MCNP6.3 and OpenMC testing of the ENDF/B-VIII.1 Graphite TSLs using FUND-ORELA-ACC-GRAPH-PNSDT-001 benchmark

Kemal Ramić, José Ignacio Marquez Damian, Travis Greene, Adimir Dos Santos, Douglas Peplow, Chris W. Chapman, Iyad Al-Qasir, Will Wieselquist

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

ReGra 2025

- From ReGra report: `https://www.osti.gov/servlets/purl/2998877`

"Benchmark worthy" down selected list of cases:

ICSBEP Identifier	Title	# of Cases	Discussion
FUND-ORELA-ACC-GRAPH-PNSDT-001	Benchmark of Neutron Thermalization in Graphite using the Slowing-Down-Time ORELA Experiment	1	Very sensitive to TSL, low benchmark uncertainties, single target material so few competing material effects
LEU-COMP-THERM-060	RBMK Graphite Reactor: Uniform Configurations of U(1.8, 2.0, or 2.4% 235U)O2 Fuel Assemblies, and Configurations of U(2.0% 235U)O2 Assemblies with Empty Channels, Water Columns, and Boron or Thorium Absorbers, with or without Water in Channels	28	Numerous different configurations with varying degree of sensitivity to TSL, low benchmark uncertainties with good characterization of the core materials
HEU-COMP-THERM-016	IGR Reactor – Uranium-Graphite Blocks Reflected by Graphite	6	High sensitivity to TSL for a k_{eff} benchmark, although also high experimental uncertainties based on measured variations. Recommended for TSL temperature validation

- FUND-ORELA-ACC-GRAPH-PNSDT-001 benchmark was designated as a "golden standard" benchmark for validation of the graphite TSLs.

- During the ReGra there was a call for the input files to be provided.
- The input files provided in the benchmark report are not correct and do not run.
- Independent review by BNL prior to the meeting confirmed this.
- As presented in the benchmark report, 30% porosity TSL gives the best agreement with the measured data:

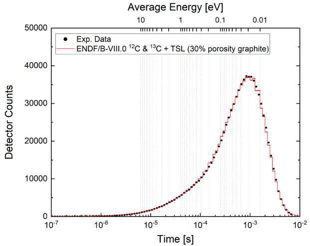


Figure 4.1-7. Comparison of experimental result of neutron slowing-down-time spectrum and calculation with ENDF/B-VIII.0 30% porosity graphite TSL.

FUND-ORELA-ACC-GRAPH-PNSDT-001 experiment summary

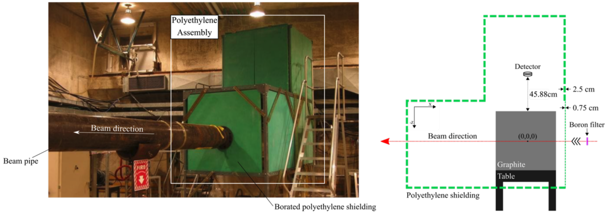
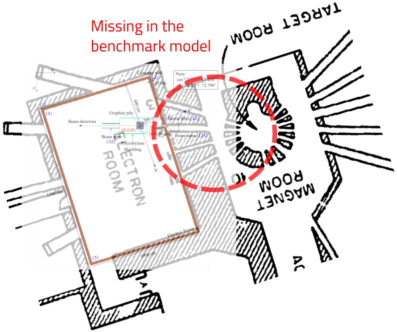


Figure 1.2-2. Photograph of the assembled experimental system showing the beam pipe and the polyethylene assembly within which the nuclear graphite pile is located in the ORELA Electron Room [3]. Note that the picture on the left shows the experiment from the back, not where neutrons come in. The orientation of the incident neutron beam is shown in the figure to the right.



- Pulsed neutron source hitting a graphite 70x70x70 cm block inside a borated polyethylene box with Li6 glass detector measuring the slowing down spectra. Relatively straightforward experiment.

