SERPENT2 at CNL: nuclear data libraries, coupled (nγ) transport, and more

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Canadian Nuclear Laboratories | Laboratoires Nucléaires Canadiens

New Nuclear Data Library based on ENDF/B-VIII.0

Temperature (K)	ZAID Extension
293.6	.03c
600	.06c
900	.09c
1200	.12c
2500	.25c
0.1	.01c
250	.02c

ENDF/B-VIII.0 library [6] (released in February, 2018),
https://www.nndc.bnl.gov/endf/b8.0/download.html

Then LANL released ACE files, 2018 (for **MCNP6** usage)

https://nucleardata.lanl.gov/ACE/Production/Lib80x.html

*ACE-2 formatted **fast ACE files** can be converted to the standard ACE files.*
***Thermal ACE files** have to be reprocessed with NJOY, with a different iwt option, to be used by SERPENT / MCNP5 .*

*95242.**c is Am-242 (with $T_{1/2}$ = 16.02 h)*

*95642.**c is Am-242-**m1** (with $T_{1/2}$ = 141 y)*

Nuclear Data Library based on ENDF/B-VIII.0

Temperature (K)	Identifier	Extension	Temperature (K)	Identifier	Extension
293.6	hh2o	.09t	293.6	od2o	.09t
341		.29t	341		.29t
350		.30t	350		.30t
550		.32t	550		.32t
563		.33t	563		.33t
293.6	dd2o	.09t	293.6	**grph**	.09t
341		.29t	293.6	almet	.09t
350		.30t			
550		.32t			
563		.33t			

Thermal ACE files has to be reprocessed with NJOY2016,
with a different iwt option, to be used by SERPENT (iwt = default, not 2).

```
mat coolant -0.812 tmp 563.0 moder sab1 1001 moder sab2 1002 moder sab3 8016
        1001.03c  -1.097378E-03
        1002.03c  -1.991992E-01
        8016.03c  -7.992177E-01
        8017.03c  -4.857071E-04
                therm sab1 hh2o.33t
                therm sab2 dd2o.33t
                therm sab3 od2o.33t
```

Nuclear Data Library based on ENDF/B-VIII.0

E70CRL and **E80CRL_D**

- E70CRL = in-house ND library in ACE format based on ENDF/B-VII.0

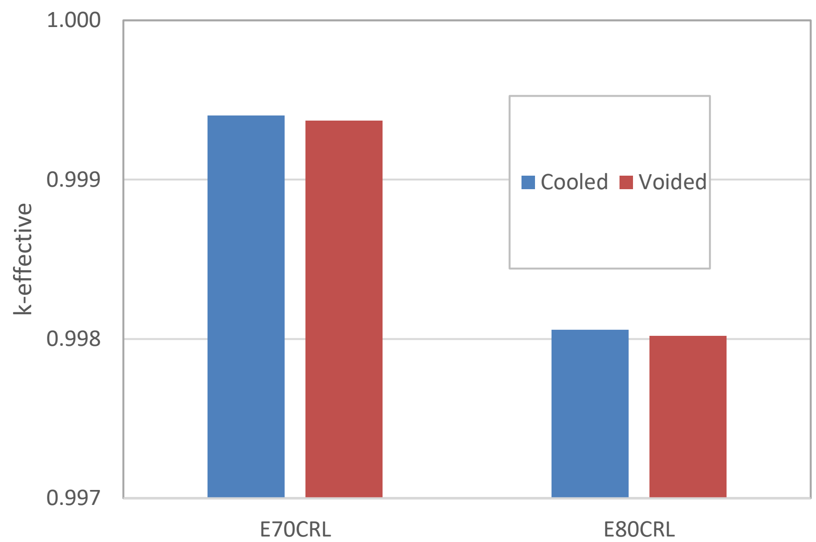
REF = D. Altiparmakov, *ENDF/B-VII.0 versus ENDF/B-VI.8 in CANDU® Calculations*, in Proceedings of PHYSOR 2010 – Advances in Reactor Physics to Power the Nuclear Renaissance, Pittsburgh, Pennsylvania, USA, May 9-14, 2010, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2010); also CW-115530-CONF-006, AECL, 2009.

- **E80CRL_D** is based on ENDF/B-VIII.0, 2018
  (neutron x-sections, decay data, and fission yield data)

```
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"
```

Nuclear Data Library based on ENDF/B-VIII.0

ZED-2 case	E70CRL	E80CRL_D
Cooled	0.999370 (60)	0.998058 (59)
Voided	0.999072 (61)	0.998019 (55)



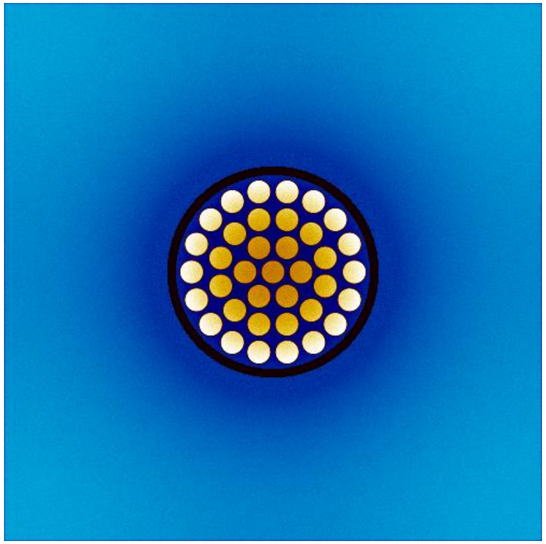
E70CRL and **E80CRL_D** ZED-2 Benchmark Results (*k*-effective, Serpent 2)

