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IRPhE and ICSBEP validation of ENDF/B-VIII.1 graphite TSLs

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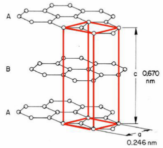
Thermalization of neutrons in nuclear graphite

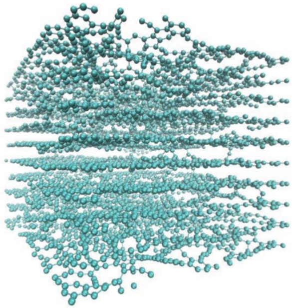
- ENDF/B-VIII.1.b1 has 5 different graphite libraries: crystalline, Sd (crystalline), 10%, 20%, and 30% porosity reactor graphite

- What is graphitization process?
  + Graphitization is the process of heating amorphous carbon for a prolonged period of time, **rearranging the atomic structure to achieve an ordered crystalline structure** that is typical of solids.

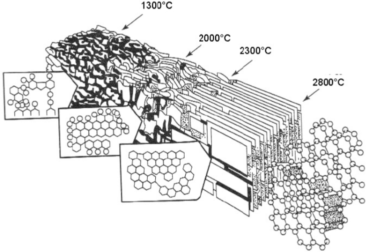
- Crystal structure for Crystalline and Sd graphite [2]:

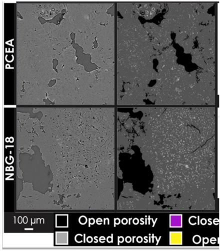


- Porous structure for 30% porosity graphite [2]:



Evolution of graphitization process, reproduced from [1]:

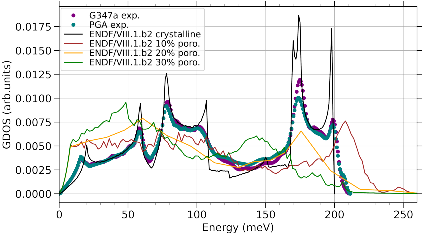




How does all this manifest itself in inelastic scattering measurements?

INS measurements of graphite

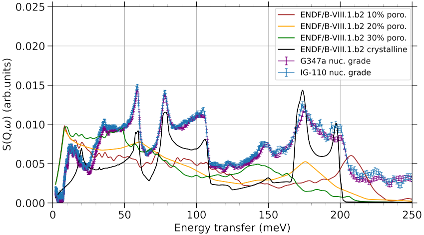
- Phonon spectrum (GDOS) measurements at ARCS instrument at SNS:

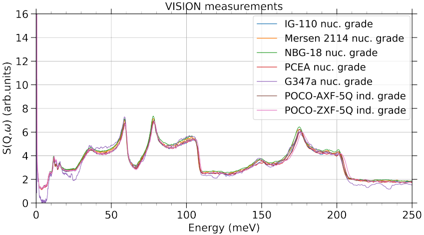


Graphite	Grain size [µm]	Density [g/cm^3]	Porosity [%]
PGA	800	1.70	25
G347a	50	1.85	17.8
IG-110	20	1.77	21.6
NBG-18	1600	1.85	17.8
PCEA	360	1.83	18
Mersen 2114	13	1.81	10
POCO-AXF-5Q	5	1.78	20
POCO-ZXF-5Q	1	1.78	20

Table 1: Properties of different types of graphite.