- The benchmark evaluation has many potential deficiencies: uncertainty analysis of the detector thickness, self-normalization instead of absolute measurements, arbitrary selection of the region for normalization, arbitrary source (spectra, position, and divergence)

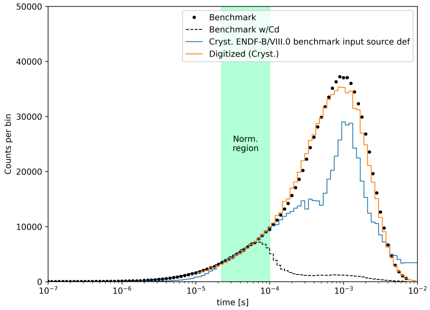
Oak Ridge National Laboratory

Fixing up the MCNP input

- To get the input running we needed to:

1. fix the cell importances: `imp:n 1` $\rightarrow$ `imp:n 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0`
2. Fix the tally times to match the benchmark report

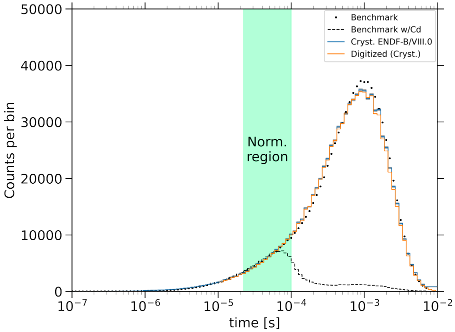
- With these changes the following result is obtained:



- To match the benchmark results we needed to:

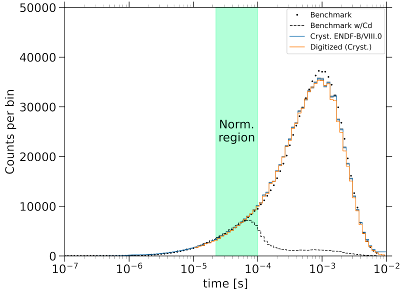
1. fix the source definition to replicate the pulse width, and remove incorrect beam divergence
   `si1 1e-10 2000 1e10` $\rightarrow$ `si1 1e-10 2 1e10`; 20 μs $\rightarrow$ 20 ns.
   `dir=d4, si4 0.99 1, sp4 0 1` $\rightarrow$ `dir=1`,
   `si4 0.99 1` corresponds to 8.1 degrees half-angle divergence.

- With these changes the following result is obtained:



OAK RIDGE National Laboratory

Reproduction of benchmark results: Crystalline TSL



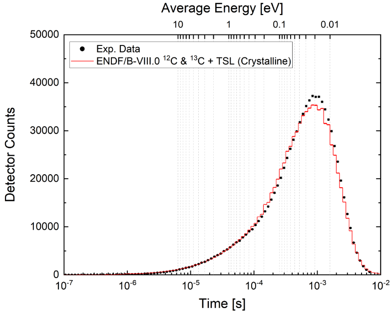
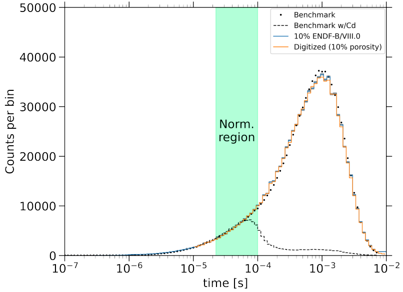


Figure 4.1-4. Comparison of the experimental result of neutron slowing-down-time spectrum and calculation with ENDF/B-VIII.0 crystalline graphite TSL.

- Our MCNP6.3 runs were done with 1e10 particles, Benchmark report results were run with MCNP6.2 with 5e10 particles.