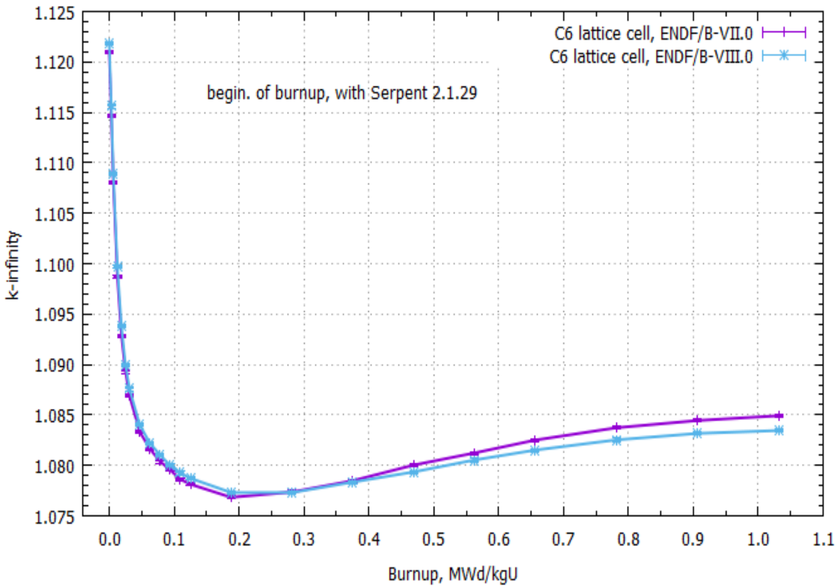
The core comprises 55 aluminum channels each containing 5 natural uranium 28-element bundles (**ZED2-HWR-EXP-001, IRPhEP Handbook**).

The new E80CRL_D library under-predicts the *k*-values by ~1.4 mk relative to those obtained with the E70CRL library

(new O-16, new S(α,β) data for D_2O in ENDF/B-VIII.0).

Nuclear Data Library based on ENDF/B-VIII.0





E70 (lib. distributed by Serpent) and **E80CRL_D** Results (*k*-effective, Serpent 2)

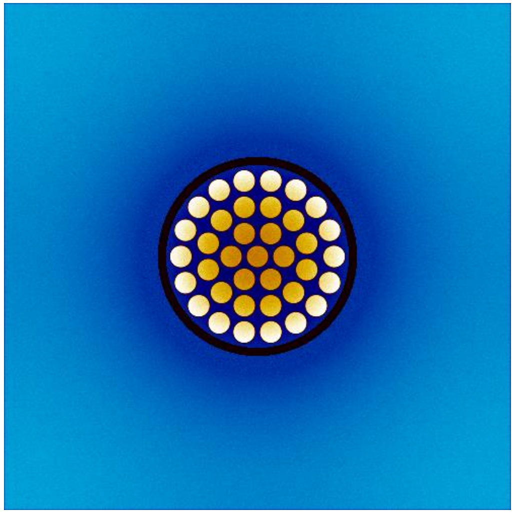
A simplified reactor lattice cell model of a 37-element CANDU-type fuel bundle was subjected to burnup with a constant bundle power of ~0.6 MW.

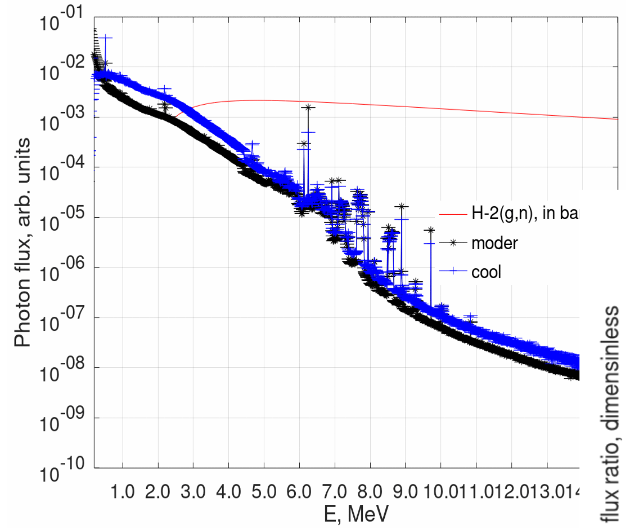
At the beginning of burnup (< 1 MWd/kgU), the k-inf values obtained with the two libraries are different by ~1 mk (100 pcm).

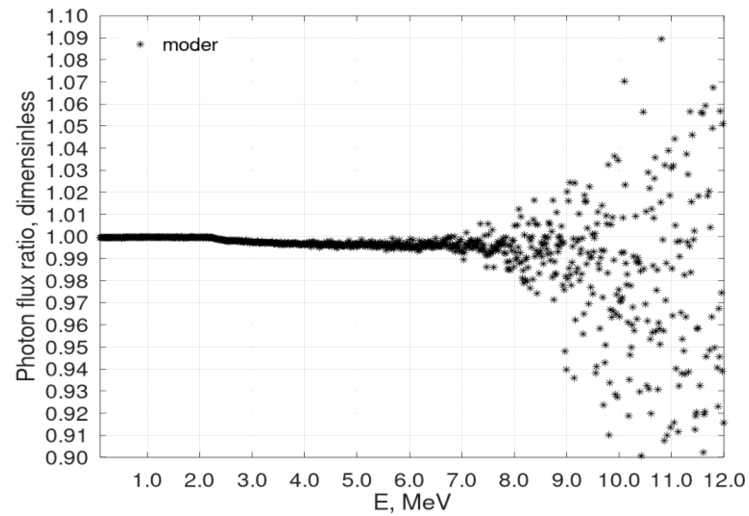
[memory usage: ~20G → ~**70G**]

% set bralib "/scratch/lib80xs/docs/sss_jeff31a.bra" : ?

