Agenda

Time (EST)	Topic	Speaker
11:00 - 11:02AM	Welcome/Housekeeping	Mr. Andrew Barto, NRC
11:02 – 11:05AM	Workshop Theme and Intro	Dr. William Wieselquist
11:05 - 11:15AM	HALEU Availability Program	Mr. William McCaughey, Director, Advanced Fuels Technologies, DOE-NE
11:15 - 11:25AM	Project Background	Mr. Don Algama, DOE-NE
11:25 - 11:35AM	Project Goals	Mr. Andrew Barto, NRC
11:35AM – 12:35PM	Discussion of Considerations for HALEU-Based Fuel Cycle Validation Basis Assessment and Benchmark Prioritization, Including: • Current HALEU-Based Reactor Landscape and Transportation Packages • Current Nuclear Data Gaps (e.g. TSL Uncertainty)	Dr. William B.J. Marshall Dr. Iyad Al-Qasir Dr. Mathieu Dupont Dr. Lisa Fassino
12:35 – 12:50PM	Open Discussion	Audience Questions
12:50 – 1:20PM	Background on Validation Methods and the need for Application Models	Dr. William B.J. Marshall Mr. Alex Shaw
1:20 – 1:50PM	Presentation of Recently Developed Criticality Safety Application Models	Dr. William B.J. Marshall Mr. Alex Shaw Dr. Veronica Karriem
1:50 – 2:15 PM	Open Discussion	Audience Questions
2:15 PM	Concluding Remarks	Dr. Will Wieselquist
	Adjourn	Ms. Lindsey Aloisi

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Workshop 1 Theme and Intro

- Demonstrate our strategy for prioritizing benchmarks
  1. Survey the field
  2. Prioritize a target application
  3. Develop an application model (today: **fresh fuel pebble transport**)
  4. Assess the validation basis
  5. Host a workshop
  6. Develop Experiment Support Opportunity (ESO) to address gaps in validation bases
  7. Rinse and repeat
- ESOs are the main vehicle for critical benchmark awards
- We are hungry for information
  - **Long lead-time on nuclear data and experiments!**
  - Existing measurements that could become benchmarks
  - From reactor designers: what are your intended transportation packages, front-end/back-end storage systems
  - Any ideas where you may need additional nuclear data or benchmarks for safe, commercial-scale operations
- Feedback methods
  - Use the chat ☺
  - Respond to feedback form (following the workshop)
  - Email DNCSH@ornl.gov
- When to ask questions?
  - Feel free to ask questions in the chat, we may answer in the chat or hold it for the discussion period
  - During the discussion period, we would like attendees to raise their virtual hands to ask questions and we'll give some preference to those versus chat-based questions

HALEU Availability Program (HAP)

02/29/24

Energy Act of 2020; Sec. 2001 “Advanced Nuclear Fuel Availability” (42 U.S.C. 16281; PL-116)

Section (A) and (C)(ii)

William McCaughey NE-42 Office Director

Authorities

- The Energy Act of 2020 authorizes the DOE to “support the availability of HA–LEU for civilian domestic research, development, demonstration, and commercial use.”
- Inflation Reduction Act in 2022 provided initial funding of $700M divided into three areas.
  - $500M to develop near-term and long-term sources of HALEU.
  - $100M to develop criticality safety BM and support vendor transportation packages
  - $100M for supporting activities.

HALEU Availability Program (HAP) Elements

Eleven Elements that Compose the Program

- Reclamation from EBR-II
- Downblending SRS & Y-12
- HALEU enrichment follow on operations at Piketon
- Enrichment in commercial quantities
- Post-enrichment deconversion
- The HALEU Consortium
- The HALEU Bank
- Physical storage
- Transportation
- NEPA
- DOE/NRC Criticality Safety for Commercial-Scale HALEU Fuel Cycle and Transportation (DNCSH) ← **This workshop**

HALEU Availability Program (HAP) Goal

- Overall goal is to kick start the industry on the road to be self sufficient.

DOE/NRC Criticality Safety for Commercial-Scale HALEU Fuel Cycle and Transportation (DNCSH)

02/29/24

Energy Act of 2020; Sec. 2001 “Advanced Nuclear Fuel Availability” (42 U.S.C. 16281; PL-116)
Section (A) and (C)(ii)

Don Algama (DOE Fed. Manager)

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Authorities

- The Energy Act of 2020 authorizes the DOE and NRC to collaborate to develop **criticality safety data**.
- Inflation Reduction Act in 2022 provided $700M, of which **$60M** is the cost estimate for this project.
- **HALEU fuel cycle** is the scope, except reactor operation step.
- **NRC** is primary customer.

Implementing Law: Energy Act of 2020, Section 2001 "Advanced Nuclear Fuel Availability"(42 U.S.C. 16281)

(A) shall develop, in consultation with the Commission, criticality benchmark data to assist the Commission in—

i. the licensing and regulation of special nuclear material fuel fabrication and enrichment facilities under part 70 of title 10, Code of Federal Regulations; and
ii. certi... u... R...

!NOT COVERED!

(B) Shall conduct research and development, and provide financial assistance to assist commercial entities, to design and license transportation packages for HA–LEU, ...ters for metal, gas, and other ...sitions;

(C) Shall, to the extent practicable—

i. by January 1, 2024, support commercial entity submission of such transportation package designs to the Commission for certification by the Commission under part 71 of title 10, Code of Federal Regulations; and
ii. encourage the Commission to have such ...designs so ...ion within 24 ...n application;

In short:

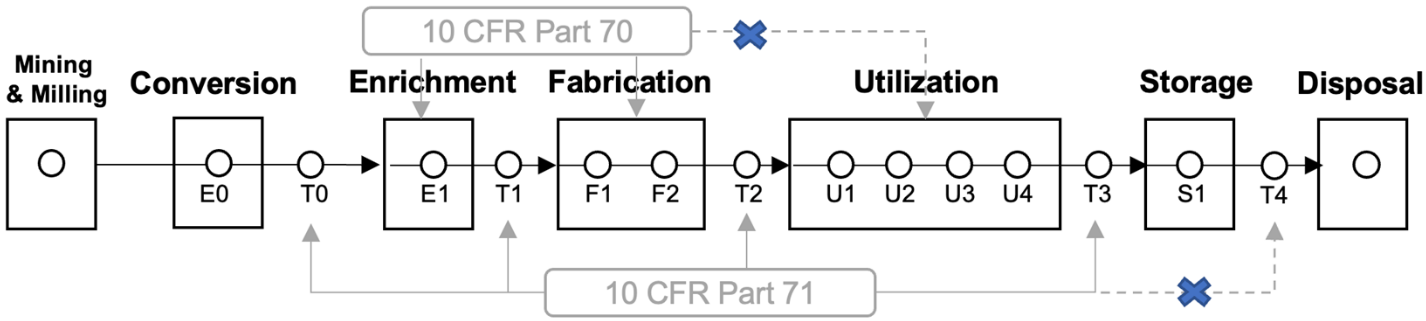
- Support the use of HALEU material –Part 70/71 crit. safety space – in reactor driven fuel cycles, e.g.: LWR, HTGR, SFR, HPR, SFR, MSR, etc. with data, methods and supporting evaluations.
- Be forward oriented.

In short:

- Enable licensees to develop quality applications that are supportive of their performance needs, and
- Support the NRC staff SER's with relevant data and updated methods.

...NERGY

Authorities: LWR Fuel Cycle Mapping

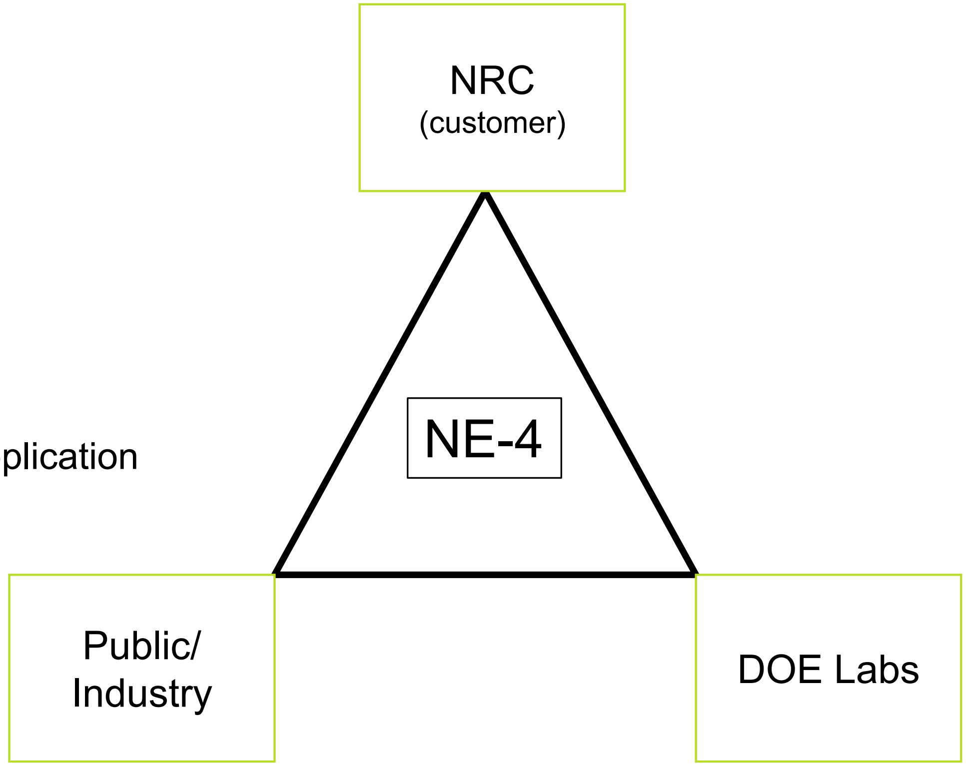


E0 – Conversion U3O8 to UF6
T0 – transportation of UF6 to enrichment facility
E1 – UF6 enrichment (<5w/o) and deconversion
T1 – transportation of UF6 to fuel fabrication facility
F1 – fabrication of UO2 fuel pellets
F2 – fabrication of LWR fuel assemblies
T2 – transportation of fresh fuel assemblies to the plant
U1 – fresh fuel staging and loading
U2 – power production
U3 – spent fuel pool/shuffle operations
U4 – on-site dry cask storage
T3 – transportation of spent fuel to off-site storage
S1 – off-site storage
T4 – transportation to disposition

Illustration of a LWR fuel cycle based on (ML21088A047) annotated with NRC regulations of interest for this effort

Who and Approach

- Customer:
  - NRC
- Partners:
  - DOE offices (NE, NNSA/NCSP, OS/NP, etc.).
  - DOE labs and universities.
  - Funded experiment opportunities.
- Approach:
  1. Develop *working* HALEU fuel cycle analysis and application models (HTGR, SFR, MSR, HPR, etc.)
  2. Conduct public workshops.
  3. **Issue experiment opportunities.**
  4. **Review and responses**.
  5. Data collection, interpretation, processing and public reports.



DNCSH Organization Structure – Management Team

Name	Project Role	Responsibilities Include
William McCaughey	DOE Office Director	Coordinate throughout DOE Complex
Don Algama	DOE Fed Manager	Coordinate throughout DOE Complex
Mark Angil	DOE Advisor	Advisor and representative for DOE HALEU Consortium
Bob Rova	DOE Experiment Support Opportunities	Implementation
Andrew Barto	NRC Program Manager	Coordinate throughout NRC Complex
William Wieselquist	National Technical Director	Coordinate technical activities, approve and review tasks, assign top-level task leads.
Lindsey Aloisi	Project Manager	Collect status, update PMP, allocate and track spending, update PICS-NE, and manage plans.

DNCSH Organization Structure – Technical Team Leads

Responsibilities	Project Role	Name
Engagement Area 1	Management and Engagement	William Wieselquist
Engagement Area 2	Quality Assurance	Travis Greene
Engagement Area 3	Survey and Summaries	Walid Metwally
Engagement Area 4	Facility Enhancements	Catherine Percher
Engagement Area 5	Reference Application Model Development	Nathanael Hudson
Engagement Area 6	Critical Benchmark Execution	Catherine Percher
Engagement Area 7	Nuclear Data Enhancement	Iyad Al-Qasir
Engagement Area 8	Simulation Methods Improvements	Rob Lefebvre
Engagement Area 9	Validation Basis Improvement	Ugur Mertyurek

Success Metrics

- Tier 1 (easily quantifiable):
  - Publicly available experiments.
  - Publicly available application models (including enabling reports).
  - Publicly available methods and approaches.
- Tier 2 (difficult to quantify):
  - Number of applications using new data/methods.
  - Number of times NRC can use new data/methods in review.

Concluding Remarks

- NRC is primary customer and project will produce publicly available data.
- Unique opportunity that will have long lasting impact on the commercial industry.
- Project application area is 10CFR70 and 10CFR71.
- Coordinate high impact experiments via experiment support opportunities available to the public. More information to follow.
- Key success metric will be in the availability of public data and models

WORKSHOP ON COLLABORATION BETWEEN DOE AND NRC FOR DEVELOPMENT OF CRITICALITY SAFETY BENCHMARKING DATA FOR HALEU FUEL CYCLE AND TRANSPORTATION

February 29, 2024

Drew Barto
Division of Fuel Management
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission

OVERVIEW

- Background
- Regulations
- Code Validation
- Existing Transportation Packages
- DNCSH Outcomes

BACKGROUND

- Office of Nuclear Material Safety and Safeguards Division of Fuel Management (NMSS/DFM) within NRC is responsible for regulation of:
  - Fuel cycle facilities under 10 CFR Part 70
  - Radioactive material (including fissile material, e.g., HALEU) transportation package designs under 10 CFR Part 71
- Regulations include requirements to maintain criticality safety under all conditions

REGULATIONS

- 10 CFR 70.61 – Subcritical under normal and credible abnormal conditions
- 10 CFR 70.64 – Double contingency principle
- 10 CFR 70.24 – Criticality monitoring
- 10 CFR 71.55 - Single packages.
  - 10 CFR 71.55(b): subcritical considering water in-leakage
  - 10 CFR 71.55(d): subcritical under normal conditions of transport (NCT)
  - 10 CFR 71.55(e): subcritical under hypothetical accident conditions (HAC)
- 10 CFR 71.59 – Package arrays.
  - Subcritical under NCT and HAC
  - Limiting number of packages under NCT or HAC used to determine Criticality Safety Index (CSI) to control package accumulation on conveyance

CODE VALIDATION

ANS 8.1 - *Nuclear Criticality Safety In Operations With Fissionable Materials Outside Reactors*:

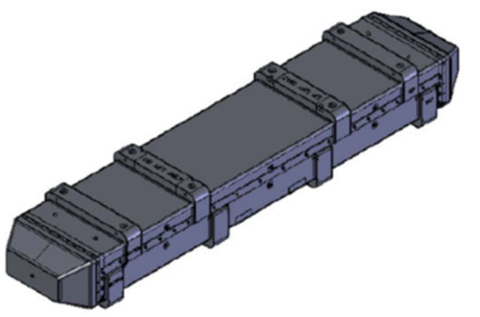
- Validation shall be performed by comparison to critical experiments, and the area of applicability for the validation should be established from this comparison
- Establish:
  - Applicability of experiments
  - Code bias and bias uncertainty
  - Trending analysis

CODE VALIDATION

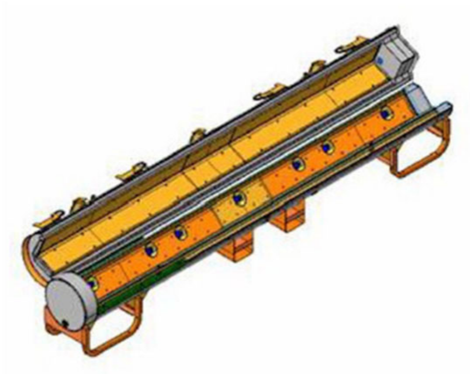
- ANS 8.24 - *Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations*
- NUREG/CR-6698 - *Guide for Validation of Nuclear Criticality Safety Calculational Methodology*
- NUREG/CR-5661 - *Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages*
- NUREG/CR-6361 - *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*
- International Criticality Safety Benchmark Evaluation Project (ICSBEP):
  - Descriptions of over 5,000 laboratory critical experiments
  - Grouped by fissile media, physical form, and neutron energy where most fissions occur
  - Many experiments representative of <5% enriched UO_2 LWR fuel; less for enrichment range of 5-20%; much less for key systems of interest (e.g., TRISO, low moderation UF_6)

EXISTING HALEU PACKAGES

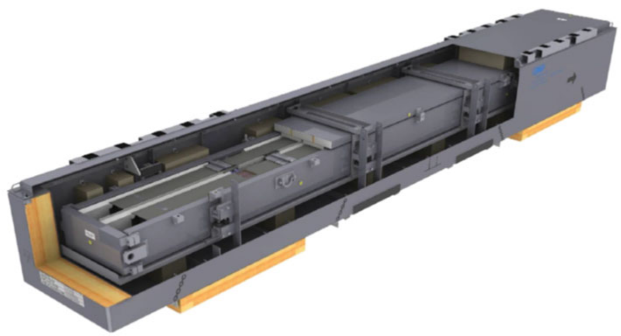
LWR Fresh Fuel:



MAP 12 and MAP 13 (71-9319)



Traveller (71-9380)



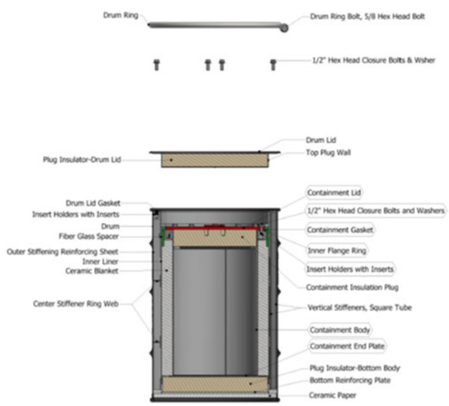
GNF RAJ-II (71-9309)

- **Certified to LEU+ range – up to 8.0% enrichment**
- **No issues with code validation**
  - Many applicable low enriched UO_2 experiments
  - Regulations require consideration of moderation by water – thermal uranium systems generally fairly easy to validate

The critical benchmarks performed at SNL with 7% enriched fuel were instrumental in certifying these package designs.