Reproduction of benchmark results: 10% porosity TSL



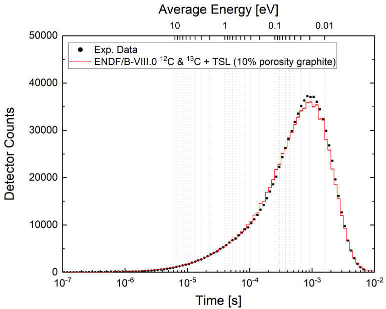
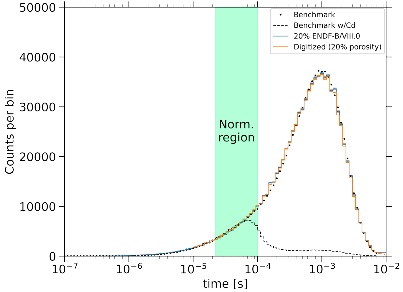


Figure 4.1-5. Comparison of experimental result of neutron slowing-down-time spectrum and calculation with ENDF/B-VIII.0 10% porosity graphite TSL.

Reproduction of benchmark results: 20% porosity TSL



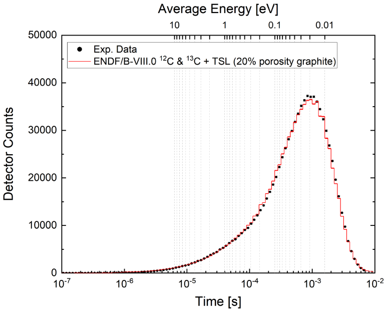
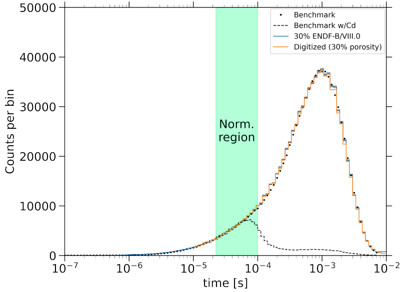


Figure 4.1-6. Comparison of experimental result of neutron slowing-down-time spectrum and calculation with 20% porous graphite TSL.

Reproduction of benchmark results: 30% porosity TSL



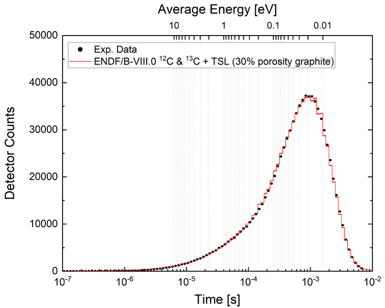


Figure 4.1-7. Comparison of experimental result of neutron slowing-down-time spectrum and calculation with ENDF/B-VIII.0 30% porosity graphite TSL.

But what is missing?

- There was no polyethylene TSL assigned to m6 material, and it should have been.

```
         6000.70c  1.41796e-03
m6       1001.70c  0.6077
         6000.70c  0.3683
         5010.70c  0.0047
         5011.70c  0.0193
m7       3006.70c  0.95
         3007.70c  0.05
m8       3006.70c  1
m9      26054.70c  0.05845
        26056.70c  0.91754
        26057.70c  0.02119
        26058.70c  0.00282
m10      5010.70c  0.90
         5011.70c  0.10
tr1     0 0 0 0.29577456 -0.95525777 0 0.95525777 0.29577456 0 0 0 1 1
```

TSL is also missing in the definition of concrete, but the impact is much smaller.

- Borated polyethylene box was only 5% borated, so polyethylene TSL applies, and it significantly contributes to the thermalization of neutrons.