- $S(Q,\omega)$ measurements at VISION instrument at SNS ORNL:





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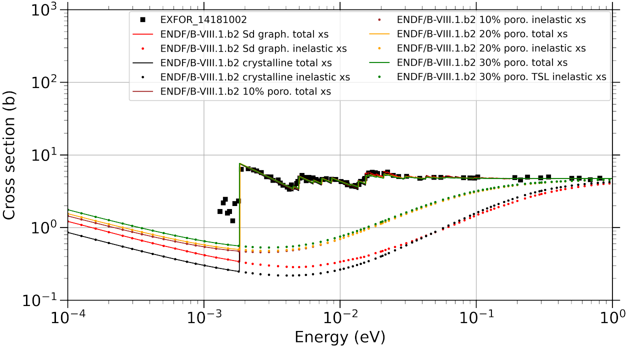
Graphite thermal transmission (total cross section) measurements

- **Sd-graphite** is the most physically accurate TSL from differential level
- The effect of porosity in 10%, 20%, and 30% TSLs was inaccurately modeled (by introducing defects on microscopic scale, when pores are a microscopic effect) which resulted in **increase of the inelastic scattering cross section**
- The actual effect of porosity is seen in **Small Angle Neutron Scattering (SANS)** cross section, and not in the inelastic cross section, and it is not quantifiable just by the percentage of the porosity, but it is a complex interplay of pore sizes and distributions



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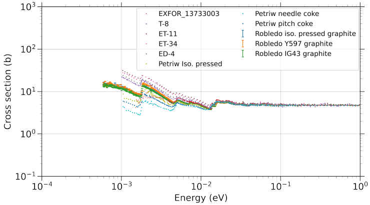
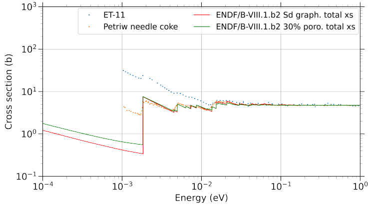
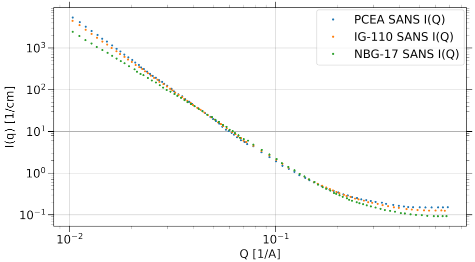
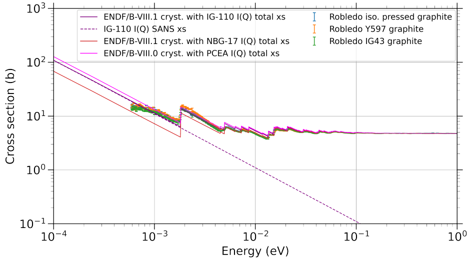
Graphite thermal transmission (total cross section) measurements

- **There are multiple of transmission measurements on different grades of nuclear graphite that show impact of SANS.**
- SANS is an elastic scattering (only change of direction)
- By measuring SANS of different grades of nuclear graphite we can reproduce their transmission.







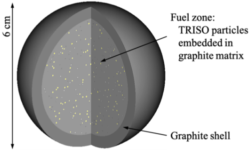


Neutronics calculations - Tools

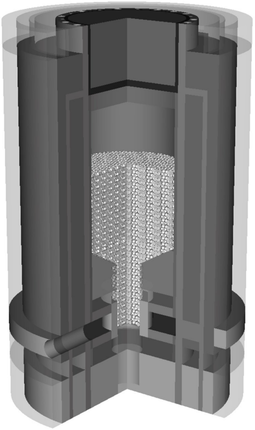
- Models of reactors or criticality benchmarks were taken from The International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE) or The International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook
- MCNP6.2
- Nuclear data libraries:
  - Continuous-energy library ENDF/B-VIII.0
  - ENDF/B-VIII.1.b2 TSL data:
    - Crystalline
    - Crystalline + Sd
    - 10% porosity
    - 20% porosity
    - 30% porosity
    - No TSL data (Carbon free gas)