Nuclear Data Library: photons







Photons:

set acelib "/path/neutron.xsdata" "/path/photon.xsdata"

Need photo-atomic data, 1000.12p

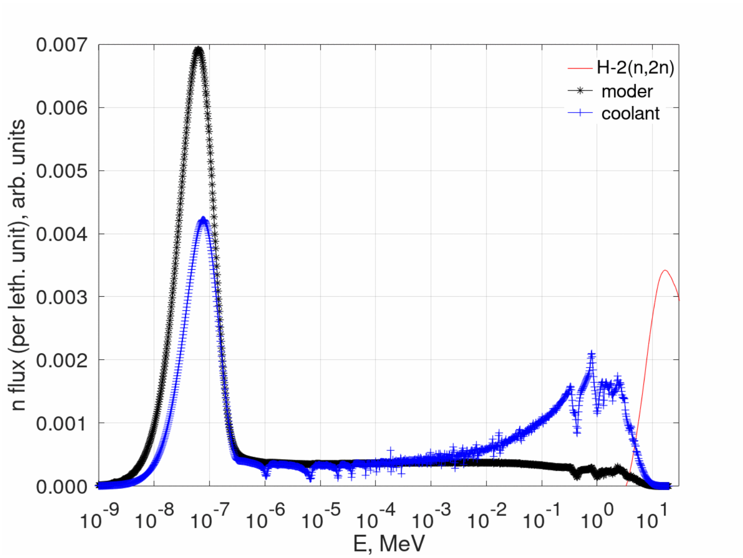
2000.12p (p files) **AND**

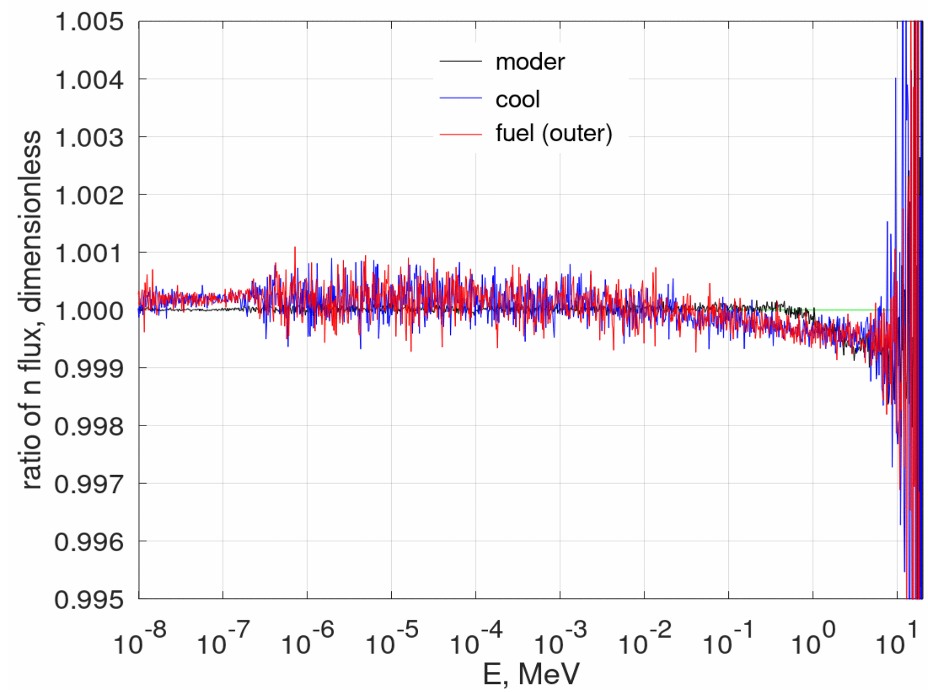
set pdatadir "/minerva/opt/SERPENT_REFDATA/photon_data"

+ (photo-nuclear option) : 1002.70u , 6012.70u, 6013.70u, … (u files)

Δk-inf ~ 0.6 mk (60 pcm), due to γ + H-2

Nuclear Data Library: photons





Photons: photo-atomic photo-nucler

set acelib "/path/neutron.xsdata" "/path/photon1.xsdata" "/path/photon2.xsdata"

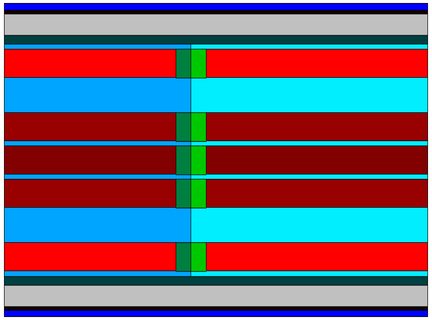
set pdatadir "/minerva/opt/SERPENT_REFDATA/photon_data"

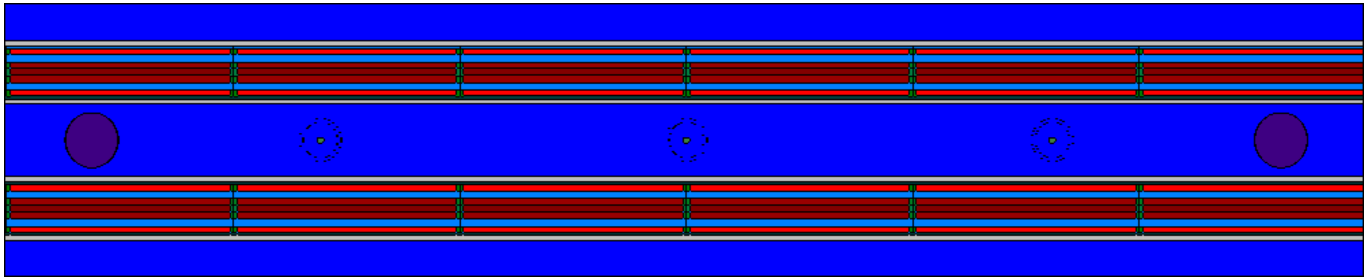
photo-nuclear option, mostly H-2(γ,n) : Δk-inf ~ +0.6 mk (+60 pcm);

compare with H-2(n,2n) : Δk-inf ~ +3 mk (+300 pcm).