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

EXISTING HALEU PACKAGES

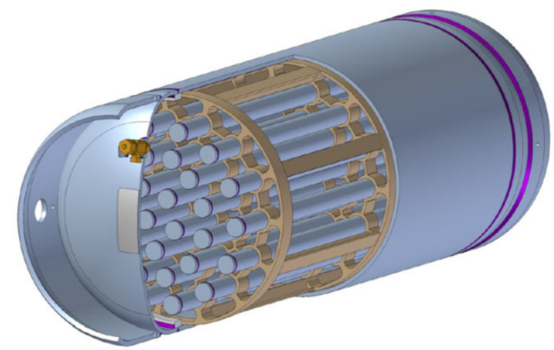


Versa Pac (71-9342)

- Varied uranium contents enriched up to 100%
- TRISO allowed
- Low mass of ^{235}U per package
- CSI 0.7 to 1.4

Optimus-L (71-9390)

- Up to 68 kg of 20% enriched TRISO compacts
- CSI = 0
- Gross weight ~9,200 lbs.



DN30-X (71-9388)

- UF_6 cylinder with internal criticality control system in overpack
- Up to 10% enriched UF_6 in 30B-10 cylinder; 20% enriched in 30B-20
- Up to 1,460 kg UF_6 in 30B-10, 1,271 kg in 30B-20 (standard 30B is 2,277 kg)
- CSI = 0.0

DNCSH OUTCOMES

- High-quality publicly available benchmark experiments, nuclear data, and evaluations applicable to wide range of HALEU systems where current data is lacking
- Will allow applicants and licensees more options for optimizing HALEU fuel cycle and transportation systems, with potentially:
  - Higher throughput fuel cycle processes
  - Higher capacity transportation package designs
  - Fewer RAIs related to code validation and criticality

Discussion of Considerations for HALEU-Based Fuel Cycle Validation Basis Assessment and Benchmark Prioritization

Lisa Fassino
Iyad Al-Qasir
Mathieu Dupont

DNCSH Workshop #1
February 29th, 2024, Germantown, MD

Outline

Introduction

Current HALEU-Based Reactor and Transportation Landscape — **Lisa Fassino**

Nuclear Data Gaps: Current Status of Thermal Scattering Laws for HALEU-Fueled Advanced Reactors — **Iyad Al-Qasir**

Review of Available Critical Experiment Benchmarks and Critical Experiment Facilities for HALEU Fuel Transport Validation — **Mathieu Dupont**

Introduction

Advanced reactors are driving a change in the nuclear power landscape

New analyses must identify where the current validation basis is and is not suitable for changing fuel cycle needs

Larger variety of fuel forms

Higher Enrichment

Higher Burnup

Oak Ridge National Laboratory

HALEU ARDP Designs and Transportation Packages

Lisa Fassino

HALEU in Advanced Reactor Designs

- **Goal:** scope the unique features of HALEU reactor fuel to determine needs for validation basis
  - **As a launching point:** begin with designs in the Advanced Reactor Demonstration Program (ARDP) using HALEU
  - 10 Designs, 9 with HALEU
    - Only 1 not planning to use HALEU (Holtec International's SMR-160)
  - **Far from an exhaustive list!** ➡

HALEU ARDP

Leads	Designs
TerraPower	Natrium
X-energy	Xe-100
Kairos Power	KP-FHR
Westinghouse Nuclear	eVinci
Southern Company and TerraPower	MCFR
BWXT	BANR
ARC	ARC-100
GA-EMS	FMR
MIT	HC-HTGR

Many more…

Let us know about public references for any additional fuel forms, storage, transportation at this email: DNCSH@ornl.gov

The MARVEL microreactor by DOE

The Aurora powerhouse reactor by Oklo

The Hermes test reactor and Hermes 2 by Kairos Power

The Ultra Safe Nuclear Corporation (USNC) micro modular reactor (MMR)

The Lightbridge helically twisted HALEU fuel for current commercial reactors

The Project Pele microreactor by the US Department of Defense (DoD) and BWXT

The Demonstration Rocket for Agile Cislunar Operations (DRACO) by the Defense Advanced Research Projects Agency (DARPA) in collaboration with the National Aeronautics and Space Administration (NASA)

The Molten Salt Research Reactor (MSRR) by the Nuclear Energy eXperimental Testing Laboratory (NEXT Lab) at Abilene Christian University (ACU)

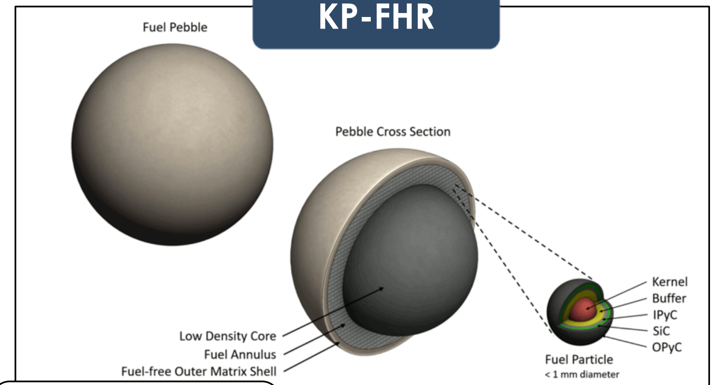
This is not an exhaustive list, either!

Summary of HALEU ARDP Characteristics

Lead	Reactor Name	Reactor Type	Neutron Spectrum	Fuel Type	Power	Enrichment (wt% ^{235}U)	Moderator	Reflector	Coolant
TerraPower	Natrium	SFR	Fast	Sodium-bonded Metallic Alloy U-10Zr Pins (Type 1)	345 MWe	19.75	N/A	—	Salt
X-energy	Xe-100	Pebble Bed HTGR	Thermal	UCO TRISO Spherical Compacts	80 MWe	15.5	Graphite	Graphite	Helium
Kairos Power	KP-FHR	Pebble Bed FHR	Thermal	UCO TRISO Annular Spherical Compacts with Low-Density Graphite Cores	140 Mwe	19.55	Pyrolytic Graphite, FLiBe	Graphite	FLiBe
Westinghouse Nuclear	eVinci	Heat-pipe Microreactor	Thermal	UCO TRISO Cylindrical Compacts	5 Mwe	19.75	Graphite	—	Sodium Heat Pipes
Southern Company and TerraPower	MCFR	MSR	Fast	Dissolved Uranium in Salt ($NaCl$-UCl_3)	800 MWe	HALEU	N/A	—	Salt
BWXT	BANR	HTGR	Thermal	UN TRISO in SiC, Carbon Matrix Compact, Additively Manufactured	50 MWth	19.75 (Baseline Design)	Graphite	—	Helium
ARC	ARC-100	SFR	Fast	Sodium-bonded U-10Zr pins	100 MWe	20 Max.; 13.1 Avg.	N/A	Stainless Steel	Sodium
GA-EMS	FMR	GFR	Fast	UO_2 Pellets	44 MWe	19.75	N/A	Zr_3Si_2 and Graphite	Helium
MIT	HC-HTGR	HTGR	Thermal	TRISO Compact	~58 MWth	—	Graphite	—	Helium

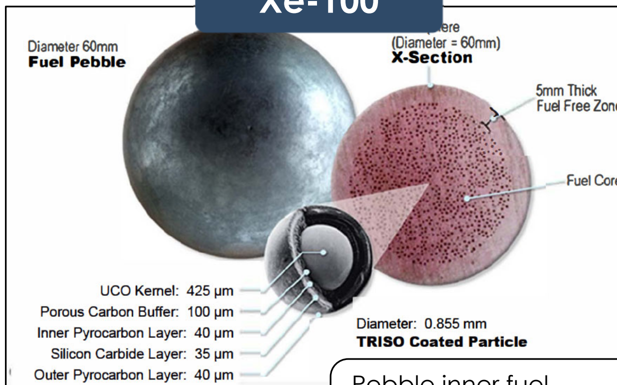
Fuel Forms Across ARDP Designs

KP-FHR



Pebble annular fuel region with UCO TRISO particles

Xe-100

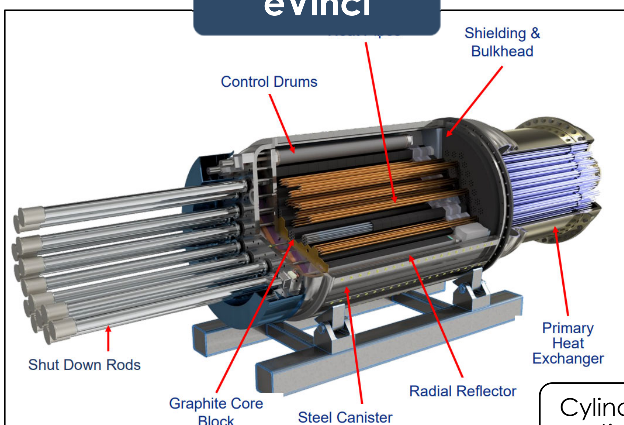


Pebble inner fuel region with UCO TRISO particles

BANR

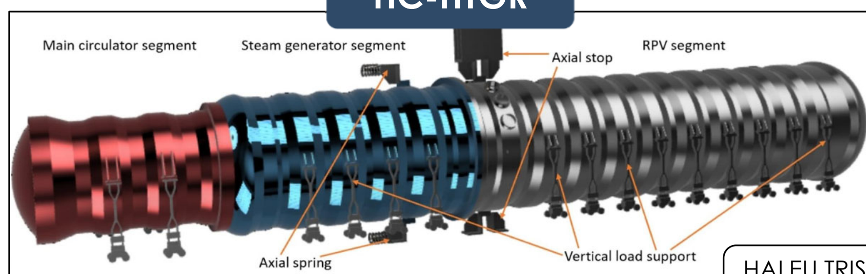
UN TRISO in SiC, carbon matrix in additively manufactured compact

eVinci



Cylindrical UCO TRISO particle compacts

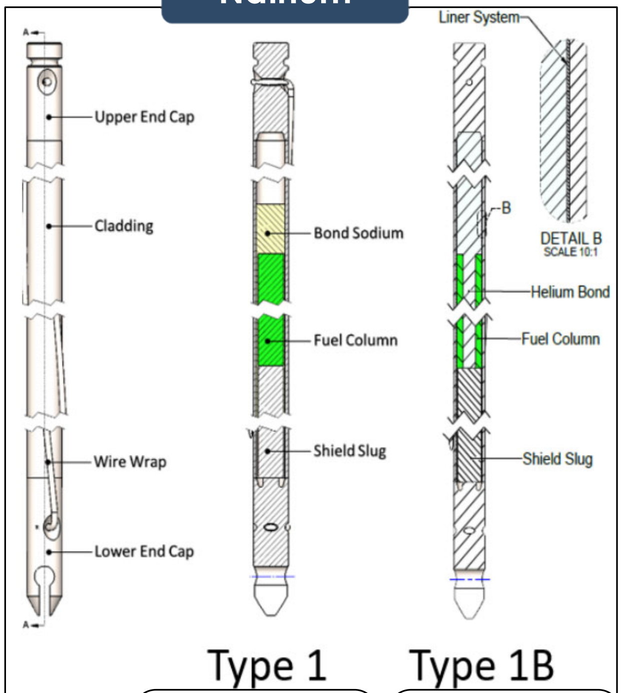
HC-HTGR



HALEU TRISO Particles Expected

Fuel Forms Across ARDP Designs

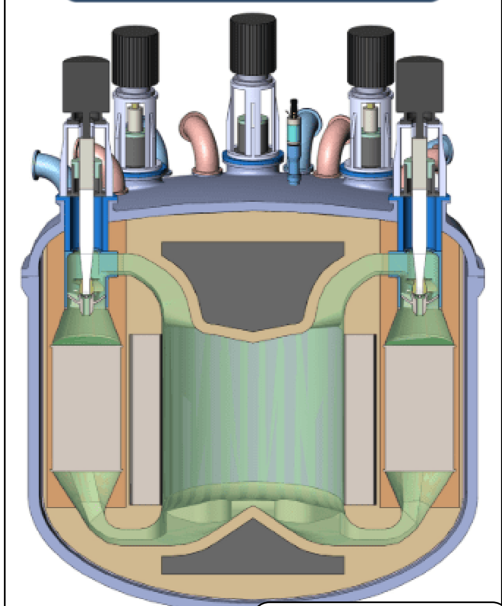
Natrium



Type 1:
Sodium-bonded
metallic alloy
U-10Zr Pins

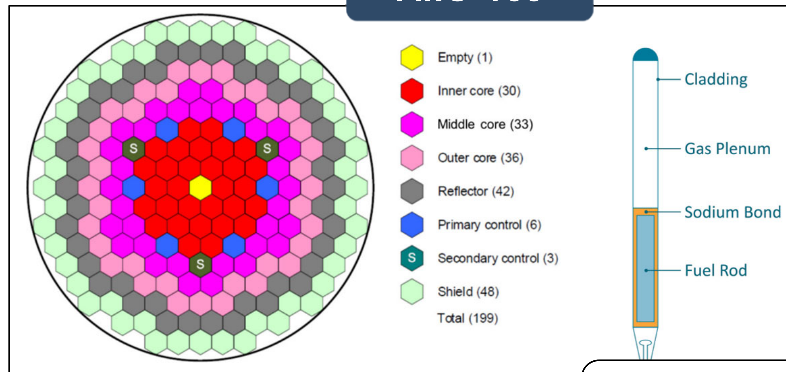
Type 1B:
Helium-bonded
metallic alloy
U-0Zr

Molten Chloride Fuel Salt



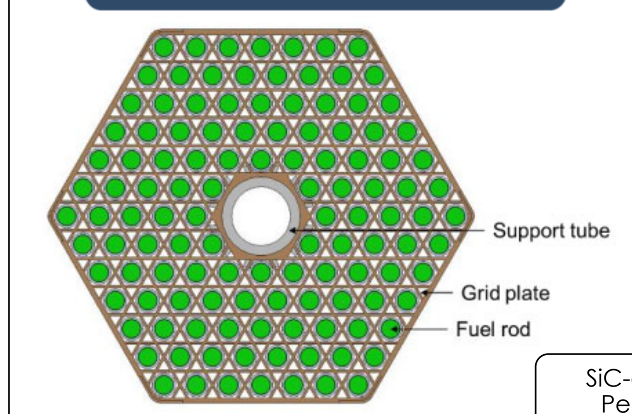
MCFR (HALEU),
MCRE (HEU)
$NaCl\text{-}UCl_3$

ARC-100



Sodium-bonded
metallic alloy
U-10Zr Pins

GA-EMS Fast Metal Reactor



SiC-clad, UO_2
Pellet Rods

Transportation Packages

- NRC lists the following transportation packages as currently involved in increased enrichment licensing activities:

RAJ-II (GNF-A)

Traveller (Westinghouse)

OPTIMUS-L (NAC)

ES-3100 (Y-12)

DN30-20 (Orano)

Versa-Pac (Orano)

TN-B1 (Framatome)

MAP-12 and MAP-13 (Framatome)

