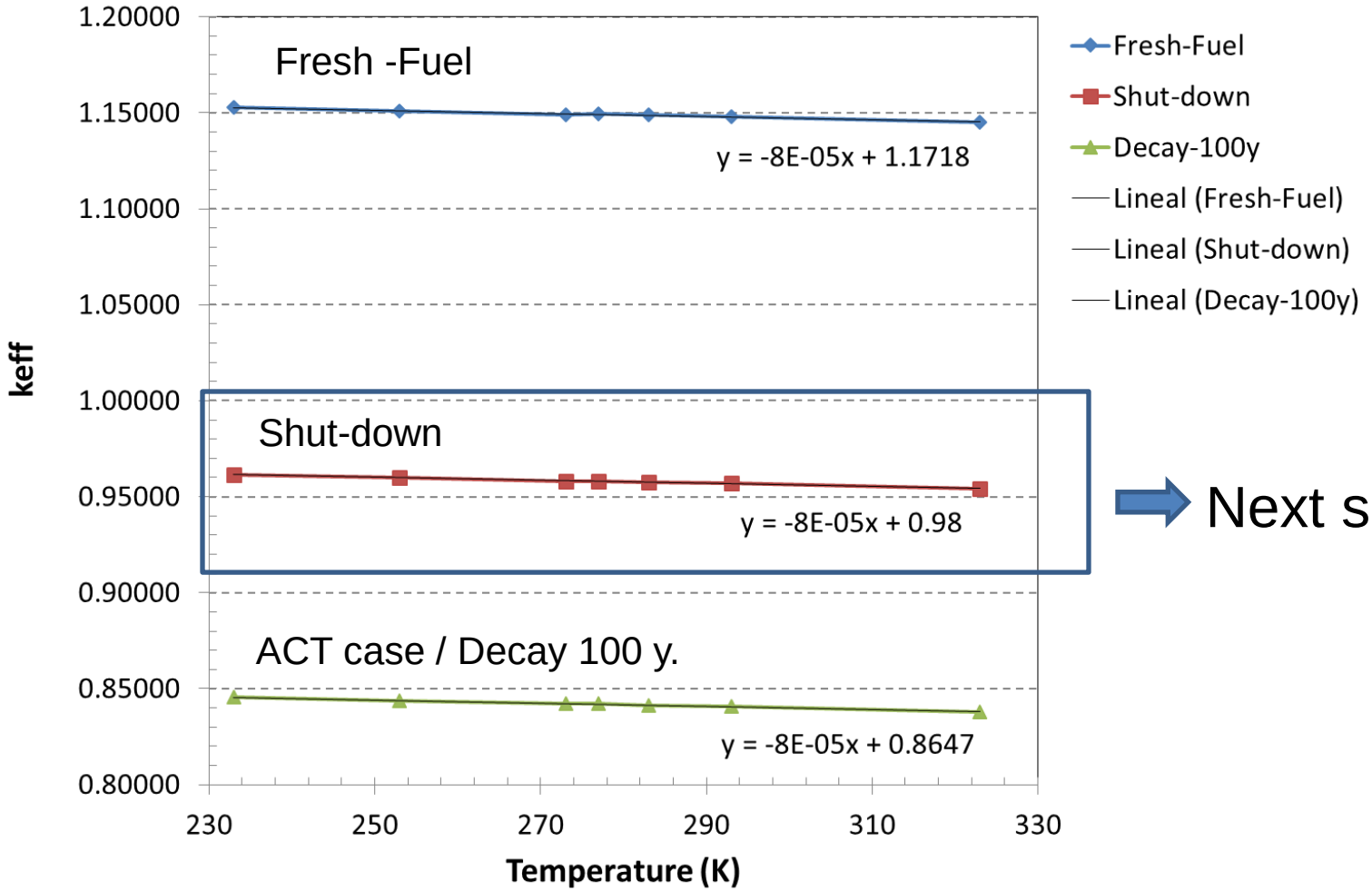
H atoms in H2O ?!!!