NJOY2016: one can generate *.*p and *.*u ACE files (B-VII.1 $\rightarrow$ B-VIII.0)

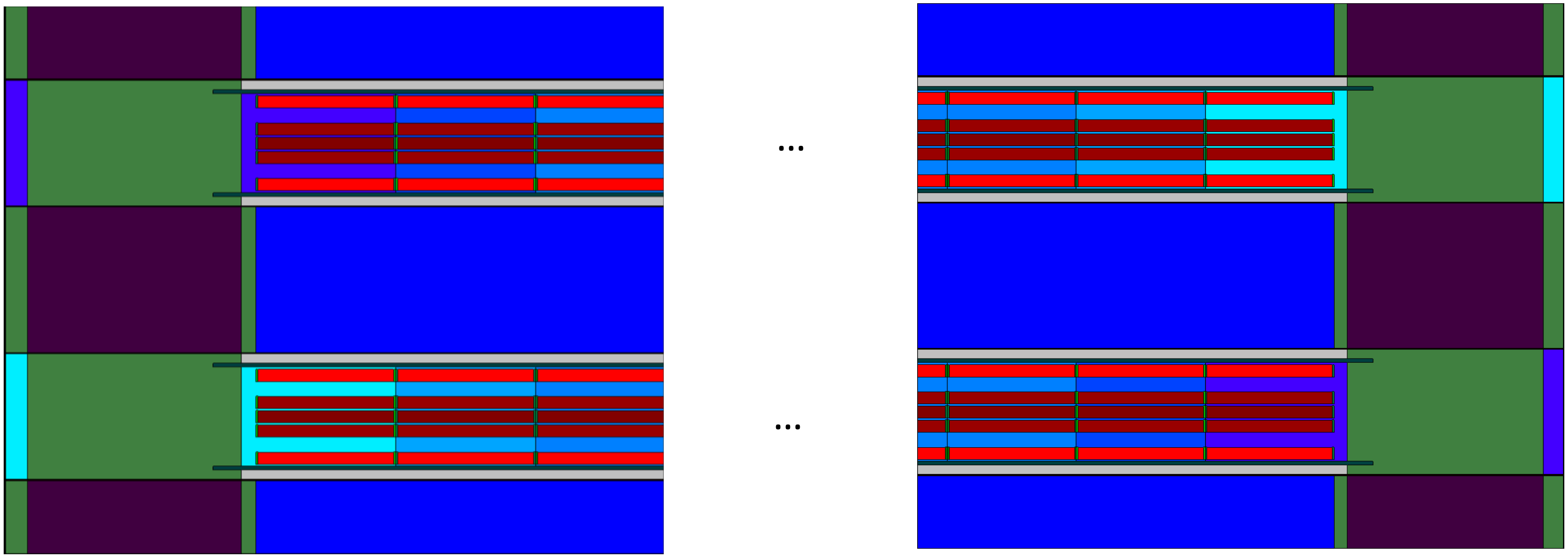
RP models with modern MC n/γ transport codes

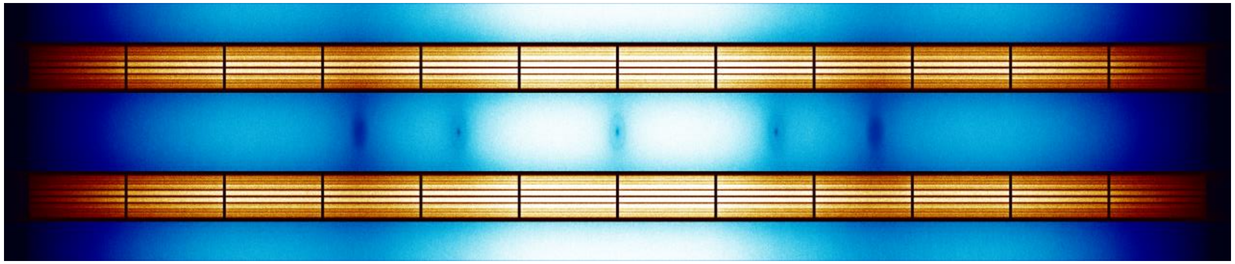




Details/refinement of reactor core components (*e.g.*, bundle end plates, LZ controllers, etc.) are developed due to necessity, *i.e.*, allowing answers to particular questions in Nuclear Engineering of CANDU (*e.g.*, peaking factors in bundle/channel power profiles, LZC reactivity worth, *etc.*)

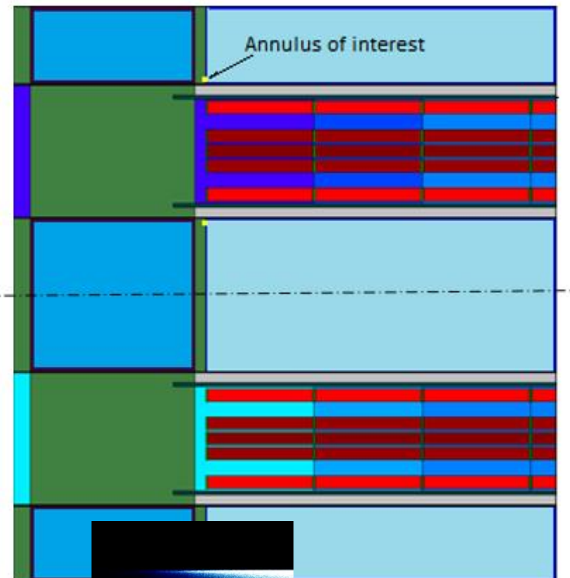
Rendition of RP models with modern MC transport codes