Up to 7 wt% ^{235}U

Up to 8 wt% ^{235}U

Up to 10 wt% ^{235}U

Up to 20 wt% ^{235}U

Up to 100 wt% ^{235}U

Summary of HALEU Transportation Package Details

Transportation Package	Owner	Fuel Type	Approved Enrichment, wt% ^{235}U	Content Limits	Approximate Dimensions, m
Traveller STD	Westinghouse	Fresh or Slightly Contaminated PWR UO_2 Assemblies or Fuel Rods	**Up to 6% for assemblies or up to 7% for fuel rods**	One assembly or one container of loose rods	5.0 x 0.7 x 1.0 (L x W x H)
Traveller XL					5.7 x 0.7 x 1.0 (L x W x H)
MAP-12	Framatome	Fresh uranium fuel assemblies	**Up to 8%**	Two assemblies	5.3 x 1.1 x 0.8 (L x W x H)
MAP-13					5.6 x 1.1 x 0.8 (L x W x H)
TN-B1	Framatome	Fresh UO_2 PWR or BWR assemblies or UC fuel rods	**Up to 5%, with request to extend to 8%**	One assembly	1.8 x 0.2 x 0.1 (inner L x W x H) 2.0 x 0.3 x 0.3 (outer L x W x H)
RAJ-II	GNF-A	BWR fuel assemblies; BWR, CANDU, or PWR rods	**Up to 5% in UC; Up to 8% in UO_2.**	Two assemblies	1.8 x 0.2 x 0.1 (inner L x W x H) 2.0 x 0.3 x 0.3 (outer L x W x H)
OPTIMUS®-L	NAC	Certain waste materials; unirradiated TRISO cylindrical compacts	**Up to 20% for cylindrical TRISO compacts**	68 kgU	0.3 x 0.5 (inner D x H) 0.5 x 0.7 (outer D x H)
DN30-10	Orano	UF_6	**Up to 10%**	98 kg fissile material, 1460 kg UF_6	0.8 x 2.1 (cylinder D x H) 1.2 x 2.4 (package D x H)
DN30-20			**Up to 20%**	170 kg fissile material, 1271 kg UF_6	
Versa-Pac 55 (VP-55)	Orano	Uranium oxides, metal, and other compounds; Uranyl nitrate crystals; TRISO fuel	**Up to 100%**	610 g ^{235}U up to 5% 505 g ^{235}U up to 10% 445 g ^{235}U up to 20% 360 g ^{235}U up to 100%	0.4 x 0.6 x 0.9 (ID x OD x H)
Versa-Pac 110 (VP-110)					0.5 x 0.8 x 1.1 (ID x OD x H)
ES-3100	Y-12	Uranium oxides, metals, alloys, compounds, and uranyl nitrate crystals	**Up to 100%**	Up to 9.682 kg ^{235}U in oxides with 921 g carbon and CSI of 0.0; Up to 35.2 kg ^{235}U in metals/alloys	1.1 x 0.5 (D x H)

Conclusions

- Fresh HALEU fuel for LWRs (up to 8%) can be transported
- Fresh HALEU fuel for ARDP reactors does not have commercial-scale packages, except maybe DN-30X and ES3100 in some cases
- Details still needed for ARDP designs to assess transportation package suitability, e.g.
  - Fuel salt characteristics for MCFR
  - Fabrication, transportation, and storage processes/plans
  - Materials/components transported in reactor (e.g. for SMRs or MMRs)
- We can only plan for what we know!

OAK RIDGE
National Laboratory

Nuclear Data Gaps: Current Status of Thermal Scattering Laws for HALEU-Fueled Advanced Reactors

Iyad Al-Qasir

Outline

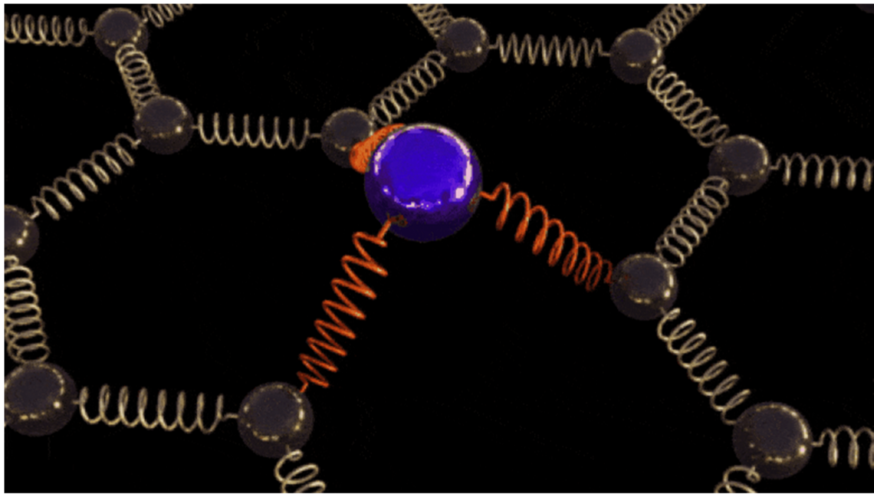
- Introduction
  - Importance of Nuclear Data
  - Thermal Neutrons
  - Neutron Moderation
- Status of Main Neutron Moderators
- Current Status Graphite TSL Sub-libraries
- Conclusions

Why Do We Need Nuclear Data?

- The effective design, operation, and eventual decommissioning of a nuclear power plant, along with licensing transportation packages for fresh or spent fuel, require extensive access to comprehensive nuclear data covering diverse radiation particles across a broad energy spectrum.
- The use of high-quality nuclear data in calculations is essential for accuracy, safety, reliability, optimization fuel performance, research, and **regulatory compliance** in various nuclear-related fields and applications.
- Nuclear data and uncertainty (aka covariance) plays a special role in similarity and validation basis assessment
- One specific category of relevant nuclear data is notably temperature-dependent and is referred to as the thermal neutron scattering law (TSL) or $S(\alpha, \beta)$.

Thermal Neutrons

- Thermal neutrons have wavelengths (~Å) comparable to the separation distances of atoms in solids.
- Hence, the thermal motion of atoms or molecules in the scattering medium can no longer be ignored
- Thermal neutron scattering law (TSL) describes the neutron scattering intensity as a function of energy and momentum transfer between the thermal neutron and the scattering medium



ENDF/B-VIII.1 TSL Sub-Libraries

	Moderators
	H /Water/ICE
1	H in H_2O (liquid)
50	O in H_2O (ice (Ih))
10	H in H_2O (ice (Ih))
51	O in D_2O (liquid)
11	D in D_2O (liquid)
2	para-Hydrogen
3	ortho-Hydrogen
12	para-Deuterium
13	ortho-Deuterium
	Be compounds
26	Be (metal)
204	Be+sd
27	Be in BeO
46	O in BeO
28	Be in Be_2C
1021	C in Be_2C
	Graphite
30	crystalline graphite
301	Graphite +sd
31	reactor-grade graphite (10% porosity)
320	reactor-grade graphite (20% porosity)
32	reactor-grade graphite (30% porosity)
	Metallic Hydrides
5	H in YH_2
7	H in ZrH
3001	Zr in ZrH_2
3002	H in ZrH_2
3006	Zr in ZrHx
3007	H in ZrHx
3011	Ca in CaH_2
3013	H1 in CaH_2
3014	H2 in CaH_2
3031	7Li in 7LiH-mixed
3032	H in 7LiH-mixed
3034	7Li in 7LiD-mixed
3035	D in 7LiD-mixed
58	Zr in ZrH
55	Y in YH2

	Fuel
71	N in UN
72	U in UN
75	U in UO_2
45	O in UO_2
76	U in UC
71	N in UN
8000	U-metal
8010	U-metal-10p
8099	U-metal-HEU
8105	U in UC-5p
8110	U in UC-10p
8147	U in UC-100P
8148	U in UC-HALEU
8149	U in UC-HEU
8150	C in UC
8155	C in UC-5p
8160	C in UC-10p
8197	C in UC-100P
8198	C in UC-HALEU
8199	C in UC-HEU
8205	U in UO_2-5p
8210	U in UO_2-10p
8248	U in UO_2-HALEU
8249	U in UO_2-HEU
8255	O in UO_2-5p
8260	O in UO_2-10p
8297	O in UO_2-100P
8298	O in UO_2-HALEU
8299	O in UO_2-HEU
8305	U in UN-5p
8310	U in UN-10p
8347	U in UN-100P
8348	U in UN-HALEU
8349	U in UN-HEU
8355	N in UN-5p
8360	N in UN-10p
8397	N in UN-100P
8398	N in UN-HALEU
8399	N in UN-HEU
8540	H in UH_3

	Filters/Structural
112	Mg (metal)
53	Al (metal)
56	Fe (metal)
59	Si
49	beta-phase SiO_2
3016	Si in SiO_2-alpha
3017	O in SiO_2-alpha
43	Si in SiC
44	C in SiC
1051	C in CF_2
1052	F in CF_2
3048	H in HF
3047	F in HF
1001	Zr in ZrC
1002	C in ZrC
3052	Al in Al_2O_3
3053	O in Al_2O_3

	FLiBe
4001	F in FLiBe
4002	Be in FLiBe
4003	Li in FLiBe

Summary of HALEU ARDP Characteristics

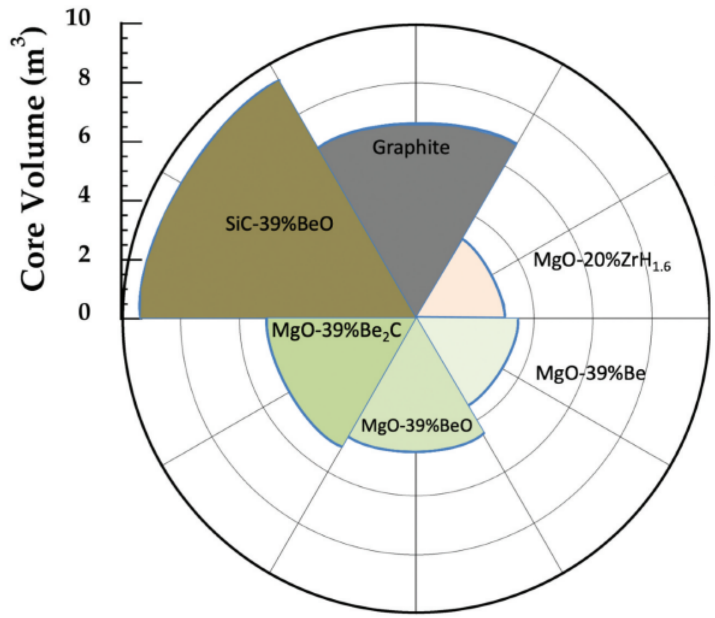
Lead	Reactor Name	Reactor Type	Neutron Spectrum	Fuel Type	Power	Enrichment (wt% ^{235}U)	Moderator	Reflector	Coolant
TerraPower	Natrium	SFR	Fast	Sodium-bonded Metallic Alloy U-10Zr Pins	345 MWe	19.75	N/A	—	Salt
X-energy	**Xe-100**	**Pebble Bed HTGR**	**Thermal**	**UCO TRISO Spherical Compacts**	**80 MWe**	**15.5**	**Graphite**	**Graphite**	Helium
Kairos Power	**KP-FHR**	**Pebble Bed FHR**	**Thermal**	**UCO TRISO Annular Spherical Compacts with Low-Density Graphite Cores**	**140 Mwe**	**19.55**	**Pyrolytic Graphite, FLiBe**	**Graphite**	**FLiBe**
Westinghouse Nuclear	**eVinci**	**Heat-pipe Microreactor**	**Thermal**	**UCO TRISO Cylindrical Compacts**	**5 Mwe**	**19.75**	**Graphite**	**—**	Sodium Heat Pipes
Southern Company and TerraPower	MCFR	MSR	Fast	Dissolved Uranium in Salt ($NaCl-UCl_3$)	800 MWe	HALEU	N/A	—	Salt
BWXT	**BANR**	**HTGR**	**Thermal**	**UN TRISO in SiC, Carbon Matrix Compact, Additively Manufactured**	**50 MWth**	**19.75 (Baseline Design)**	**Graphite**	**—**	**Helium**
ARC	ARC-100	SFR	Fast	Sodium-bonded U-10Zr pins	100 MWe	20 Max.; 13.1 Avg.	N/A	Stainless Steel	Sodium
GA-EMS	FMR	GFR	Fast	UO_2 Pellets	44 MWe	19.75	N/A	**Zr_3Si_2 and Graphite**	Helium
MIT	**HC-HTGR**	**HTGR**	**Thermal**	**TRISO Compact**	**~58 MWth**	**—**	**Graphite**	**—**	Helium

Neutron Moderation

- Typical core moderator and reflector materials consist of relatively simple compounds of a simple material type or simple composition (e.g, H_2O, D_2O, Be, BeO, Graphite, ZrH_2).
- Recently, compact thermal fission reactors are of increased interest due to their potential lower and controlled construction cost, enhanced safety, and portability to remote areas.
- They are also considered as a point-source for process industrial heat
- The compact nature of these cores requires good neutron economy

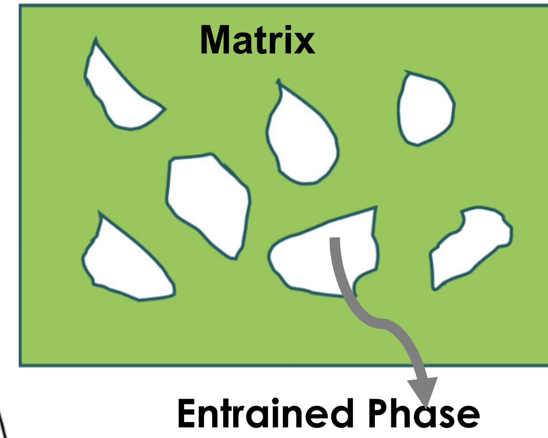
Example: Two Phase Composite Moderator

	Entrained Phase	Matrix Phase
Scattering	High	Fair
Absorption	Low	Low
Thermal Conductivity	Fair	High
Radiation resistivity	Fair	Good
Mechanical Stability	Fair	Good
Examples	Graphite, Be, **$Be_4{}^{11}B$**, BeO, **Be_2C**, **YH_{2-x}**, **ZrH_{2-x}**	MgO, SiC



Be_2C: reacts with moisture to form Be(OH)2. However, as an entrained phase it will not

YH_{2-x}, **ZrH_{2-x}**: High dense matrix forms barriers that prevents hydrogen leakage



Entrained Phase refers to a phase or component of a mixture that is carried along or transported by another medium or phase.

MgO-based composite moderators can exhibit considerably smaller critical volumes when compared to nuclear graphite

Snead et al., *J. Asian Ceram. Soc.* **10**, 9 (2022).

Neutron Moderators Status

Material	Available TSL ENDF Files	Differential Measurement	Integral Measurements	Benchmark* Experiments.
Graphite	Yes	Yes	Yes	Yes
$ZrH_{1.6}$ & ZrH_2	Yes	Yes	Yes	Yes
YH_2	Yes	Yes	Yes	**No**
Be metal	Yes	Yes	Yes	**No**
BeO	Yes	**No**	Yes	**No**
MgO	**No****	**No**	Yes	**No**
Be_2C	Yes	**No**	**No**	**No**
FLiBe	Yes	**No**	**No**	**No**
SiC	Yes	**No**	**No**	**No**
Zr_3Si_2	**No**	**No**	**No**	**No**

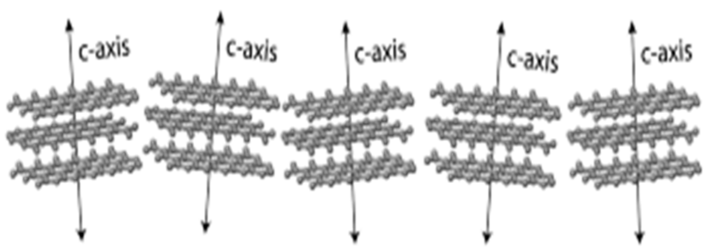
* These experiments involve fuel compositions ranging from 5 to 19.75 wt% enrichment with ^{235}U and exhibit a neutron flux of < 0.625 eV

** The MgO TSL sub-library has been submitted to the Cross Section Evaluation Working Group (CSEWG) for approval and inclusion in the ENDF database; at this writing, approval is pending.