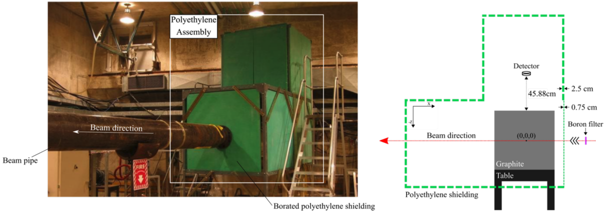
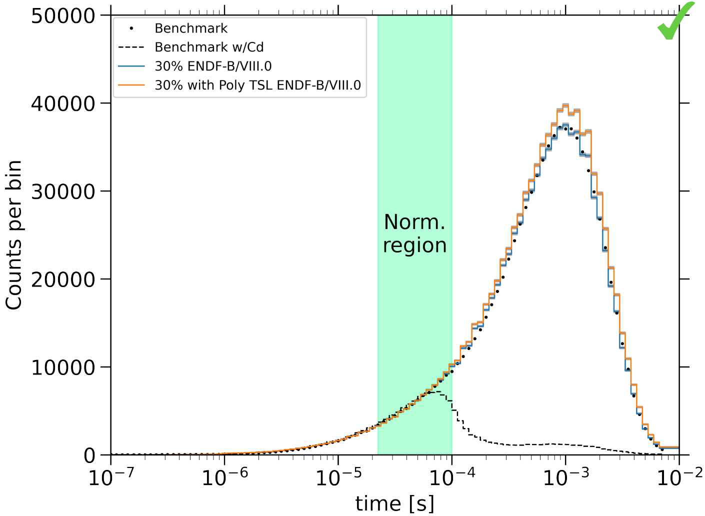
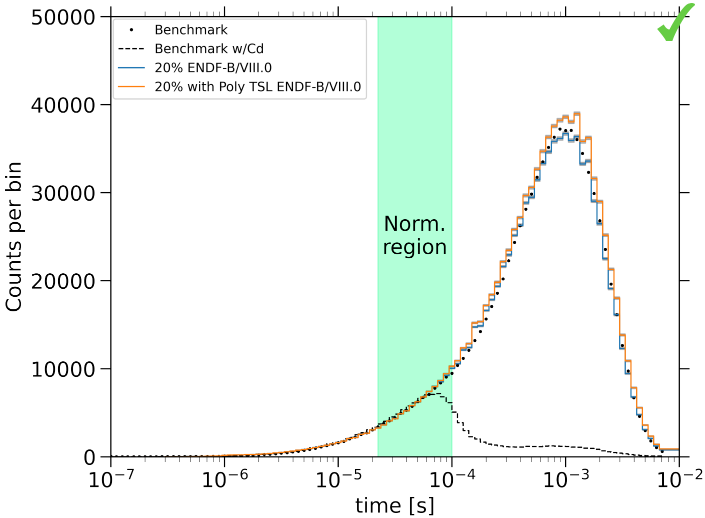


Figure 1.2-2. Photograph of the assembled experimental system showing the beam pipe and the polyethylene assembly within which the nuclear graphite pile is located in the ORELA Electron Room [3]. Note that the picture on the left shows the experiment from the back, not where neutrons come in. The orientation of the incident neutron beam is shown in the figure to the right.

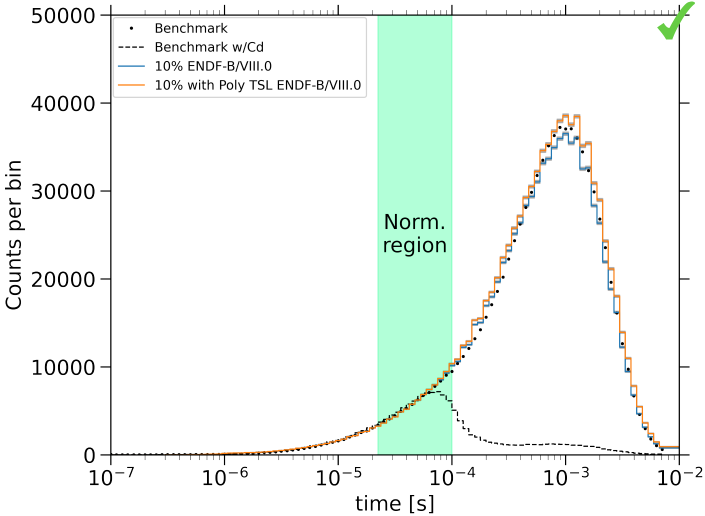
Benchmark results with Polyethylene TSL included: 30% porosity TSL