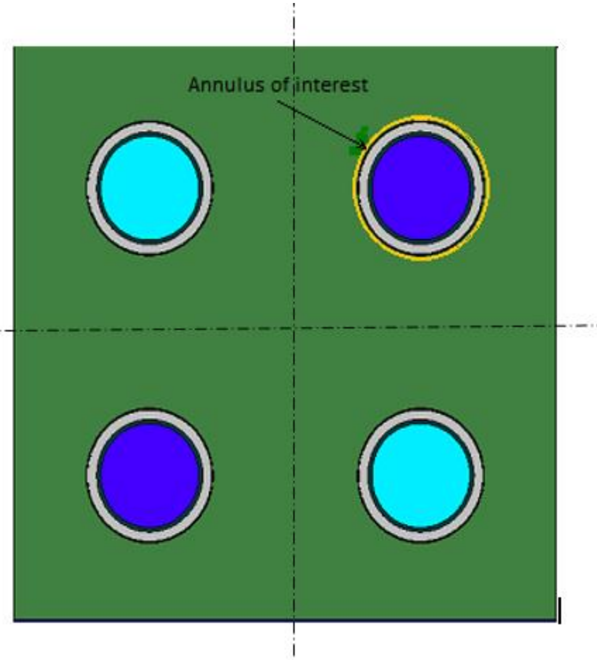


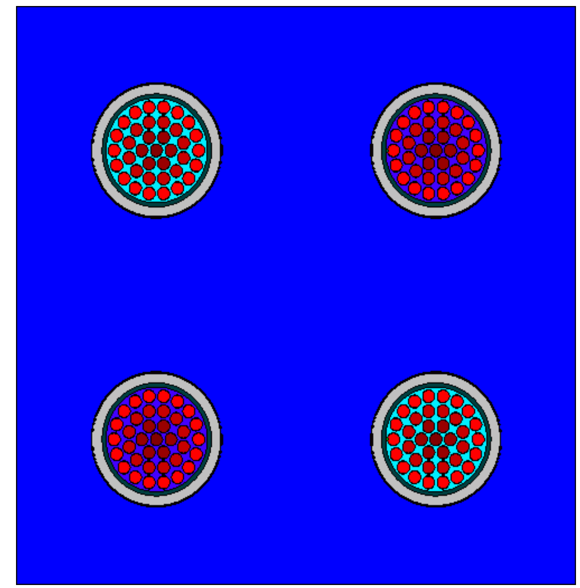


Present calculations using diffusion codes (SORO/RFSP) cannot capture the details of components (*e.g.*, PT roll joints, garter springs, *etc.*) important for material degradation analyses. These details can be included in modern MC simulations.

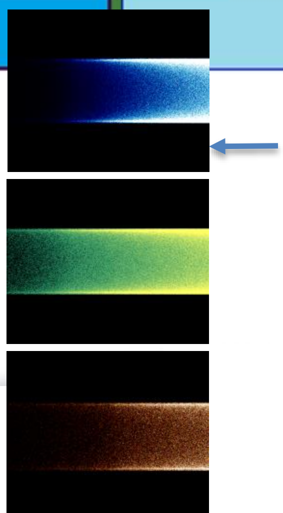
MC simulation examples: CT - Tube Sheet connection in 4-channel model with 12×4 37-el. Bundles