Current Status of Graphite TSL Sub-libraries

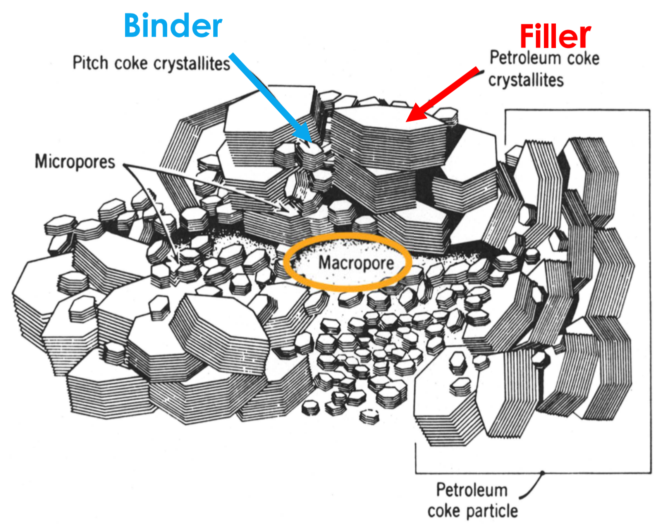
Graphite

- **Crystalline Graphite**
- **Density ~2.26 g/cm³ (HOPG)**
- Huge number of small nearly perfect micro-crystallites that have the same c-axis but with different orientations in x-y plane
- Very close to the Ideal, perfect or theoretical graphite.

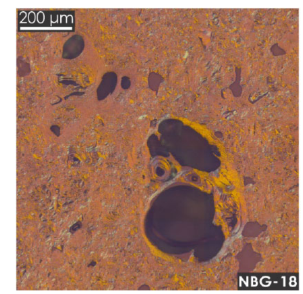


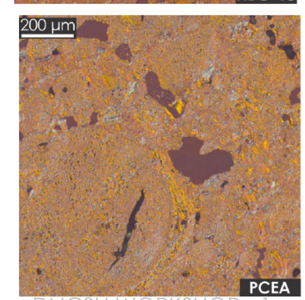
	Graphite
30	crystalline graphite
301	Graphite +sd
31	reactor-grade graphite (10% porosity)
320	reactor-grade graphite (20% porosity)
32	reactor-grade graphite (30% porosity)

- **Nuclear Graphite**
- **Density(1.5~1.90) g/cm³**
- Complex Microstructure- contains crystallite (filler and binder) & pores
- The size and shape of grains and pores vary from one graphite grade to another.



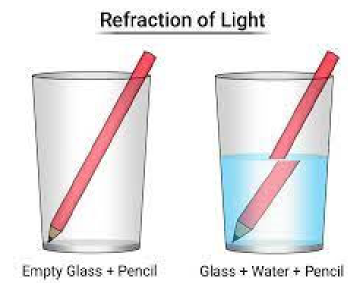
Contescu & Paul, ORNL/TM-2022/1839

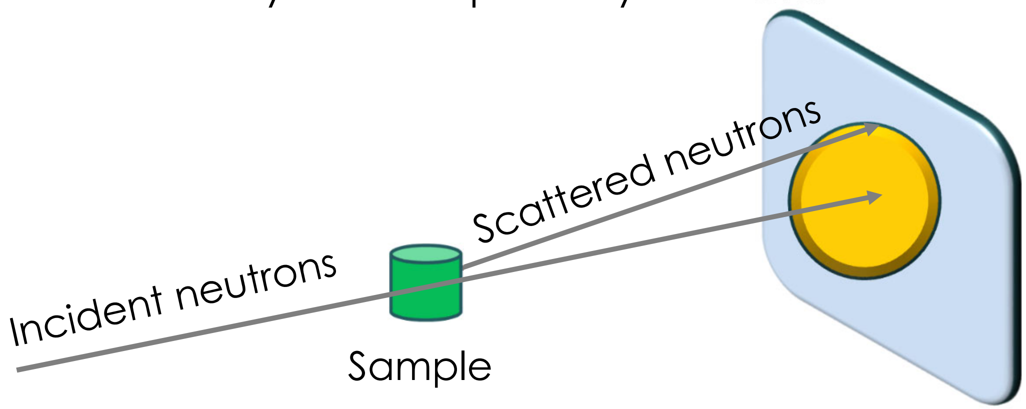


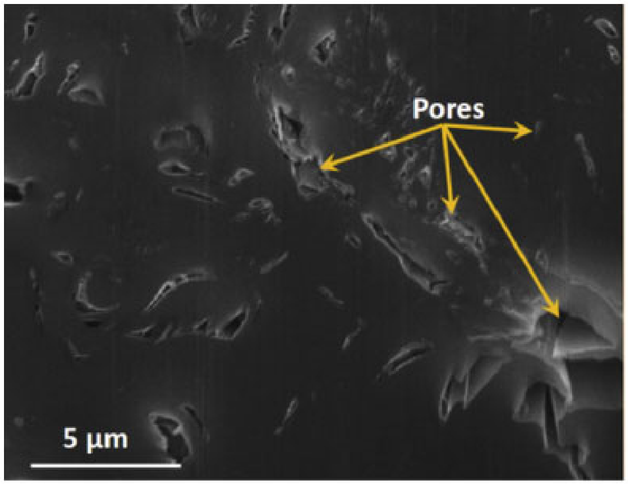


Small Angle Neutron Scattering (SANS)

- SANS is an elastic scattering phenomenon where neutrons **diverges** from their incident beam by a small scattering angle (generally, $2\theta < 10$ deg), as it penetrates through a sample.
- In **nuclear graphite**, SANS occurs on cracks, voids, pores, etc., where the continuous distribution of carbon density is interrupted by defects.





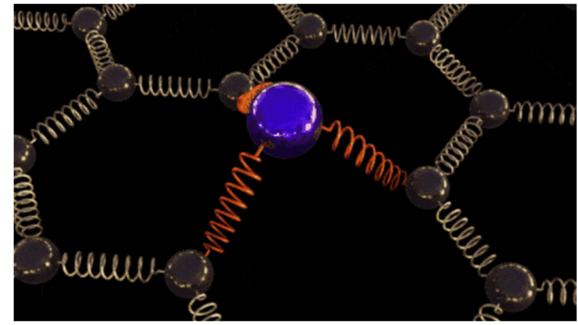


Liu et al., J. Nucl. Mater. ***493***, *246-54, (2017)*

Graphite: Inelastic + Elastic + SANS
Others : Inelastic + Elastic

Thermal Scattering Law (TSL), S(α, β)

Energy Transfer
Momentum transfer

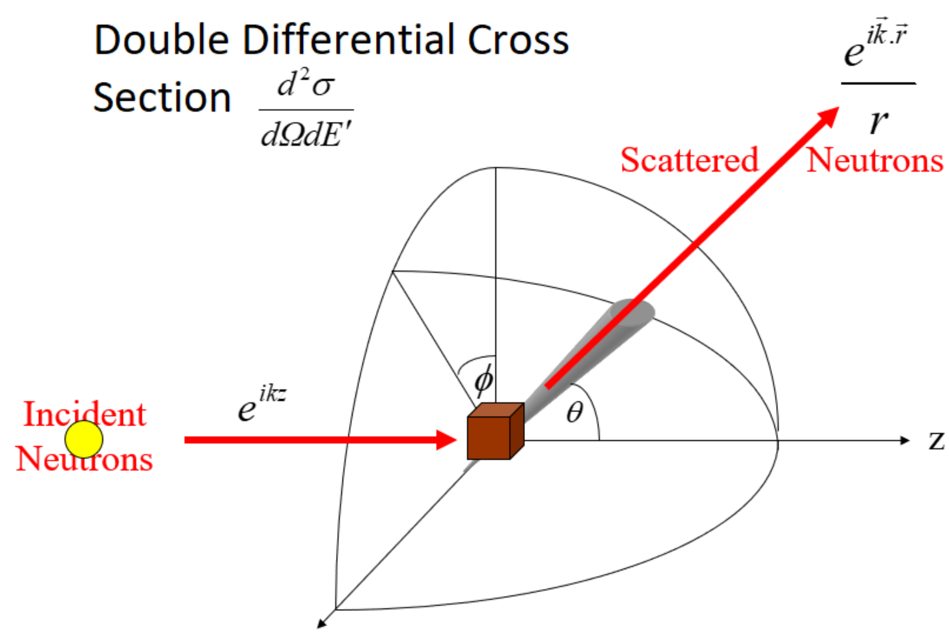


$$\frac{d^2\sigma}{dE'\,d\Omega} \cong \frac{\sigma_{coh}+\sigma_{incoh}}{4\pi k_B T}\sqrt{\frac{E'}{E}}\, e^{-\beta/2}\sum_{P=1}^{P} S_s(\alpha,\beta)$$

$$\Rightarrow S_s(\alpha,\beta)=\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\beta\tau}e^{-\gamma^2(\tau)}\,d\tau$$

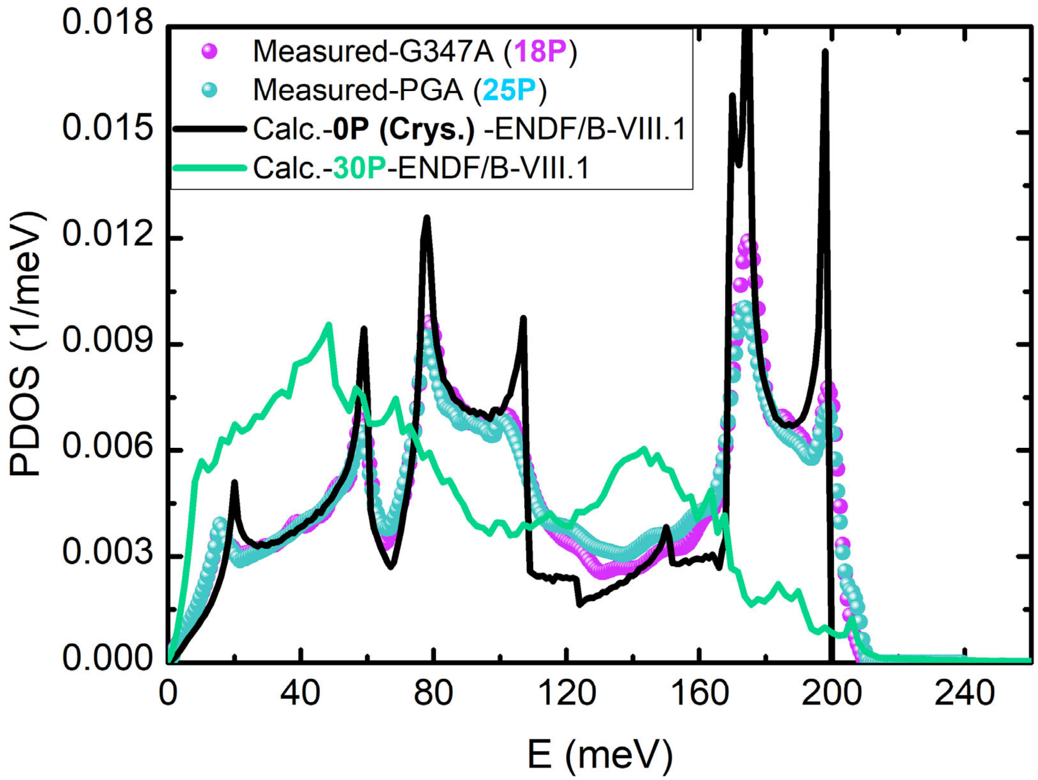
$$\gamma^2(\tau)=\alpha\int_{-\infty}^{\infty}\frac{\rho(\beta)[1-e^{i\beta\tau}]e^{\frac{-\beta}{2}}}{2\beta\sinh(\beta/2)}\,d\beta$$

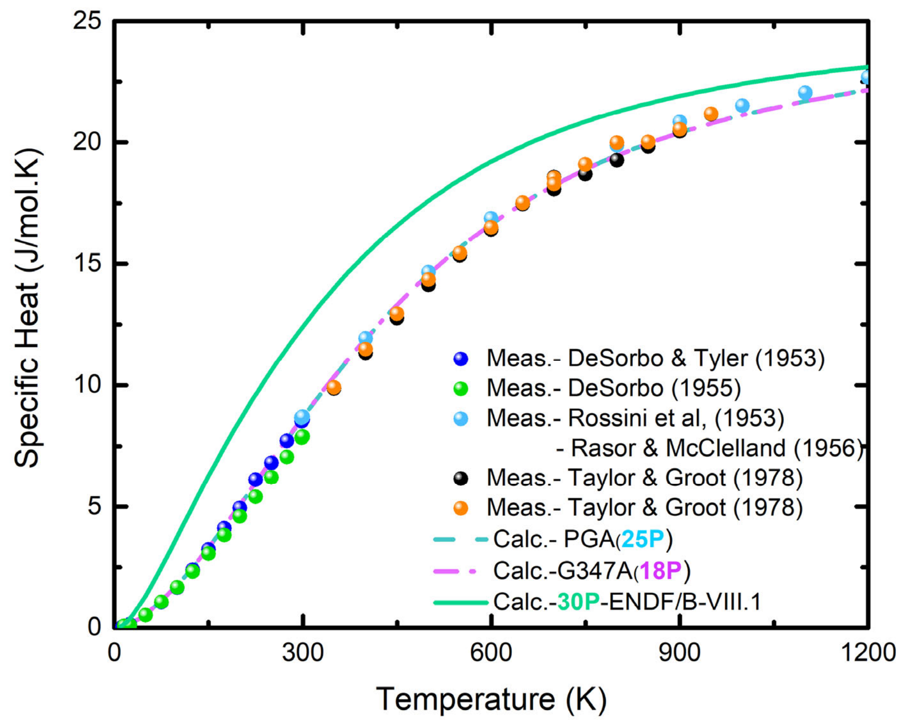
Double Differential Cross Section $\frac{d^2\sigma}{d\Omega dE'}$



All we need to calculate the scattering law is the phonon density of states (PDOS), $\rho(\beta)$

ARCS Measurements of Phonon Density of States (PDOSs)





- ✓ **Specific heat as well as S(α , β) are both functions of the PDOS, $\rho(\omega)$**
- ✓ **Different graphite grades, show similar measured PDOS & specific heat**
- ✓ **30P-PDOS & Specific heat shows significant deviations from measured values**

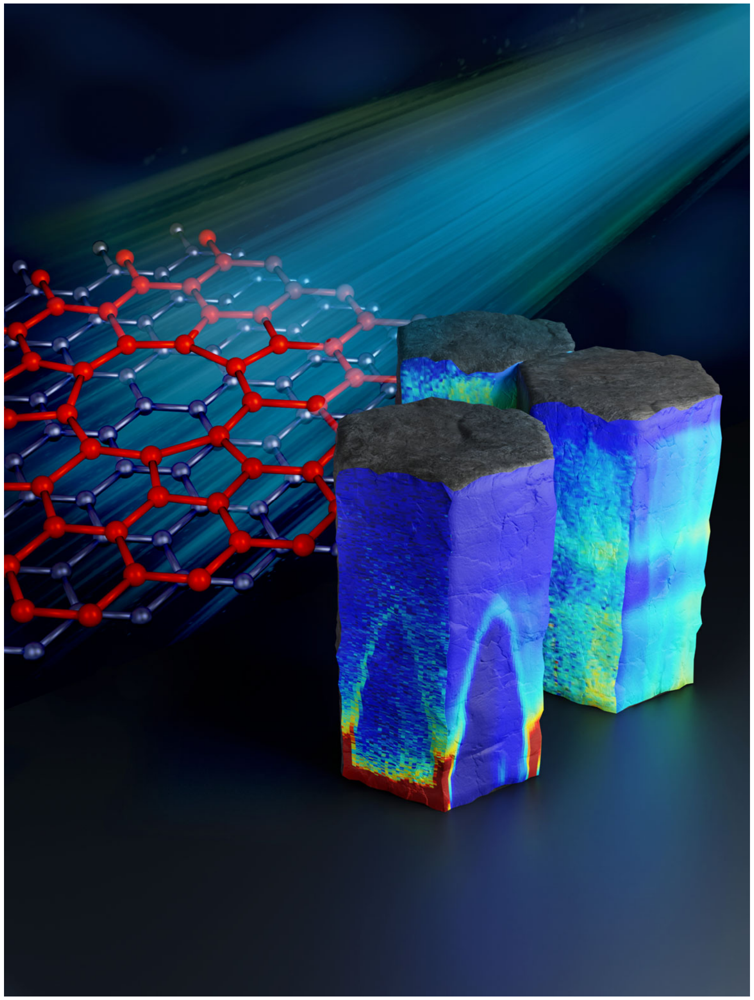
Al-Qasir et al., Neutron thermalization in nuclear graphite: A modern story of a classic moderator, Annals of Nuclear Energy **161**, 108437 (2021)

Conclusions

- Thermal moderators are not adequately covered across all necessary types of experiments
- High-fidelity nuclear graphite neutronics calculations require **inelastic+elastic+SANS** and pore size distribution
- A standardized approach for generating or preserving TSL 2D covariance data related does not exist—currently investigating relevance for criticality safety