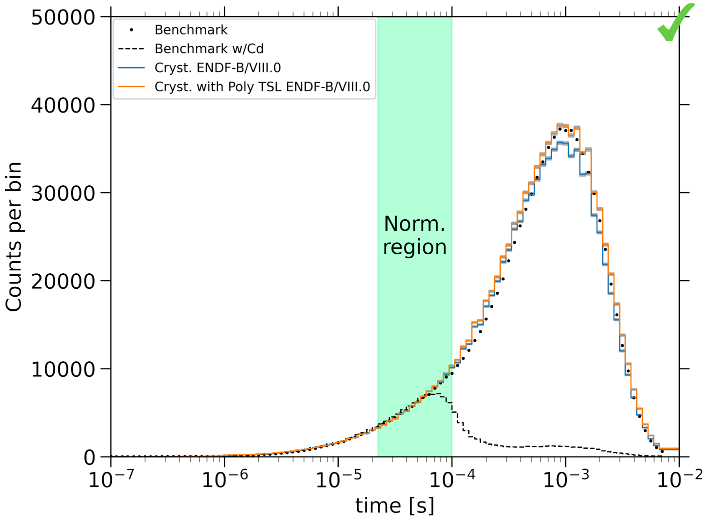
Benchmark results with Polyethylene TSL included: 20% porosity TSL



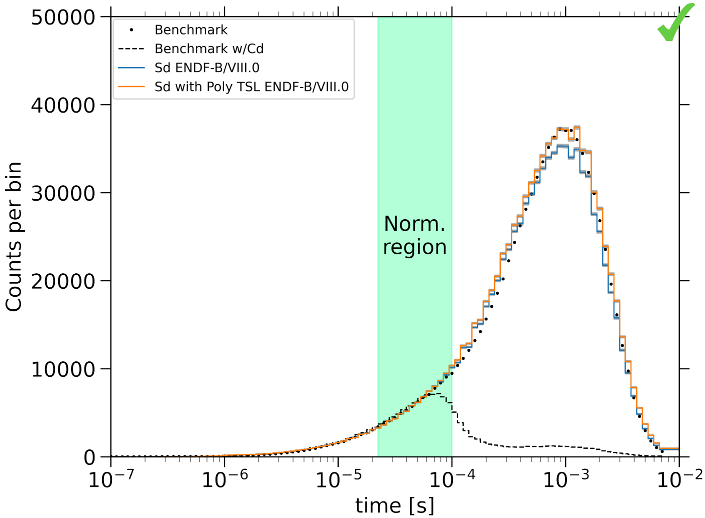
Benchmark results with Polyethylene TSL included: 10% porosity TSL



Benchmark results with Polyethylene TSL included: Crystalline TSL



Benchmark results with Polyethylene TSL included: Crystalline Sd TSL



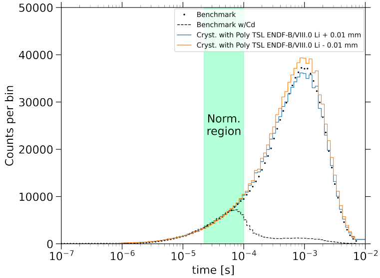
OAK RIDGE National Laboratory

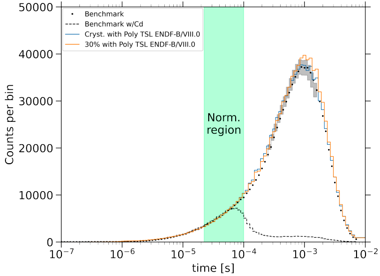
Benchmark uncertainty under-representation