Model 1: HTR-10

- 10 MWth Pebble-bed High Temperature Gas-cooled Reactor
- Relevant characteristics:
  - UO_2 fuel density: 10.4 g/cm^3
  - ^{235}U enrichment: 17 wt.%
  - TRISO packing fraction: $\sim$9%
  - Number of particles per pebble: 8,385
  - Pebble radius: 3 cm (fuel zone: 2.5 cm)
  - Graphite densities indicate porosities between 19-30%
    - Dummy pebbles: 18.6%
    - Fuel pebbles (matrix, shell): 23.5%
    - Reflector and carbon brick: up to 30%
- HTR-10 initial criticality:
  - 9,627 fuel pebbles
  - 7,263 dummy pebbles
  - 61% packing fraction
  - Room temperature
  - Fresh fuel



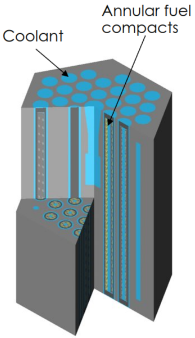
HTR-10 fuel pebble



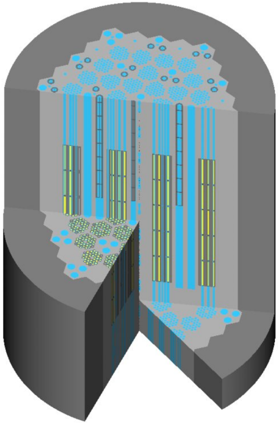
SCALE model of the HTR-10

Model 2: HTTR

- 30 MWth Prismatic High Temperature Gas-cooled Reactor
- Relevant characteristics:
  - UO_2 fuel density: 10.39 g/cm^3
  - ^{235}U enrichment: 3.4-9.9 wt.%
  - TRISO packing fraction: 30%
  - Number of particles per fuel compact: 12,987
  - Fuel compact inner radius/outer radius/length: 1 cm/2.3 cm/3.9 cm
  - Graphite densities indicate porosities between 22-25%:
    - Graphite overcoat and cladding: 24.8%
    - Graphite reflector around blocks: 24.0%
    - Graphite in blocks: 22.2%
- HTTR criticality experiment:
  - Configuration with fully loaded core (30 fuel blocks)
  - Room temperature
  - Fresh fuel



HTTR fuel block



SCALE model of the HTTR

MCNP: Impact of graphite TSL evaluation on the HTR-10

TSL library	293 K, just structure		293 K, just pebbles		293 K, both	
Cross section data	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]
Crystalline+ Sd					1.00722 ± 0.00008	+722
Crystalline					1.00678 ± 0.00008	+678
10% porosity	1.00663 ± 0.00008	+663	1.01045 ± 0.00008	+1045	1.01018 ± 0.00008	+1018
20% porosity	1.00639 ± 0.00008	+639	1.01261 ± 0.00008	+1261	1.01181 ± 0.00008	+1181
30% porosity	1.00579 ± 0.00008	+579	1.01480 ± 0.00008	+1480	1.01321 ± 0.00008	+1321
HTR-10 exp.					1.00000 ± 0.00370	

1. **In graphite structure → Increased inelastic xs slows down neutrons to get absorbed in surrounding materials** → fission goes down → k_{eff} **goes down**
2. **In pebbles → Increased inelastic xs slows down neutrons to get absorbed in the fuel** → fission goes up → **k_{eff} goes up**
3. When used for all materials, two effects compete, but pebble effect wins out

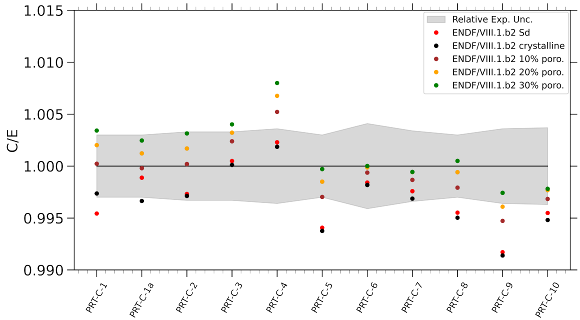
- **As the inelastic goes up, k_{eff} goes up for all cases using ENDF/B-VIII.1 porosity TSLs.**