Material	Available TSL ENDF Files	Differential Measurement	Integral Measurements	Benchmark Experiments
Graphite	Yes	Yes	Yes	Yes
$ZrH_{1.6}$ & ZrH_2	Yes	Yes	Yes	Yes
YH_2	Yes	Yes	Yes	No
Be metal	Yes	Yes	Yes	No
BeO	Yes	No	Yes	No
MgO	No	No	Yes	No
Be_2C	Yes	No	No	No
FLiBe	Yes	No	No	No
SiC	Yes	No	No	No
Zr_3Si_2	No	No	No	No

Thank you

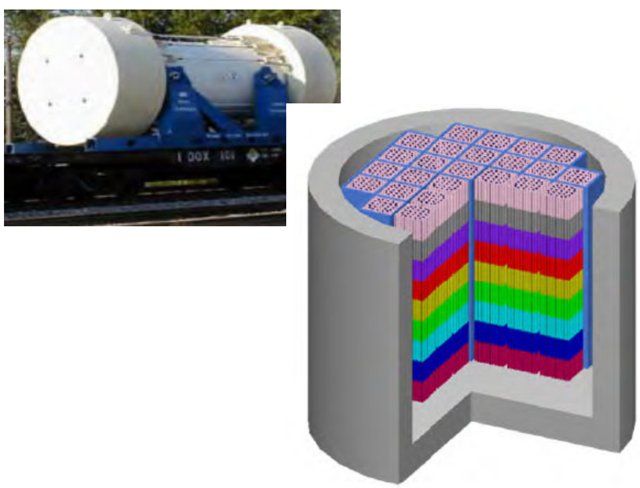


Review of Available Critical Experiment Benchmarks and Critical Experiment Facilities for HALEU Fuel Transport Validation

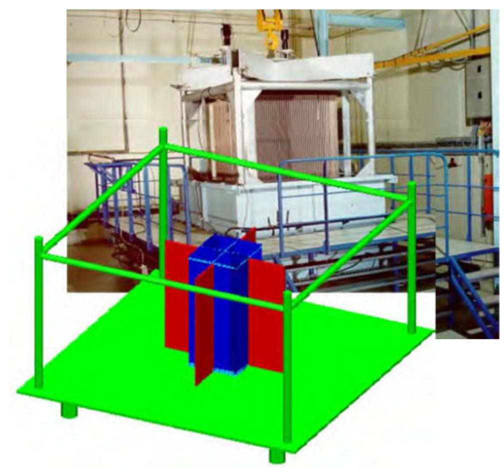
Mathieu Dupont

Introduction to HALEU fuel validation

- Computational validation [1]: determine the bias and bias uncertainty between calculations and observations
- Criticality safety: Compare k_{eff} values of critical experiment benchmarks and application models



Application



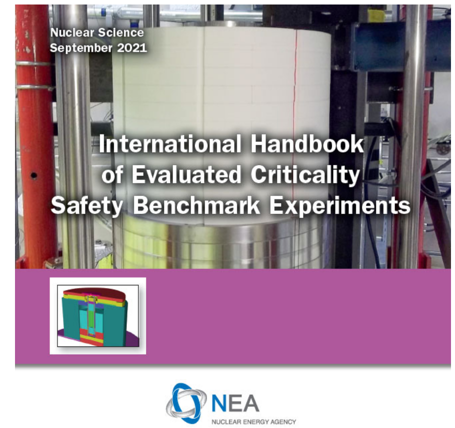
Critical Experiment

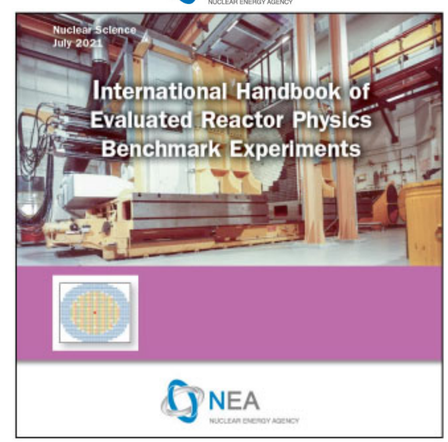
Introduction to HALEU fuel validation

- What we need: Critical experiment benchmark as similar as possible to the application to be validated
  - Fuel enrichment: HALEU 5-20 wt% ^{235}U, most advanced reactors are close to 20 wt% ^{235}U
  - Moderator/reflector material: graphite, FLiBe
  - Neutron energy spectrum: thermal and fast
  - Structural materials: wide range
  - Fuel form: Uranium compacts, TRISO particle-like, fuel salt, metal
- What do we have?

Review of available critical experiments for HALEU validation

- Two best sources from Nuclear Energy Agency (NEA):
  - International Criticality Safety Benchmark Evaluation Project (ICSBEP) [2]: wide range of critical experiments, focus on the light water reactor validation
  - International Reactor Physics Benchmark Evaluation Project (IRPhEP) [3]: focus on reactor physics experiments, some critical configurations available
- The handbooks provide thousands of benchmark experiments from dozens of countries with an assessment of data integrity, quantification of experimental uncertainties, and thorough technical review with established deployment process





Review of available critical experiments for HALEU validation

- Experiments potentially relevant for HALEU validation from the handbooks
- Experiments quality and correlation
- Upcoming experiments
- Conclusions and recommendations

Review of available critical experiments for HALEU validation

- **Experiments potentially relevant for HALEU validation from the handbooks**
- Experiments quality and correlation
- Upcoming experiments
- Conclusions and recommendations

Review of available critical experiments for HALEU validation

In ICSBEP handbook:

Characteristic of Interest for HALEU Fuel Validation	Number of Evaluations	Number of Experiments
^{235}U enrichment 5 to 21 wt%	74	431
^{235}U enrichment 5 to 9 wt%	26	247
^{235}U enrichment 9 to 21 wt%	48	184
^{235}U enrichment 18 to 21 wt%	13	36
^{235}U enrichment 9 to 21 wt% and uranium metal	13	29
^{235}U enrichment 9 to 21 wt% and UF_4	2	6
^{235}U enrichment 9 to 21 wt% and UO_2 in TRISO particles	1	5
UF_4-UF_6 any enrichment	10	110
Uranium metal of any enrichment	195	799
Uranium salts any enrichment	0	0

OAK RIDGE National Laboratory

Review of available critical experiments for HALEU validation

In IRPhE handbook:

Characteristic of interest for HALEU Fuel Validation	Number of evaluations	Number of Experiments
Potentially relevant to HALEU fuel forms	15	54
Uranium salt any enrichment	1	1
UO_2 in TRISO and BISO particles	7	27
^{235}U enrichment 18 to 21 wt% and uranium metal or graphite moderator	4	7

Review of available critical experiments for HALEU validation

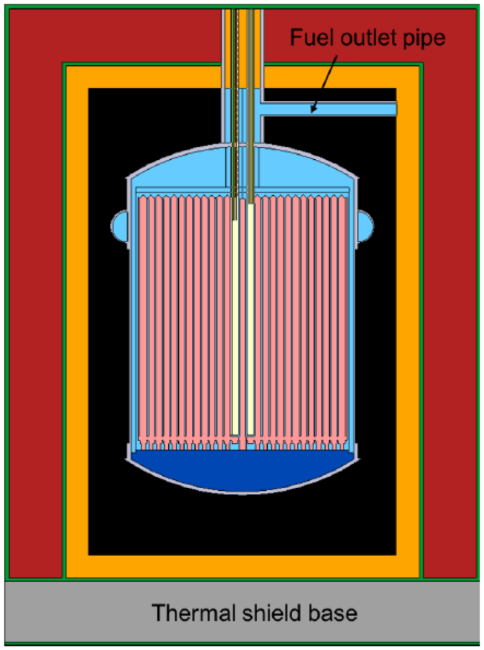
- Experiments potentially relevant for HALEU validation from the handbooks
- **Experiments quality and correlation**
- Upcoming experiments
- Conclusions and recommendations

Review of available critical experiments for HALEU validation

- Good validation suite:
  - As high as possible number of applicable critical experiments
  - As low as possible experimental uncertainty
  - As high as possible variety of experimental facilities to reduce experimental correlations [4]
- What is the current status on quality and correlation of HALEU validation critical experiments?

Review of available critical experiments for HALEU validation

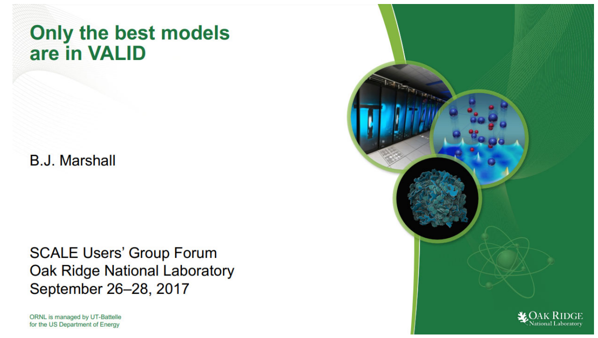
- Experimental uncertainty:
  - ICSBEP: Mostly good, some outliers IEU-COMP-THERM-009-001 with an experimental uncertainty of 600 pcm and IEU-COMP-MIXED-002-008 with a Calculated/Expected ratio of 1.044
  - IRPhEP: Mostly high uncertainty, for example Molten Salt Reactor Experiment (MSRE) has an experimental uncertainty of 420 pcm on k_{eff} and a k_{eff} C/E ratio of 1.0215: known deficiencies exist



MSRE benchmark model core [5]

Review of available critical experiments for HALEU validation

- Additional review of the quality of critical experiments may be needed, such efforts already exist:
  - ORNL Verified, Archived Library of Inputs and Data (VALID) [6]: peer-reviewed criticality benchmarks sensitivity data files
  - WPNCS subgroup 8 (SG-8) [7]; “Preservation of Expert Knowledge and Judgement Applied to Criticality Benchmarks”



VALID [8]

Initial Efforts Organizing WPNCS SG-8:
Preservation of Expert Knowledge and Judgement Applied to Criticality Benchmarks

William Wieselquist,[1] John D. Bess,[2] Douglas Bowen,[1] Isabelle Duhamel,[3] Ian Hill,[4] Nicolas Leclaire,[3] William B. J. Marshall,[1] Catherine Percher,[5] Ellen Marie Saylor,[1] Shuichi Tsuda[4]

[1]*Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, USA, wieselquiswa@ornl.gov*
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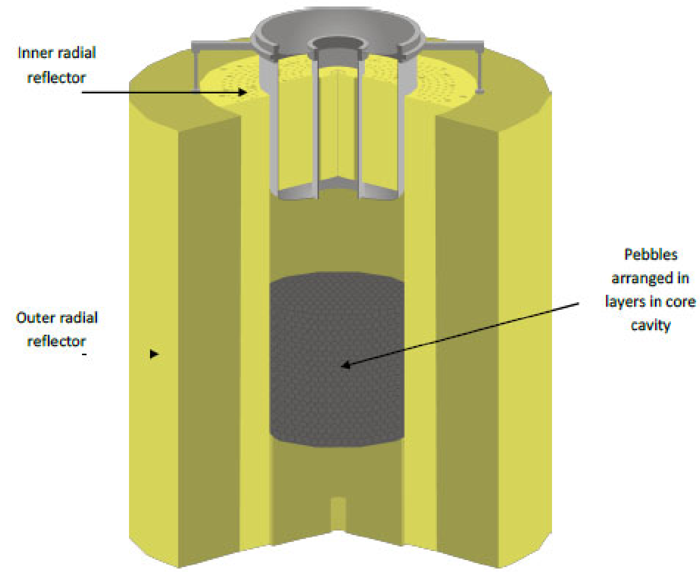
[5]*Lawrence Livermore National Laboratory (LLNL), Livermore, CA, USA*

https://dx.doi.org/10.13182/T123-32977

WPNCS SG-8 [7]

Review of available critical experiments for HALEU validation

- Experimental correlations:
  - From both ICSBEP and IRPhEP handbooks, 616 experiments in 104 evaluations were identified
  - Many come from the same facilities: experimental correlations exist
  - Example: PROTEUS-GCR



Generic HTR-PROTEUS configuration [9]

Review of available critical experiments for HALEU validation

- Experimental correlations:
  - 11 PROTEUS-GCR experiments from 4 evaluations come from the same PROTEUS facility operated at the Paul Scherrer Institute (PSI) in Switzerland
  - All have around 300–400 pcm experimental uncertainty, from the same ^{235}U isotopic content, resulting in 250–300 pcm keff
  - Correlation within and between the evaluations, so the resulting computational bias for all the experiments and evaluations from the same facility will be similar

- **Critical experiments from different facilities are recommended**

Review of available critical experiments for HALEU validation

- Experiments potentially relevant for HALEU validation from the handbooks
- Experiments quality and correlation
- **Upcoming experiments**
- Conclusions and recommendations

Upcoming experiments potentially relevant for HALEU validation [10]

Experiment	Characteristic of Interest for HALEU Fuel Validation	Facility/ Organization / country	Status	Potential issues
AGN-201M Reactor Benchmark [11]	19.5 wt% microspheres coated with graphite	University of New Mexico, USA	Expected benchmark completion in 2025	Lack of characterization of the fuel plates
IPEN/MB01 reactor conversion to 19.75 wt% metallic plates fuel [12]	19.75 wt% U_3Si_2-Al metal fuel	IPEN, Brazil	Experiments ongoing	Evaluation plans not officially announced
The Deimos Experiment [13]	19.9 wt% TRISO particles in cylindrical graphite compacts	Los Alamos National Laboratory/NCERC, USA	Experiments ongoing	Evaluation plans not officially announced
MARVEL Reactor [14]	19.75 wt% TRIGA uranium zirconium hydride metal fuel	Idaho National Laboratory, USA	Under construction	Goal is to demonstrate microreactor technologies, not critical benchmark
ROSE Critical Facility [15]	21 wt% UO_2 rods	Joint Institute for Power and Nuclear Research, Belarus	Experiments performed and evaluated	Evaluation not in ICSBEP format

Review of available critical experiments for HALEU validation

- Experiments potentially relevant for HALEU validation from the handbooks
- Experiments quality and correlation
- Upcoming experiments
- **Conclusions and recommendations**

Conclusions and recommendations

1. High number of critical experiments are available in the HALEU fuel enrichment range
2. High number of critical experiments are available in the thermal, intermediate and fast neutron spectra
3. A low number of experiments with TRISO particle-based fuels or similar, with questionable uncertainty, and only one experiment in development (DEIMOS)
4. Only one Uranium salt critical experiment benchmark is available, with very high uncertainty and C/E ratio (MSRE), and the only one in development not planned to be a benchmark (MCRE [16])
5. No critical experiments with depleted HALEU fuel exist for the back-end validation
6. Experimental correlations could be reduced by performing experiments in new facilities
7. Quality of evaluations can be ensured (low uncertainty) by performing experiments in already trusted facilities with potential new equipment

Review of available critical experiments facilities for HALEU validation

- Where to perform new critical experiments?
  - Established critical experiment facilities
  - University research reactors
  - Other facilities

Lists are non-exhaustive, from analysis of the handbooks and recent NEA efforts [17] [18]

Review of available critical experiments facilities for HALEU validation

Most promising facilities:

Facility, Organization	Location, Status	Advantages	Disadvantages
NCERC, Los Alamos National Laboratory [19]	USA, Operational	TRISO experiment ongoing, broad staff experience designing critical experiments and ICSBEP/IRPhE evaluation	Hazard category 2 facility, no water allowed, time and money consuming, low availability
SPRF/CX, Sandia National Laboratories [20]	USA, Operational	Room to install new critical machines, broad staff experience designing critical experiments and ICSBEP/IRPhE evaluation, existing fuel rods enriched around 7%	Facility in air force base, no critical experiment machine for new HALEU fuel, low availability
ZED-2, Chalk River, Canadian Nuclear Laboratories [21]	Canada, Operational	HALEU fuel research ongoing, staff experience designing critical experiments and ICSBEP/IRPhE evaluation, announced facility availability for international collaborations	Procure HALEU fuel could be a challenge
New STACY, Japan Atomic Energy Agency [22]	Japan, Operational Mid 2024	Staff experience designing critical experiments and ICSBEP/IRPhE evaluation, announced facility availability for international collaborations	Not yet operational, so delays could occur
IPEN/MB01, Instituto de Pesquisas Energéticas e Nucleares [23]	Brazil, Operational	Broad staff experience designing critical experiments and ICSBEP/IRPhE evaluation, new core with metallic rods within HALEU enrichment range	No communicated plans for international collaboration

Review of available critical experiments facilities for HALEU validation

University-led facilities:

Facility, Organization	Location, Status	Advantages	Disadvantages
Reactor Critical Facility, Rensselaer Polytechnic Institute [24]	USA, Operational	Flexible reactor, critical experiments experience	No experiments are in a ICSBEP or IRPhE evaluation
Illinois Microreactor Demonstration Project, University of Illinois Urbana [25]	USA, Licensing stage, not built	Use of TRISO-like fuel	Not built yet, no flexibility once built, potentially not suitable for benchmarking
Molten Salt Nuclear Reactor Research, Abilene Christian University [26]	USA, Licensing stage, not built	Use of Uranium salt fuel	Not built yet, no flexibility once built, potentially not suitable for benchmarking
Missouri S&T Reactor, Missouri University of Science and Technology [27]	USA, Operational	Use of 19.75 wt% Uranium silicide fuel	No critical benchmarking experience
Kyoto University Critical Assembly, Kyoto University [28]	Japan, Core upgrade in progress	Modern upgrade	Not built yet, potential loss of flexibility and capabilities once built

Review of available critical experiments facilities for HALEU validation

- Other notable facilities:
  - VENUS [29], operated by SCL CEN at Mol, Belgium
  - LR-0 [30], operated by the Nuclear Research Institute Řež plc at Husinec, Czech Republic
  - RSV Tapiro [31], operated by the Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), located in Rome, Italy
  - CROCUS [32], operated by Polytechnique Federale (EPFL) in Lausanne, Switzerland
  - UTR [28], located at the Kindai University in Japan
  - DOME and LOTUS testbeds [33], located at Idaho National Laboratory (MCRE), USA
  - Nextgen MURR [34], operated by University of Missouri, USA
  - Other university research reactors such as TRIGA reactors

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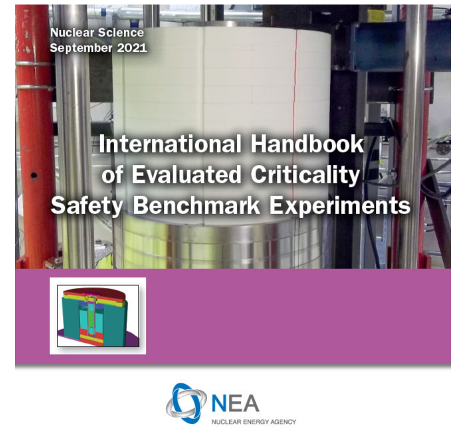
Questions ?