2.1.9 Uncertainty in Position and Dimensions of the Detector

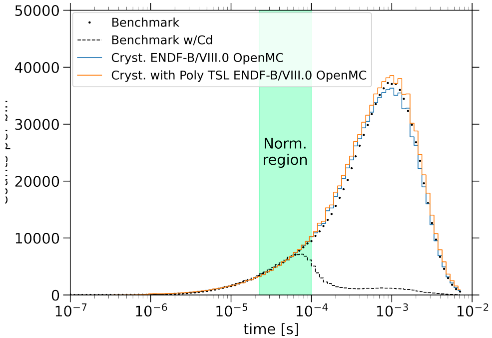
The distance from the detector to the graphite assembly was measured directly by a tape ruler with around 2 mm uncertainty and the detector is aligned to the center of the assembly and neutron beam. The dimensions of the lithium in the detector were 7.62 cm in diameter and 1 mm in thickness. The impact from both these uncertainties is assumed to be negligible to the measured spectrum for the graphite pile. Further properties such as the density, enrichment, and impurities of the lithium in the detector are also negligible. The impacts from these uncertainties would be significantly less than those from the characteristics of the graphite pile which were themselves negligible. Therefore, we can assume the impact from these uncertainties for the detector will not impact the results.

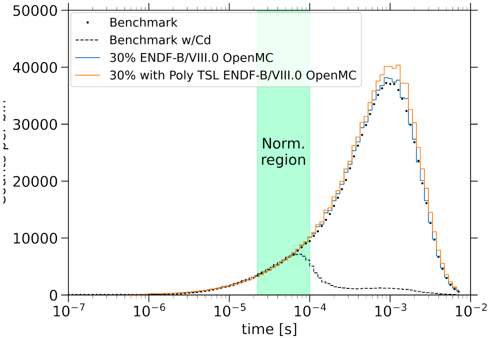
- Among the things we have checked, the uncertainty due to Lithium glass detector thickness (±20%, T. Zhou PhD thesis) has the biggest impact. There are possibly things we did not have time to investigate, so the benchmark uncertainty needs to be re-evaluated comprehensively.





OpenMC model

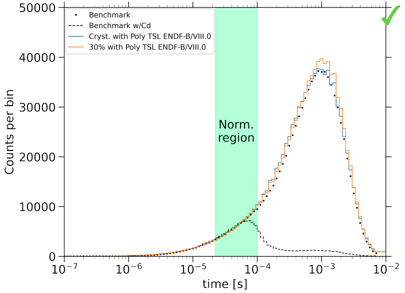




Results are qualitatively similar to MCNP, with proper asymptotic behavior at long times. Differences are likely due to the way MCNP and OpenMC model the detector (tally multiplier in pure Li6 in MCNP vs. absorption scoring in real material in OpenMC). Care must be taken when comparing results from different Monte Carlo codes.

Summary & Conclusions

- All the inputs, runs, output, and postprocessing data are available upon request and have already been provided to the ICSBEP coordinator. Also available at `https://github.com/ramic-k/ICSBEP_and_IRPHE_graphite_benchmarks`.
- During ReGra workshop, validity of the graphite TSLs was judged by giving a lot of weight to this single benchmark, but the results are not reproducible with the provided input.
- When the results are reproduced, it was determined that the crucial omission of polyethylene TSL was made, and that the corrected model does not support the benchmark results as provided in the benchmark report.
- With the new understanding of the results of this benchmark, and with the data presented by us during ReGra, in none of the studied benchmarks does the recommendation from Graphite TSL evaluators to match the porosity TSL with the assumed porosity in the benchmark give agreement with the benchmark. The increase in C/E values stems from the unphysical inelastic scattering found in the porosity TSLs.
- The benchmark evaluation as is potentially has many deficiencies, and it should be re-evaluated.
- We do have a working really slow SCALE model.



Acknowledgements

- This work was performed under the framework of DOE / US Nuclear Regulatory Commission (NRC) collaboration for Criticality Safety support for the commercial-scale HALEU fuel cycles project (DNCSH).
- This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a Department of Energy Office of Science User Facility using NERSC award ERCAP0033587.

SCALE results