III. Comparison IceWater cross-sections



IV. Keff as a function of Temperature

- Nuclear Data: JEFF-3.3T3 + IceWater Bariloche's CAB model



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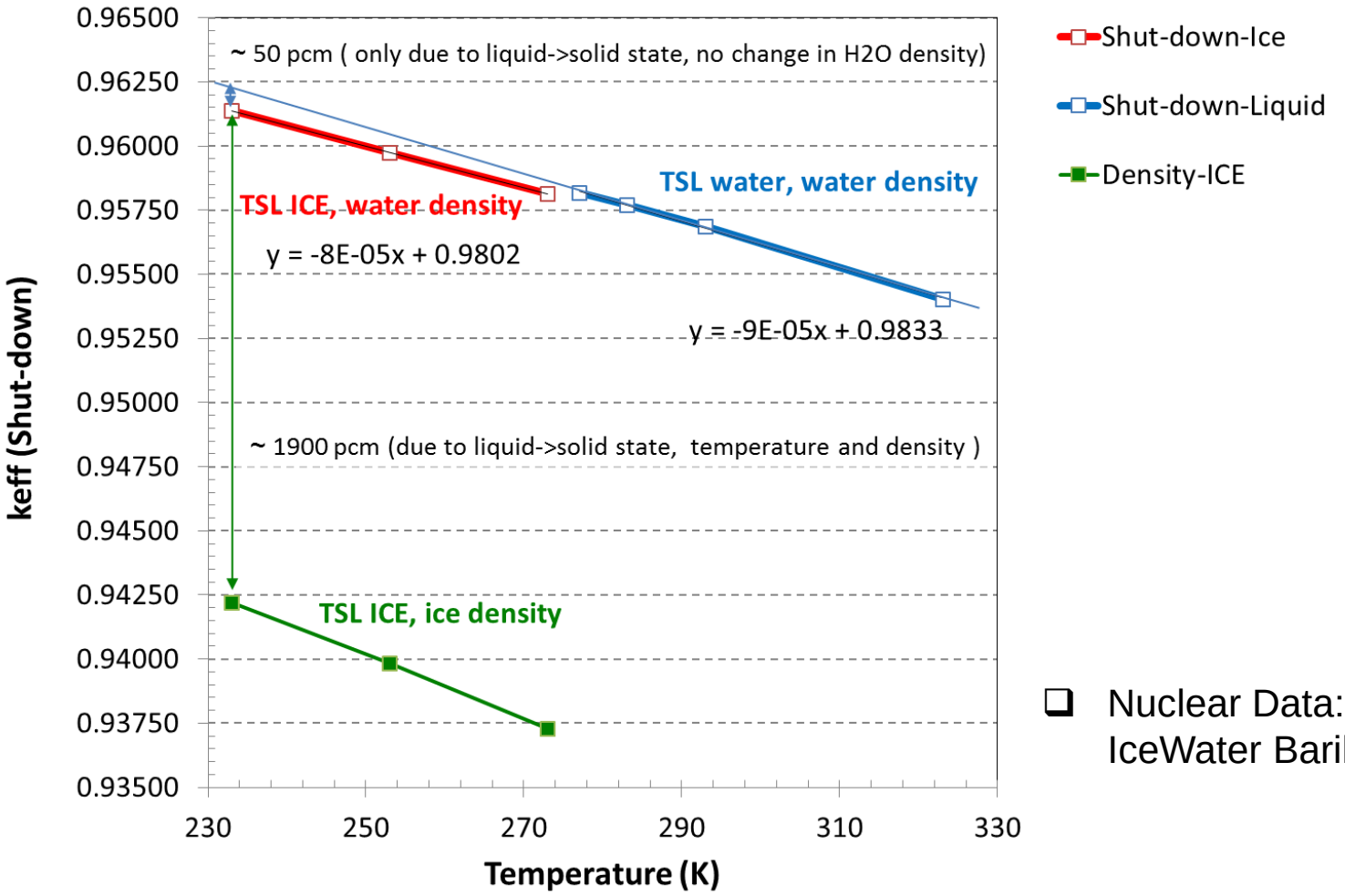
Keff as a function of Light Water Temperature and Density