Review of available critical experiments for HALEU validation

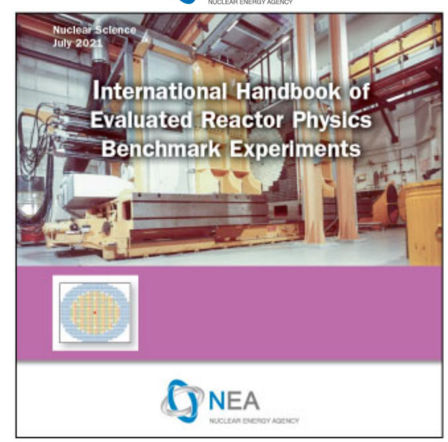
- Comments on ICSBEP and IRPhE handbooks available critical experiments:
  - High number of critical experiments in the HALEU fuel enrichment range, neutron spectrum
  - Only one evaluation and 5 cases with TRISO fuel at 20.91 wt% ^{235}U (IEU-COMP-THERM-008)
  - No Uranium salts experiments in ICSBEP handbook, only one in IRHPhE handbook
  - More critical experiments related to advanced reactors in IRPhE handbook, but potentially more uncertainty because criticality is not the main focus

Review of available critical experiments for HALEU validation

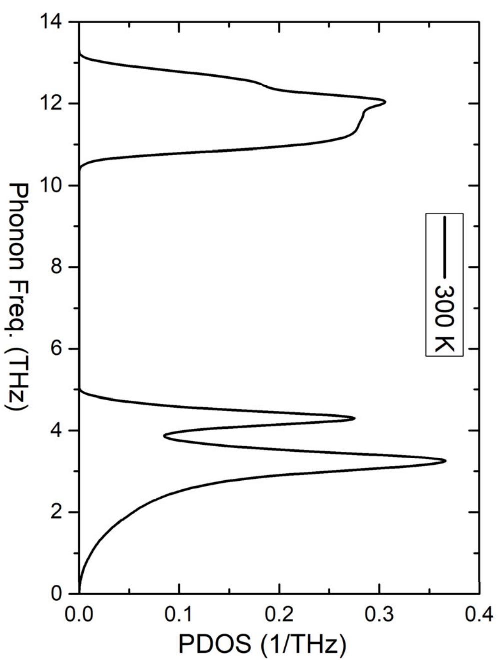
- ICSBEP Handbook 2021:
  - 26 contributing countries
  - Over 80,000 pages
  - More than 5000 approved benchmarks

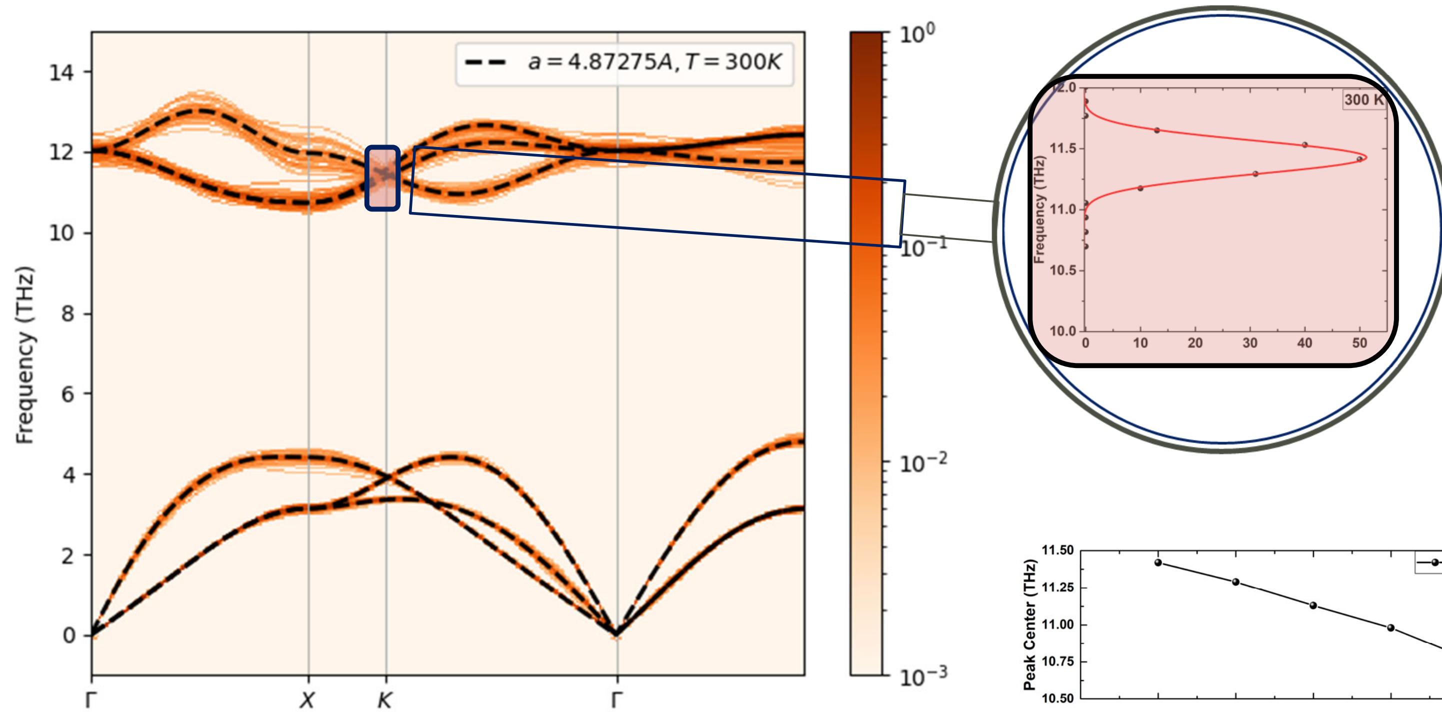


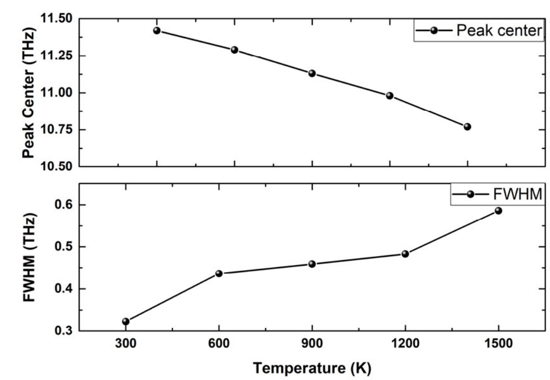
- IRPhE Handbook 2021:
  - 25 contributing countries
  - 57 reactor facilities
  - 165 approved benchmarks



Phonon Calculations at High Temperatures
T = 300 K







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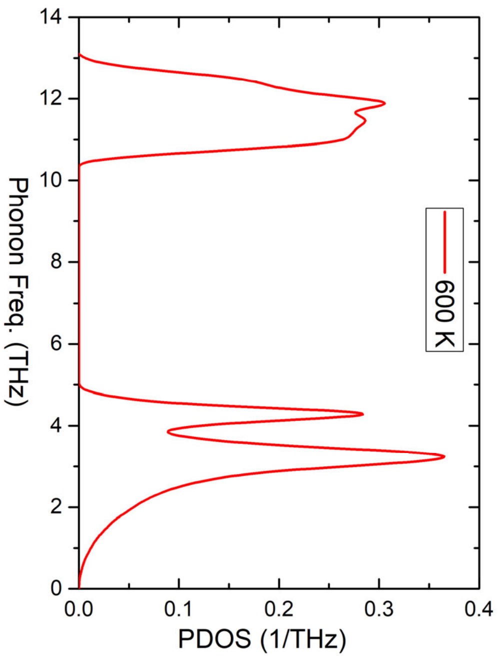
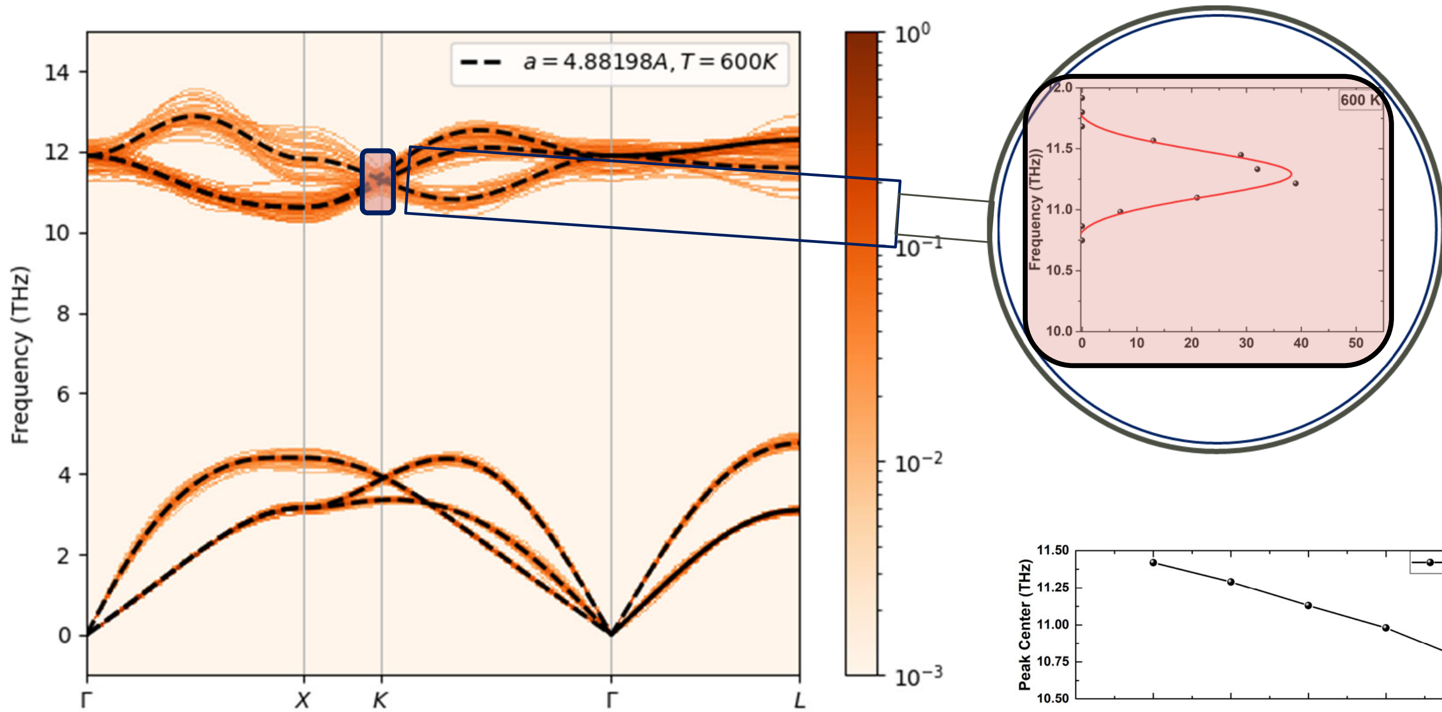
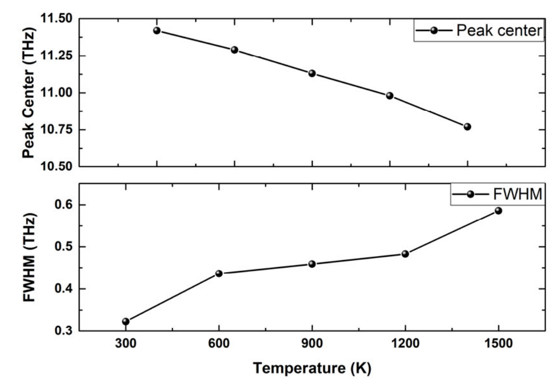
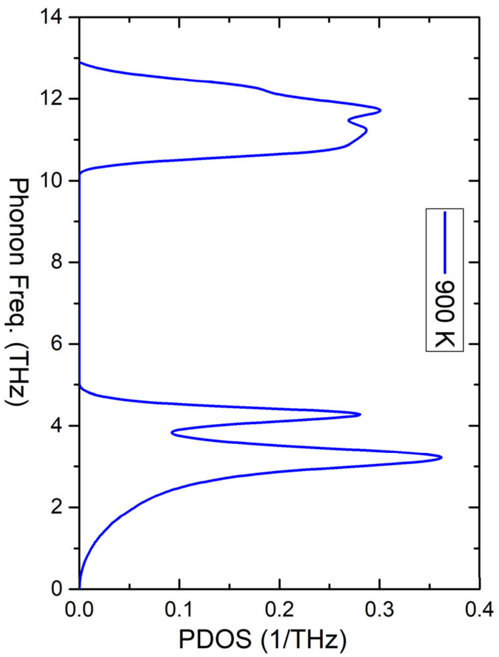
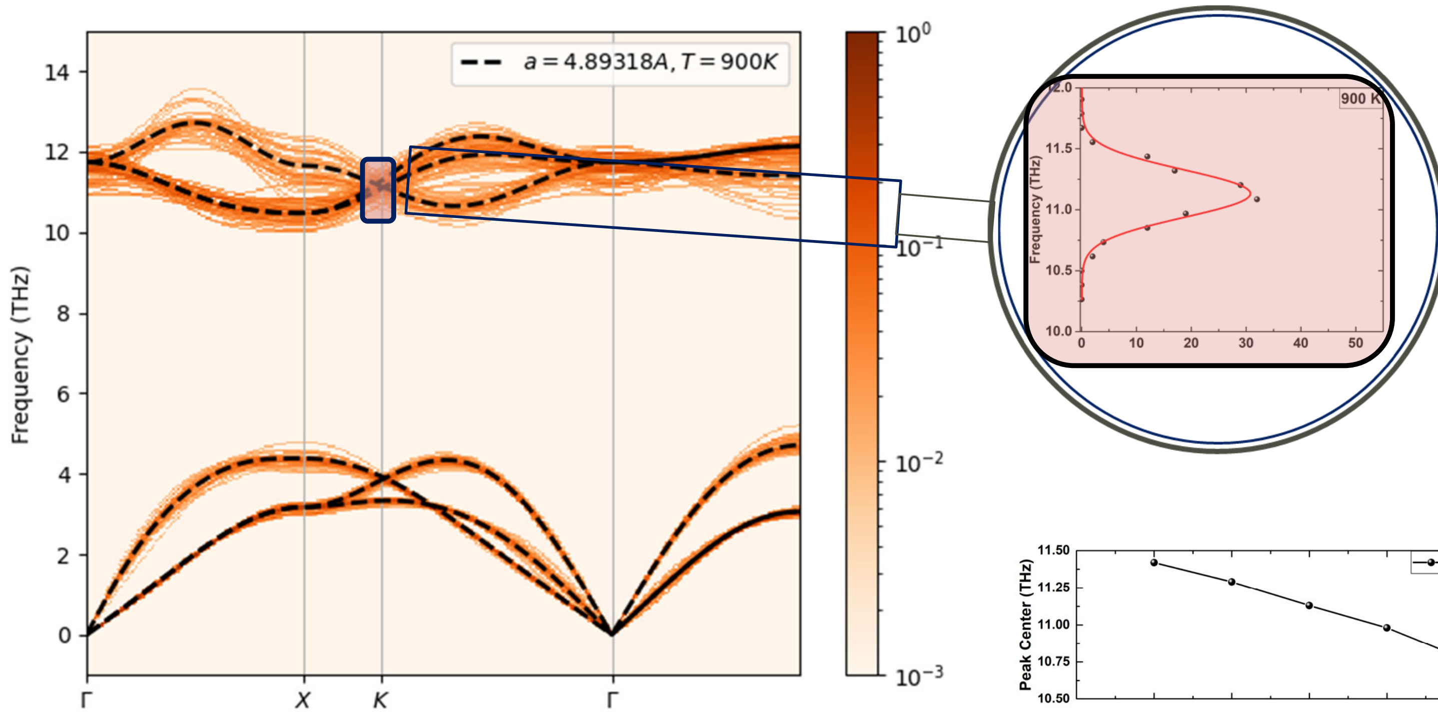