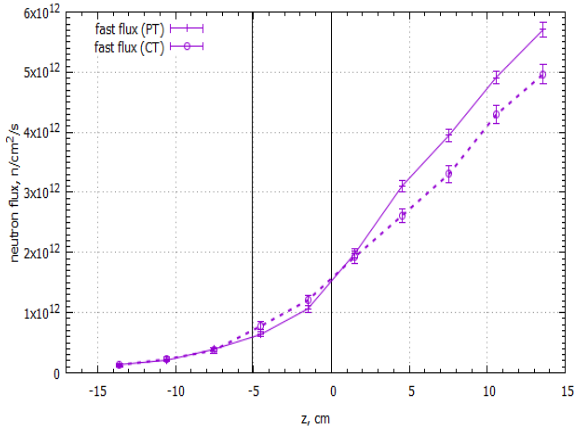


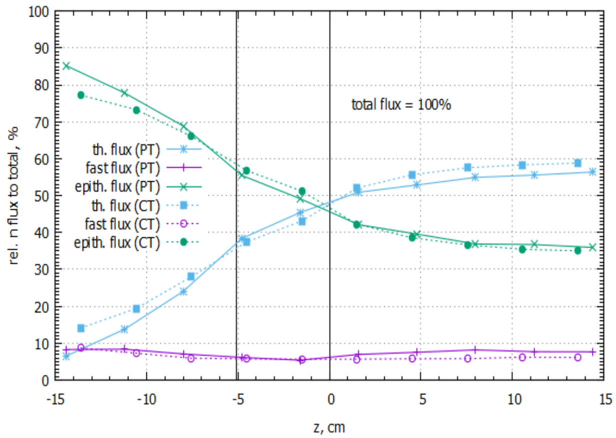
th.
epith.
fast

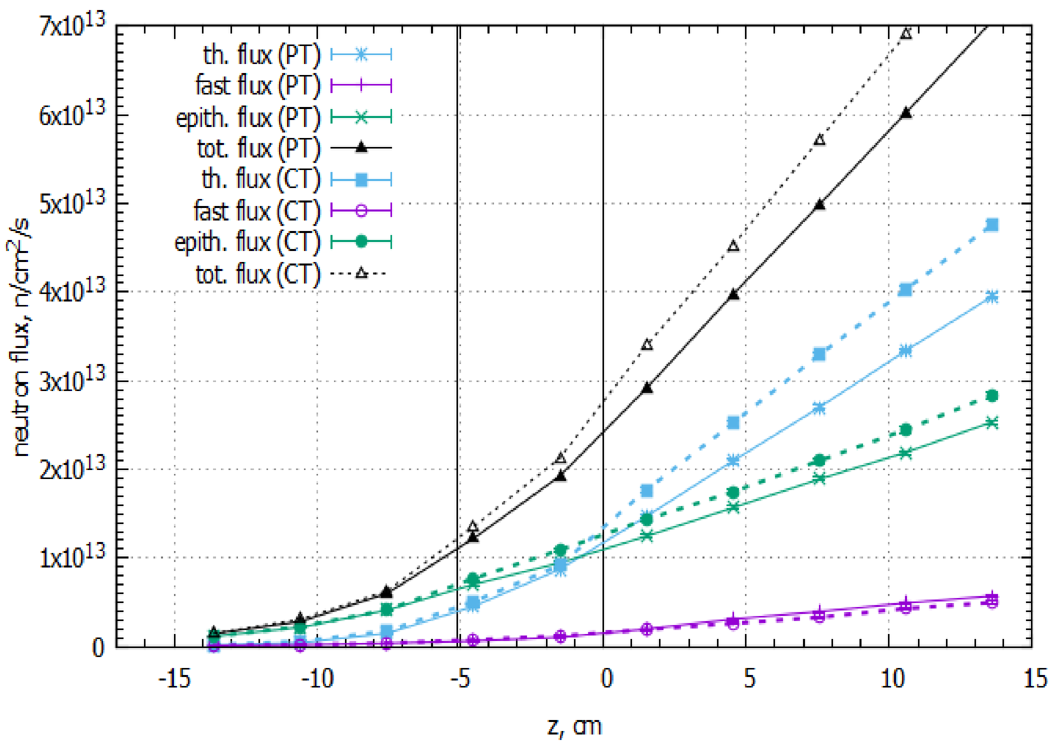


- 2D projection of thermal (blue), epithermal (green), and fast (orange) neutron flux along CT, covering ~ 30 cm of CT length, (15 cm in the active area & 15 cm outside of active area);
- Neutron spectra have been obtained in the simulations at Tube Sheet (TS), CT, and PT around CT – TS joint.

Example 1: CT - TS connection in 4-channel model







Neutron flux profile along CT and PT near the calandria tank (TS: ~ –5 to 0 cm); thermal, epithermal, fast, and total, 15 cm in the active area / 15 cm outside of it.

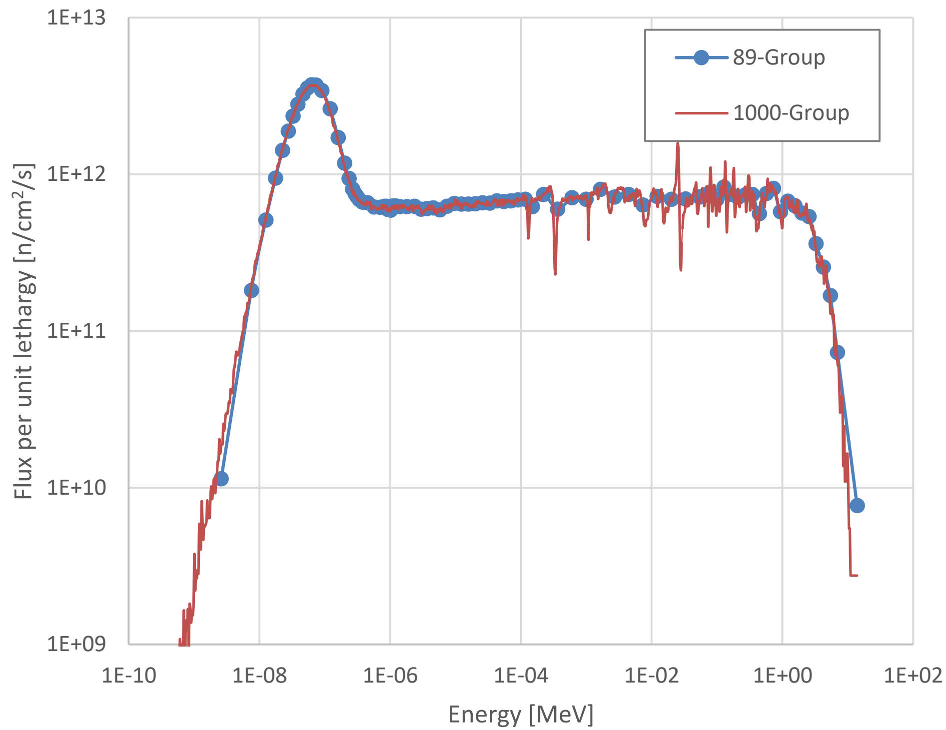
Spectral indices at the periphery are *not* the same as those of the active area.

Example 2: CT - TS connection in 4-channel model

TS annulus:
Total n flux ~ 1.8×10^{13} n/cm²/s, (one-ch. power ~ 7.2 MW);

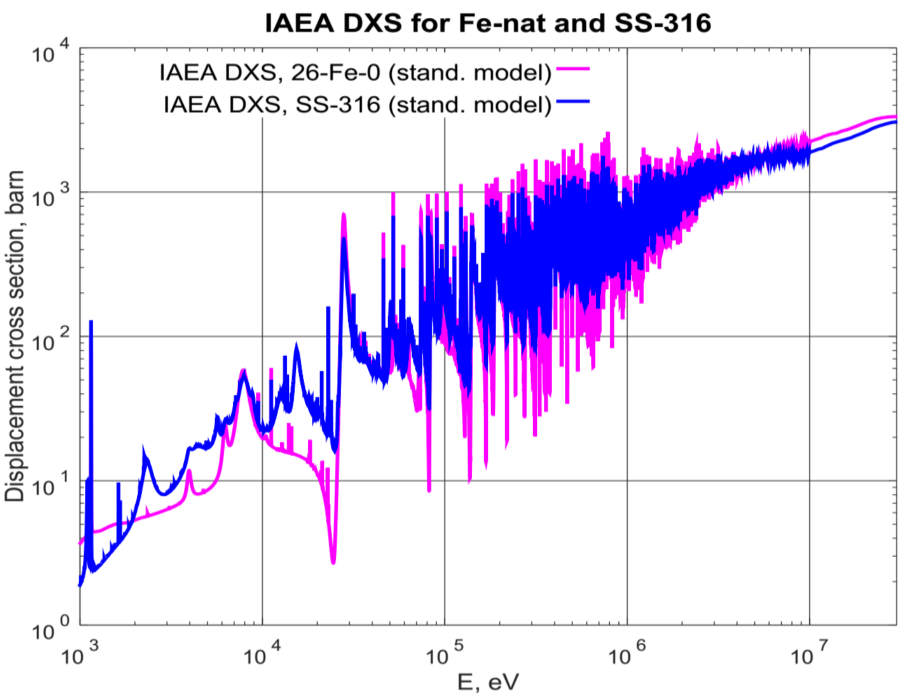
Fast flux (***E* > 1.0 MeV**):
~ 4.7% from total neutron flux.
Fast flux (***E* > 0.1 MeV**):
~ 14% from total neutron flux.
Thermal: ~ 41% (*E* < 0.625 eV).