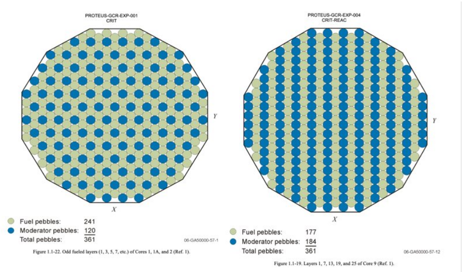
MCNP: Impact of graphite TSL evaluation on the HTTR

TSL library	Conf. 1		Conf. 2		Conf. 3		Conf. 4		Conf. 5	
Cross section data	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]
Crystalline+ Sd	1.01668	+1188	1.01983	+1583	1.01713	+1363	1.02177	+1857	1.01535	+1245
Crystalline	1.01662	+1182	1.02032	+1632	1.0173	+1380	1.02194	+1874		
10% porosity	1.019	+1420	1.02205	+1805	1.01971	+1621	1.02442	+2122	1.01828	+1538
20% porosity	1.02029	+1549	1.02384	+1984	1.02112	+1762	1.02585	+2265	1.01961	+1671
30% porosity	1.02187	+1707	1.02542	+2142	1.02302	+1952	1.02731	+2411	1.02137	+1847
HTTR exp.	1.0048 ± 0.0103		1.004 ± 0.01		1.0035 ± 0.0078		1.0032 ± 0.0080		1.0029 ± 0.0068	

- **As the inelastic goes up, k_{eff} goes up for all cases using ENDF/B-VIII.1 porosity TSLs.**

MCNP: Impact of graphite TSL evaluation on the PROTEUS





- Due to **increase in the inelastic xs** for porous TSLs, combined with the HCP pebble arrangements for Cores 1-3, which amplifies the effect due to decreased probability of leakage, porous TSLs seem like they provide a better k_{eff} values
- **As the inelastic goes up, k_{eff} goes up for all cases using ENDF/B-VIII.1 porosity TSLs.**

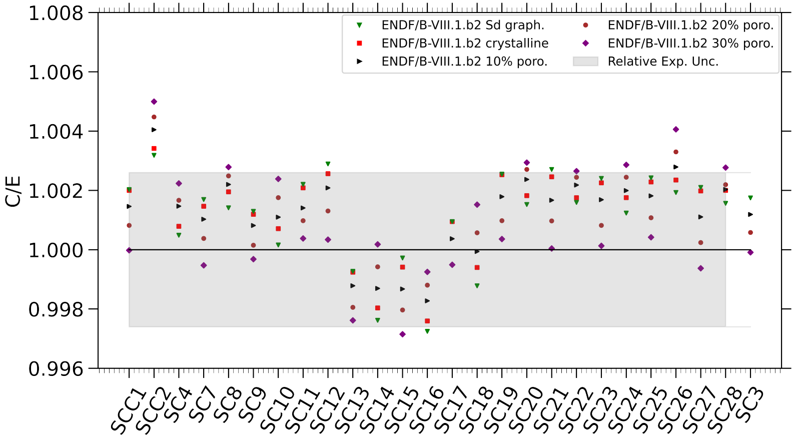
- PROTEUS-GCR-EXP-001
  - Cores 1, 1A, 2, and 3
  - **Hexagonal Close Packing**
  - 1:2 Moderator-to-fuel Pebble Ratio
- PROTEUS-GCR-EXP-002
  - Cores 4
  - **Random Packing**
  - 1:1 Moderator-to-fuel Pebble Ratio
- PROTEUS-GCR-EXP-003
  - Cores 5,6,7, and 8
  - **Columnar Hexagonal Point-on-Point Packing**
  - 1:2 Moderator-to-fuel Pebble Ratio
- PROTEUS-GCR-EXP-004
  - Cores 9 and 10
  - **Columnar Hexagonal Point-on-Point Packing**
  - 1:1 Moderator-to-fuel Pebble Ratio