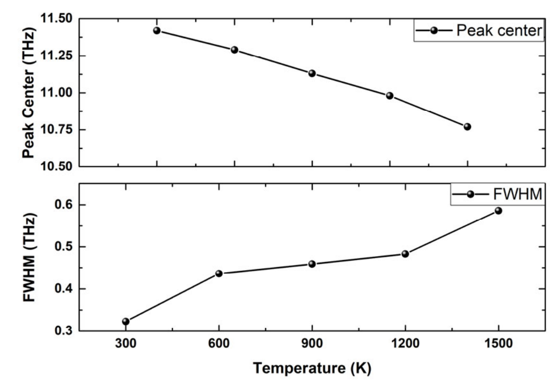




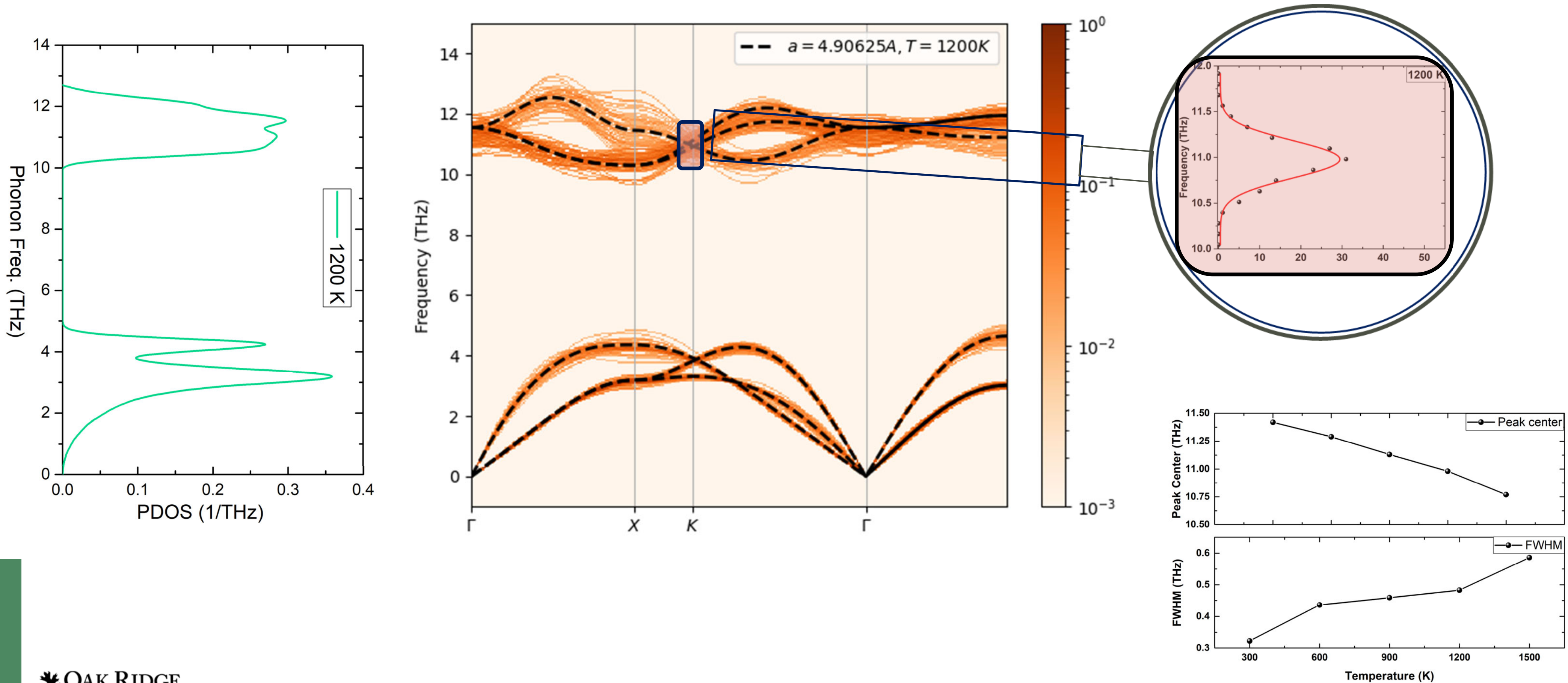
Phonon Calculations at High Temperatures T = 900 K



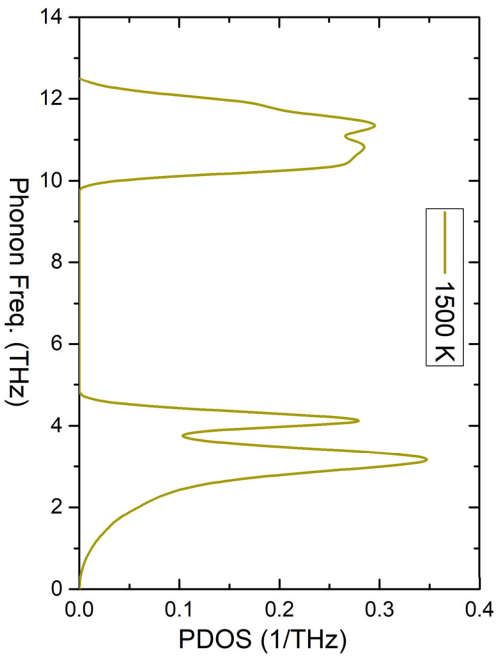


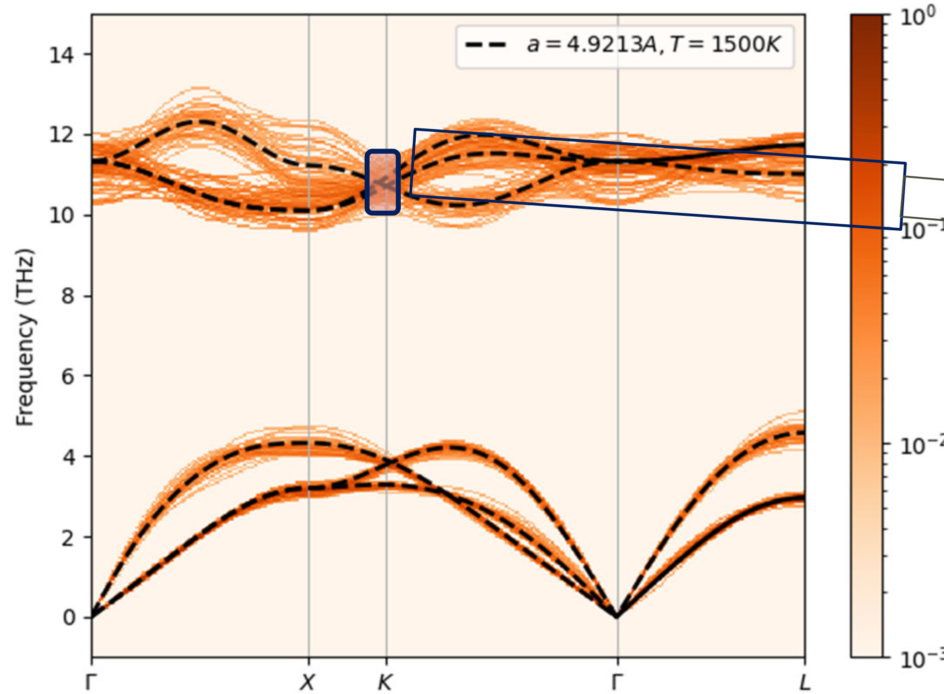


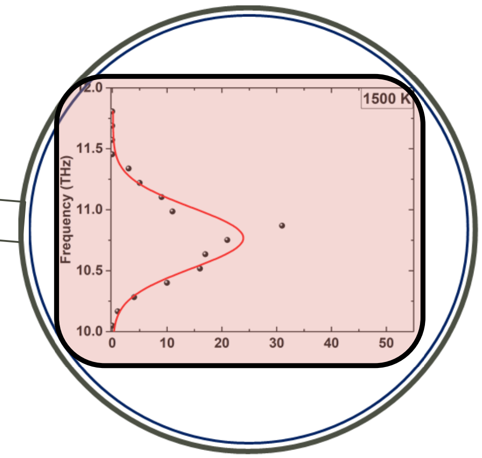
Phonon Calculations at High Temperatures
T = 1200 K

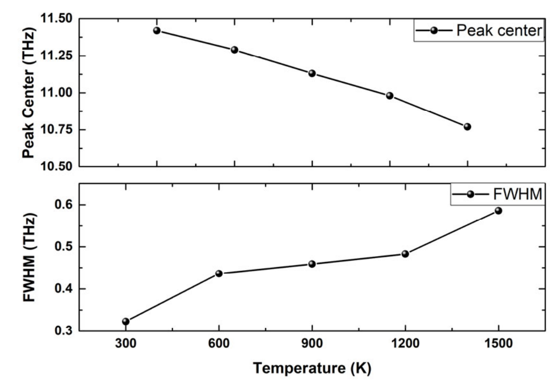


Phonon Calculations at High Temperatures
T = 1500 K



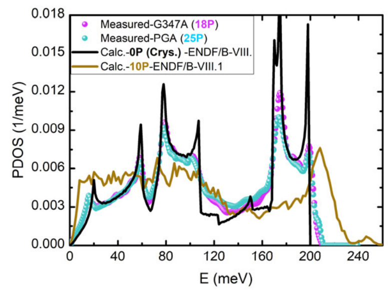


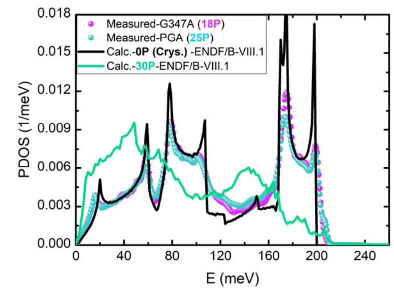


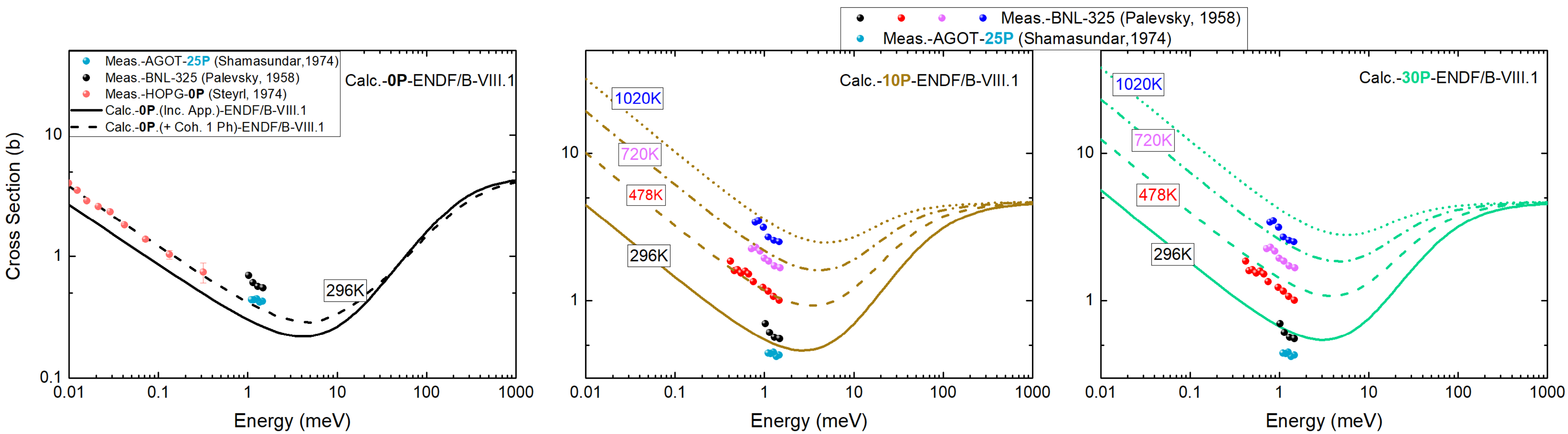


Oak Ridge National Laboratory

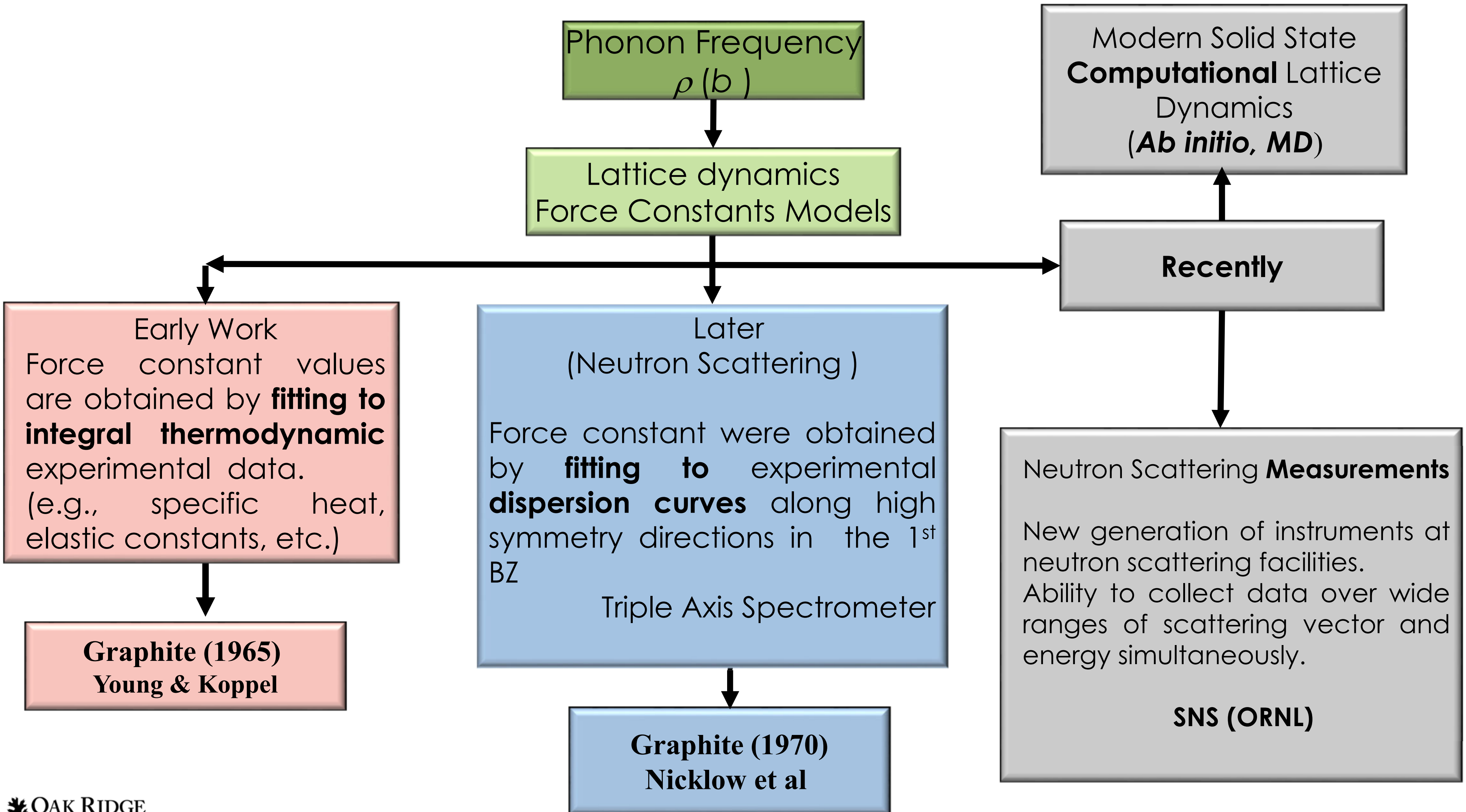
Inelastic Scattering XS







- ✓ As the temperature increases, both the 10P & 20P ENDF/B-VIII.1cross sections overestimate the measured cross sections of Palevsky.
- ✓ The higher the temperature, the higher overestimation. This is due to the phono excess in the low energy part of the PDOSs