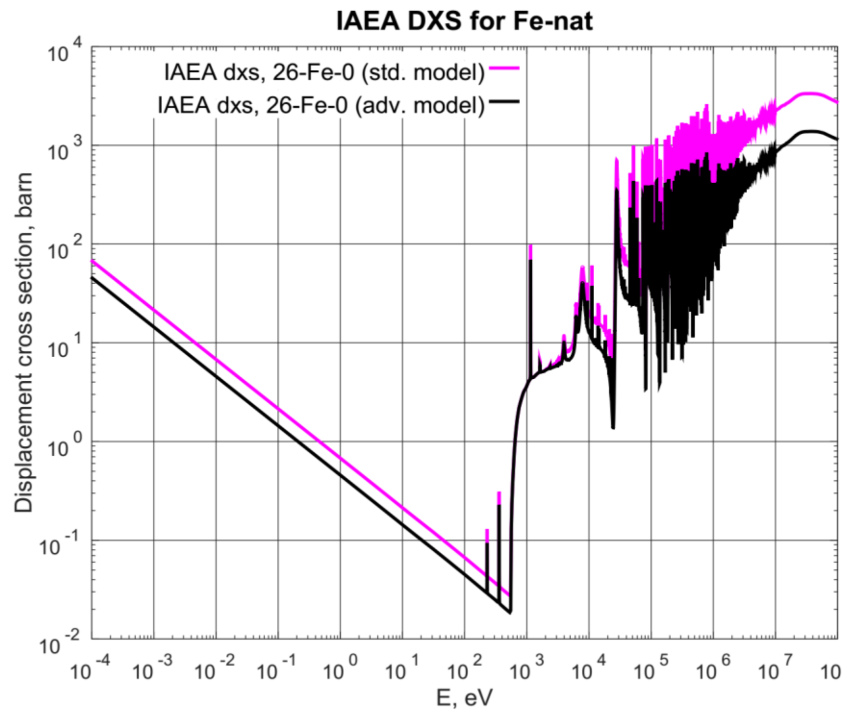
(Stat. (MC) uncertainty < 1%)



The region of interest in SS tube sheet: annulus of 2.5 cm radial width outside of CT, bounded by the inner tube-sheet surface next to the moderator and another parallel surface ~ 1.0 cm from the tube-sheet surface.

IAEA material damage cross section database (DXS)





Displacement Cross Section (DXS) database (maintained by Nuclear Data Services, IAEA),
https://www-nds.iaea.org/public/download-endf/DXS/ : there are files in ACE, *.*y (readable ?)

SS-316 : σ_{dpa} = 8.10 b (th.), 17.93 b (epith.), 880.87 b (fast), w. **standard (NRT) model.**

It can be used to estimate ***t*** **(*dpa* ~ 10)** ~ 130 years for the annulus of TS (near CT - TS).

However, ***t*** **(*dpa* ~ 10)** ~ 365 years using DXS, advanced models for $\sigma_{dpa}(E)$.

Coupling Serpent2

contact person: **Dan Wojtaszek** , daniel.wojtaszek@cnl.ca

- Model Molten Salt Reactor Experiment
- Using Serpent2 multi-physics interface
- Python script
  - power from Serpent2 detector files → TH code input
  - temperature and density from TH code → Serpent2 .ifc

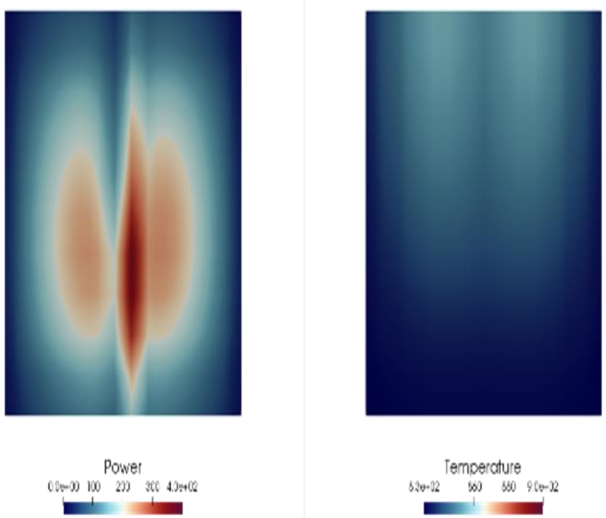
Coupling Serpent2:
Zig-zag noise growing in amplitude during transient