MCNP: Impact of graphite TSL evaluation on the HCT-016 (IGR reactor)

	Configuration 1		Configuration 2		Configuration 3		Configuration 4	
Cross section data	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]	k_{eff}	Δk [pcm]
Crystalline+ Sd	1.00538 ± 0.00008	+538	1.00104 ± 0.00008	+104	1.00219 ± 0.00008	+219	1.00587 ± 0.00008	+587
Crystalline	1.00463 ± 0.00008	+463	1.00017 ± 0.00008	+17	1.00183 ± 0.00008	+183	1.00521 ± 0.00008	+521
10% porosity	1.00924 ± 0.00008	+924	1.00551 ± 0.00008	+551	1.00647 ± 0.00008	+647	1.01043 ± 0.00008	+1043
20% porosity	1.01145 ± 0.00008	+1145	1.00800 ± 0.00008	+800	1.00906 ± 0.00008	+906	1.01283 ± 0.00008	+1283
30% porosity	1.01320 ± 0.00008	+1320	1.00986 ± 0.00008	+986	1.01095 ± 0.00008	+1095	1.01472 ± 0.00008	+1472
HCT-016 exp.	1.00000 ± 0.01100		1.00000 ± 0.01100		1.00000 ± 0.01100		1.00000 ± 0.01100	

- **As the inelastic goes up, k_{eff} goes up for all cases using ENDF/B-VIII.1 porosity TSLs.**

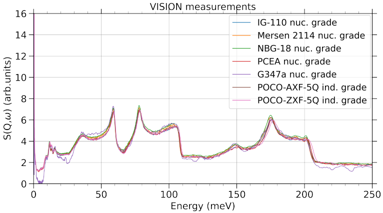
MCNP: Impact of graphite TSL evaluation on the LCT-060 benchmark

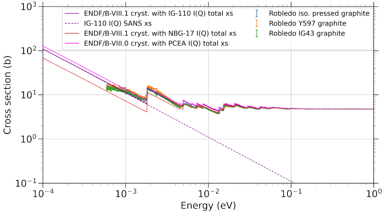


- **For cases with water in the fuel or absorber channels → as the inelastic goes up in graphite TSLs it lowered the k_{eff} values, due to increased absorption.**
  Cases without water in the fuel or absorber channels → as the inelastic goes up, k_{eff} goes up using ENDF/B-VIII.1 porosity TSLs.

Summary & Conclusions

- Compared different benchmarks (with unknown graphite) using MCNP6.2 and ENDF/VIII.1 graphite TSLs.
- All the benchmarks show that the increase in the inelastic cross section of the porous graphite libraries lead to a significant increase in the k_{eff}.
- ENDF/B-VIII.0 and ENDF/B-VIII.1 ”porous” graphite libraries should not be used because they lead to an overestimation of k_{eff} and shouldn’t be used in the design of advance reactors with graphite or critical benchmarks containing graphite. They need to be **removed** from ENDF library.
- Porosity in graphite manifests itself through SANS (macroscopic structural effect) and not through increase in the inelastic cross section (microscopic structural effect) as represented in porous ENDF TSLs.
- **Graphite is a perfect example of why both INS and transmission measurements are need! Without INS measurements we would be misled by the atomistic modeling, and without transmission measurements we would not see the effects of SANS.**





Acknowledgements

- This work is supported under the framework of the US Department of Energy/US Nuclear Regulatory Commission Collaboration for Criticality Safety Support for 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 at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.
- This research used resources of the Compute and Data Environment for Science at ORNL, which is supported by DOE SC under Contract No. DE-AC05-00OR22725.
- Computational resources were also provided by the Rensselaer Polytechnic Institute Center for Computational Innovations, more specifically the Artificial Intelligence Multiprocessing Optimized System supercomputer.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.