Figure. keff results at shut-down

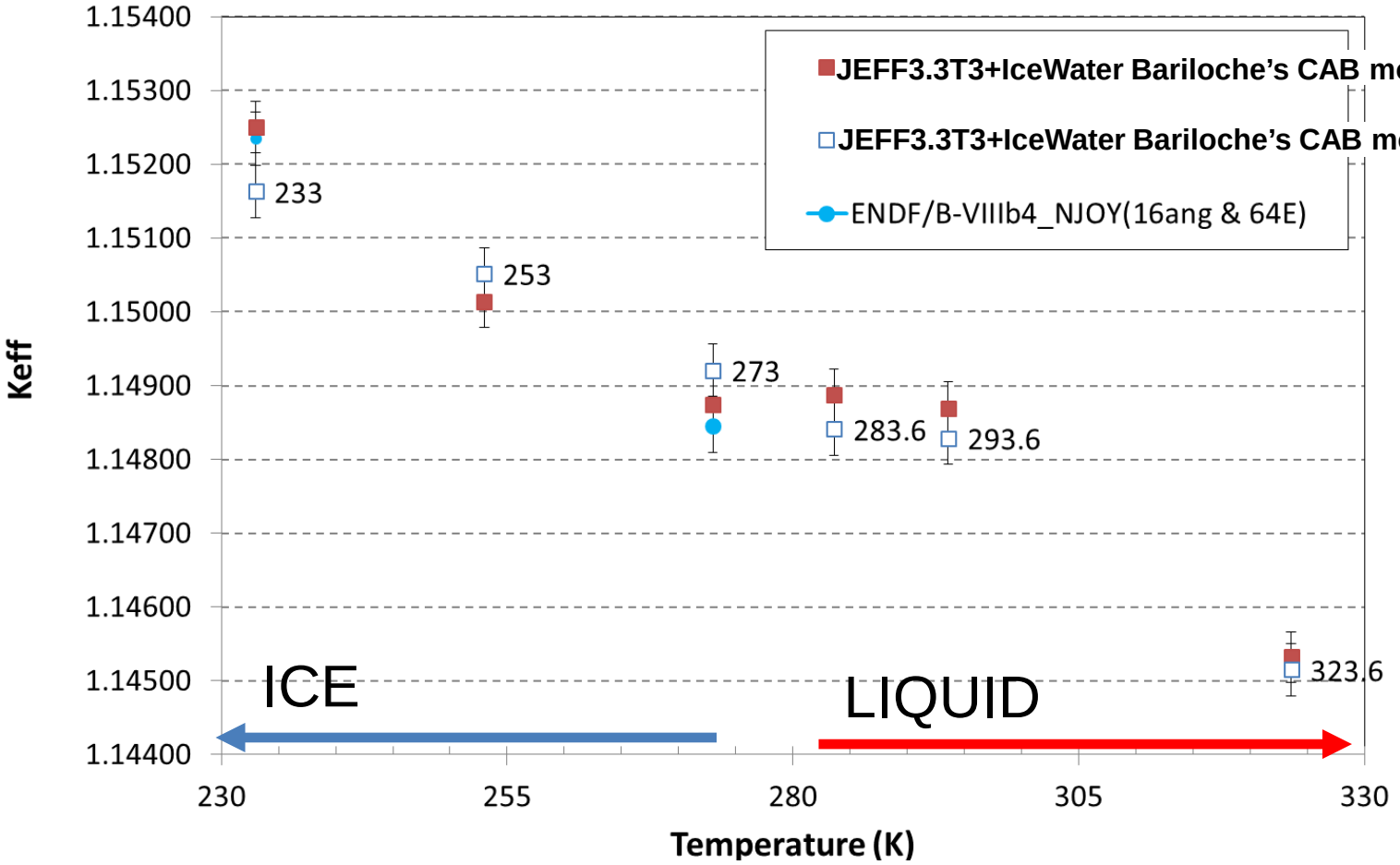


- Nuclear Data: JEFF-3.3T3 + IceWater Bariloche's CAB model

❑ Keff as a function of NJOY options

❑ Nuclear Data: “JEFF-3.3T3 + IceWater Bariloche’s CAB model” and ENDF/B-VIIIb4

Figure. keff results for fresh-fuel Benchmark Phase-VII



V. Conclusion

- ❑ Testing the new ICE-water libraries ✓

- o Reactivity change – Temperature and state of H2O

- o Importance of NJOY options (angle and energy bins)

- o “JEFF-3.3T3+IceWater Bariloche´s CAB model” versus ENDF/B-VIIIb4
  - Proposal in JEFF-3.3: To adopt IceWater Bariloche´s CAB model

Acknowledgment

- Thanks UPM & CSN providing MCNP PHASE-VII's inputs