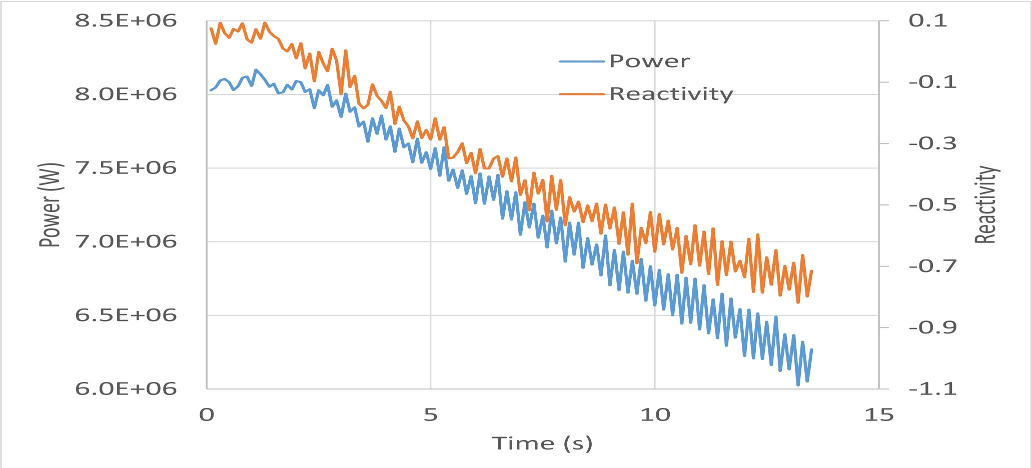
10 million neutrons

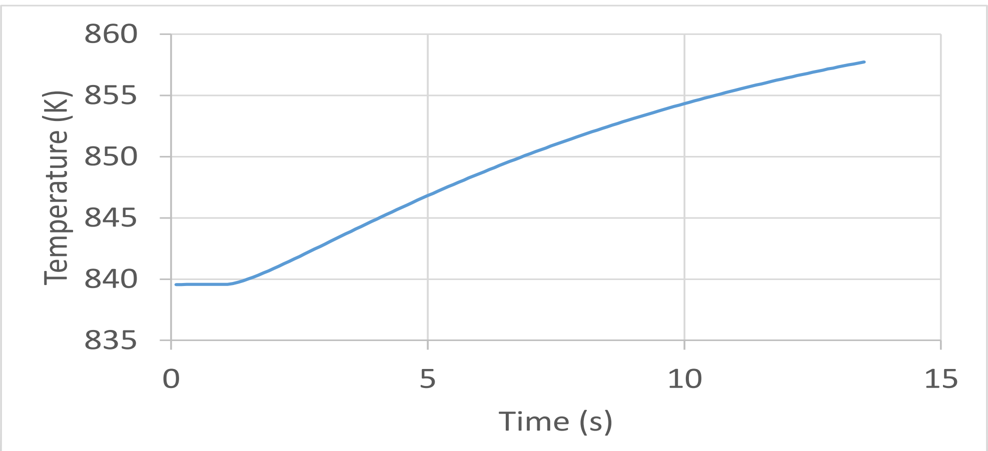
200 batches

Serpent2 + Relap5-3D

Start:



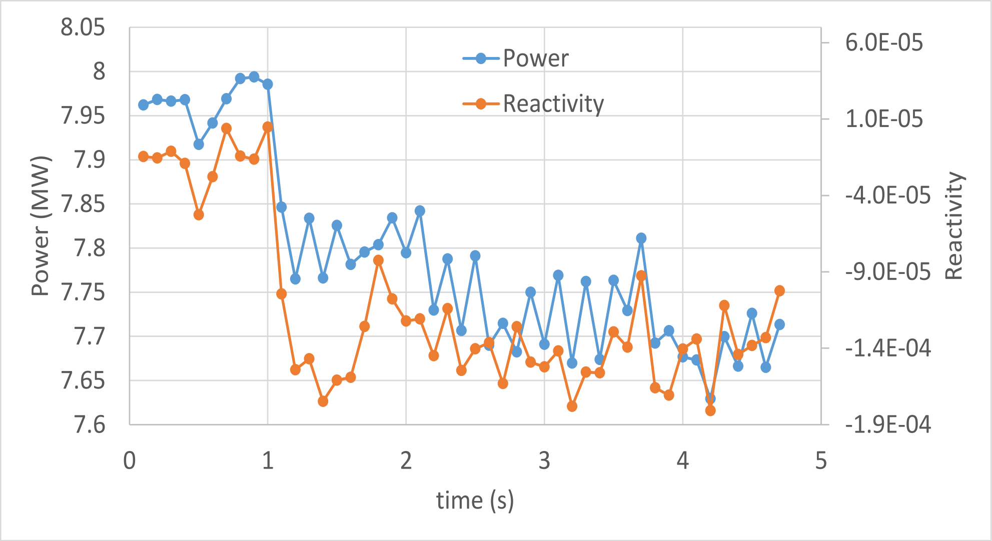


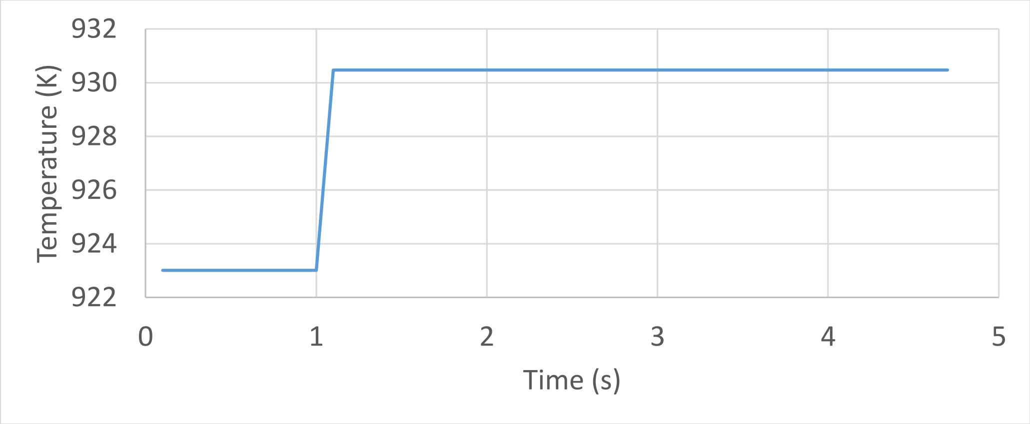


Serpent2:

Zig-zag noise growing in amplitude during transient

Similar effect with temperature step transient.





Conclusion

- **ENDF/B-VIII.0-based nuclear data library is available for Serpent2 applications at CNL**
- **For ZED-2 international benchmarks, we have Serpent full core models**
- **Coupled transport with photo-nuclear option: very interested in this option, can help with further testing**
- **Numerous application for Serpent2 in reactor physics R&D, such as material damage/dosimetry analysis, coupled physics-TH applications, etc.**

Acknowledgement

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