Phonon Frequency
ρ (b)
Lattice dynamics
Force Constants Models
Early Work
Force constant values are obtained by **fitting to integral thermodynamic** experimental data. (e.g., specific heat, elastic constants, etc.)
Graphite (1965)
Young & Koppel
Later
(Neutron Scattering)
Force constant were obtained by **fitting to dispersion curves** along high symmetry directions in the 1st BZ
Triple Axis Spectrometer
Graphite (1970)
Nicklow et al
Recently
Modern Solid State **Computational** Lattice Dynamics
(***Ab initio, MD***)
Neutron Scattering **Measurements**
New generation of instruments at neutron scattering facilities.
Ability to collect data over wide ranges of scattering vector and energy simultaneously.
SNS (ORNL)

TSL Sub-Libraries Evolution

ENDF/B-III (1960s)

- ✓ General Atomics (GA)
- ✓ GASKET Code
- ✓ Various approximations
- ✓ Limited number of TSL sub-libraires

ENDF/B-VI (1990s)

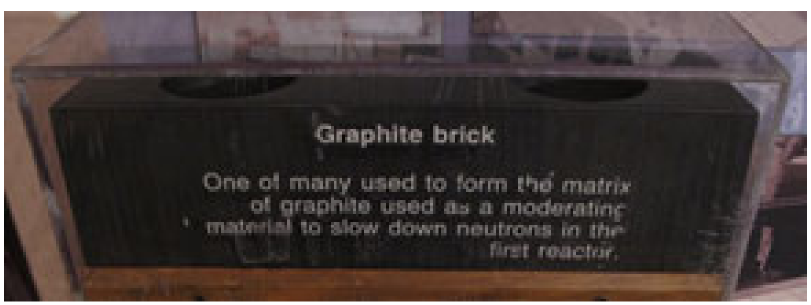
- ✓ LANL
- ✓ LEAPR/THERMR- NJOY Code
- ✓ Coh. and Incoh. elastic scattering
- ✓ Multi-Phonon expansion
- ✓ Extended energy and momentum transfer grides
- ✓ TSL sub-libraires for new materials

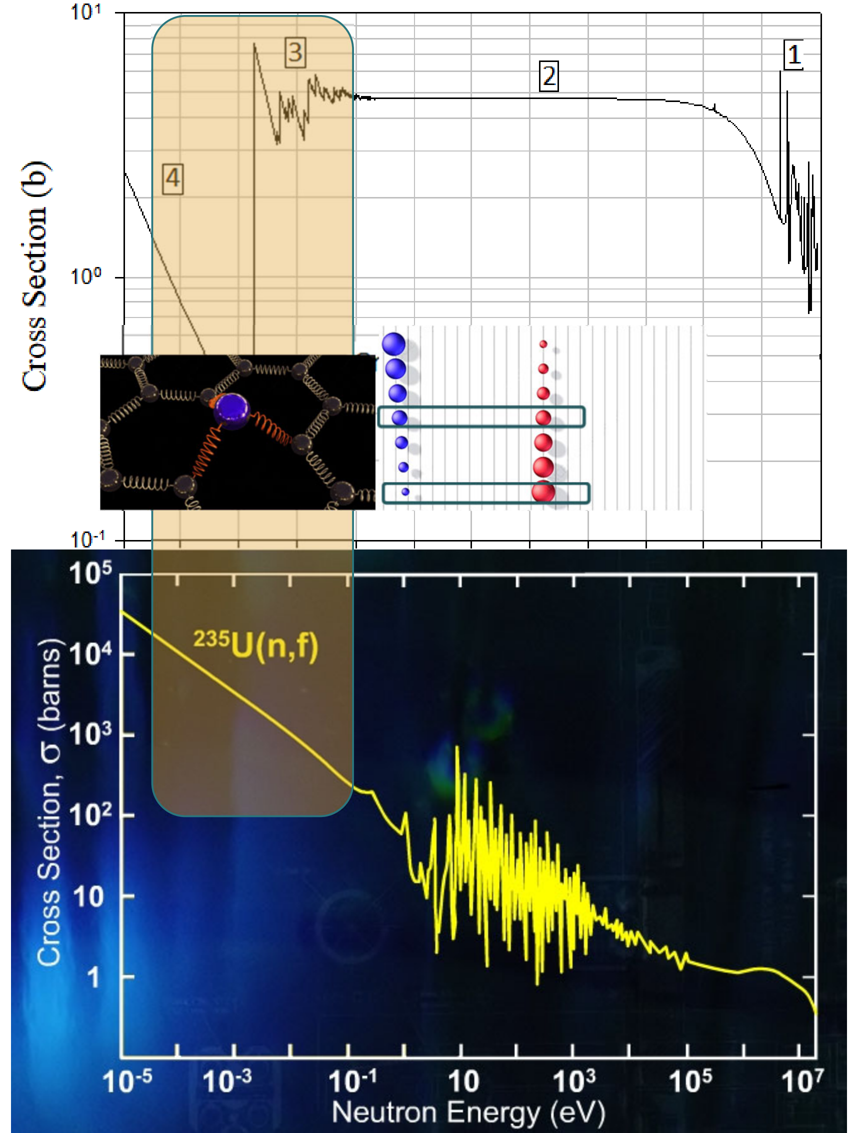
ENDF/B-VIII (2010s)

- ✓ National labs, Universities
- ✓ NJOY/FLASH/ NJOY-NCRYSTAL
- ✓ Modern Solid State computational techniques (e.g., DFT, MD)
- ✓ Coherent 1-phonon inelastic scattering
- ✓ About 100 TSL sub-libraries generated so far

Neutron Moderation

- *Slowing Down: Region 2*
- $Thermalization \begin{cases} Region\ 3 & \quad Elastic\ Scattering \\ Region\ 4 & \quad Inelastic\ Scattering \end{cases}$
- High Purity (low boron content)
- High Thermal Conductivity
- High Strength
- Good stability under irradiation
- High oxidation Resistivity
- Low anisotropy
- Low Cost

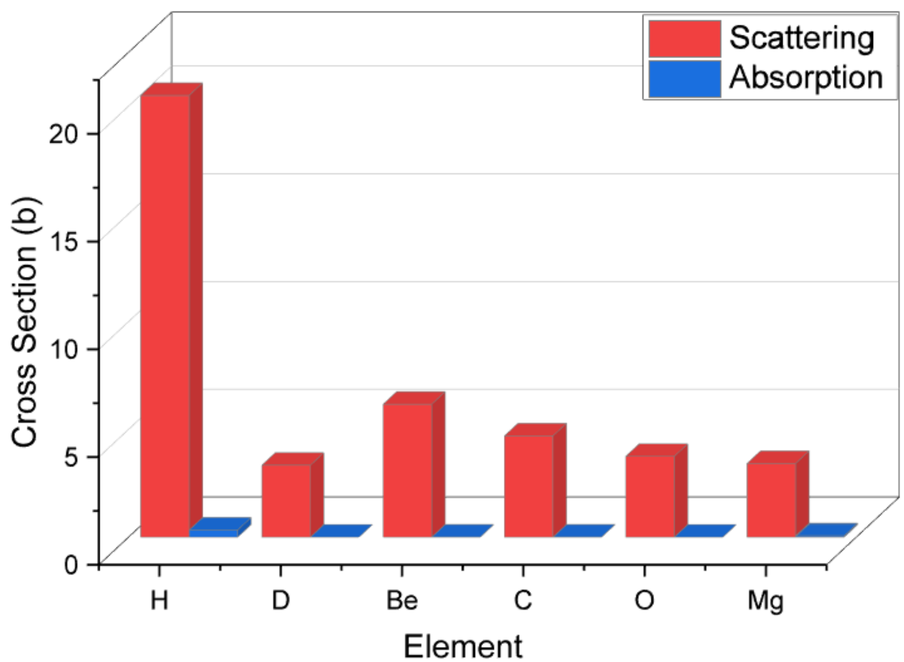


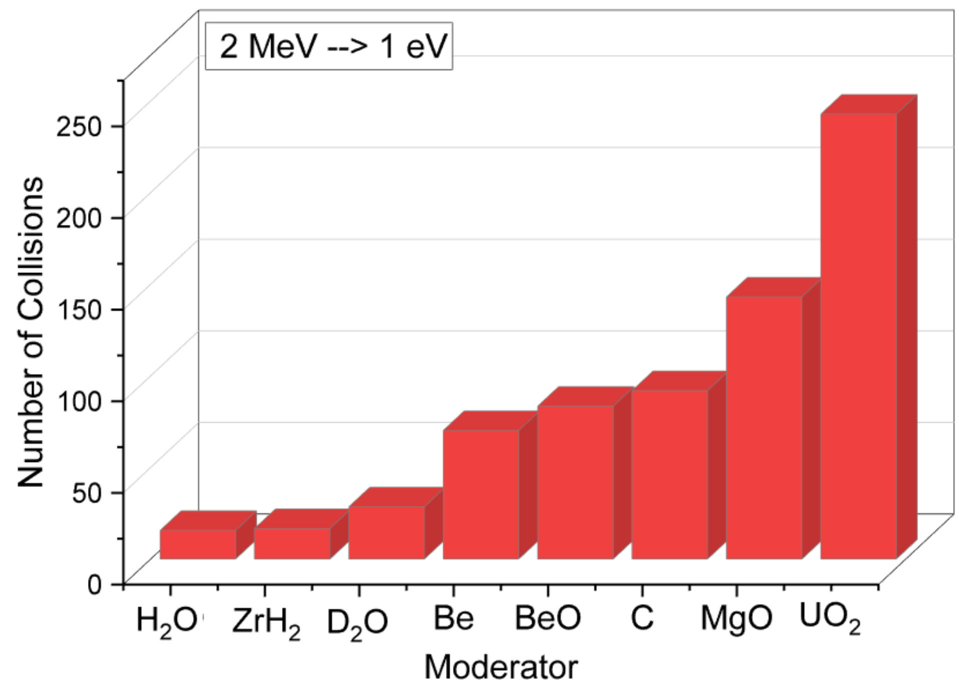


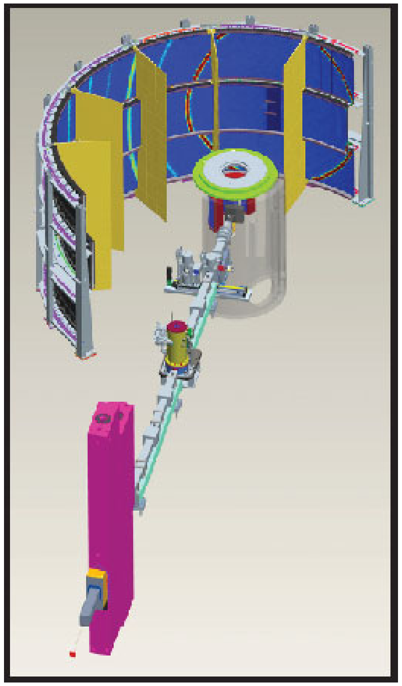
OAK RIDGE National Laboratory

Neutron Moderation

- High scattering cross section
- Low Atomic Mass Number

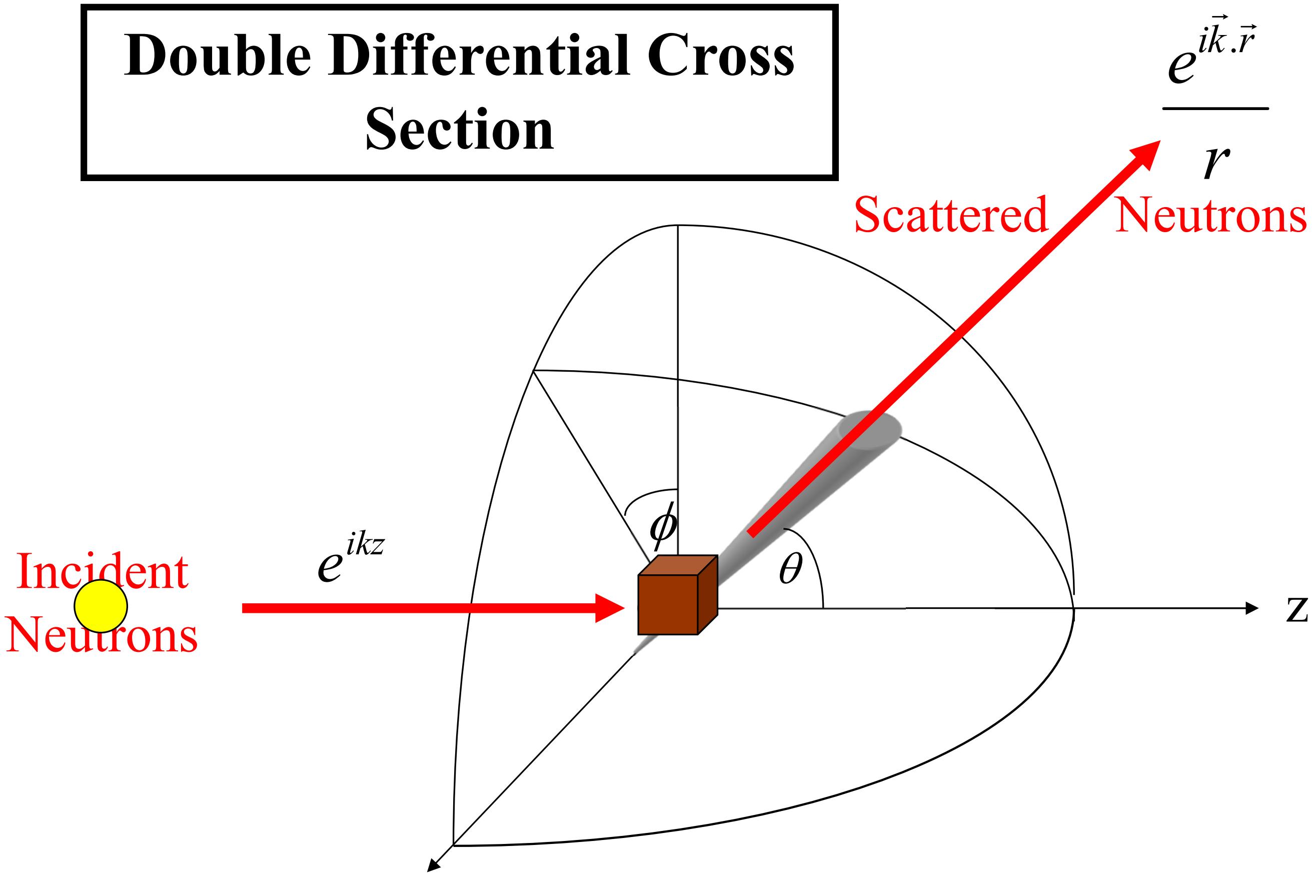






ARCS/ORNL

Double Differential Cross Section



$$\frac{d^2\sigma}{d\Omega dE'} = \text{(\textbf{Number of neutrons scattered into} } d\Omega \text{ \textbf{per second with final energy between} } E' \text{ \textbf{and} } E' + dE' \text{) / } \Phi \, d\Omega \, dE'$$

TSL Sensitivity and Uncertainty

- Established formats and procedures exist for representing covariances in various types of ENDF reaction data.
- Transport codes, like SCALE, calculate sensitivity to 1D scattering, but they do not directly address TSL. Covariance data are accessible for all neutron files, but not for the 2D TSL.
- Presently, no published ENDF evaluations include covariance data for TSL or its corresponding scattering cross sections.
- Additionally, there is a lack of a standardized approach for generating or preserving covariance data related to TSLs.
- Ongoing initiatives such as the Global Nuclear Data System (GNDS) and the Working Party on International Nuclear Data Evaluation Cooperation (WPEC), subgroup 42/44/48, actively explore thermal scattering covariances.
- Recent efforts have focused on evaluating covariances in thermal neutron scattering for moderators like H_2O, D_2O, and graphite[1,2,3].

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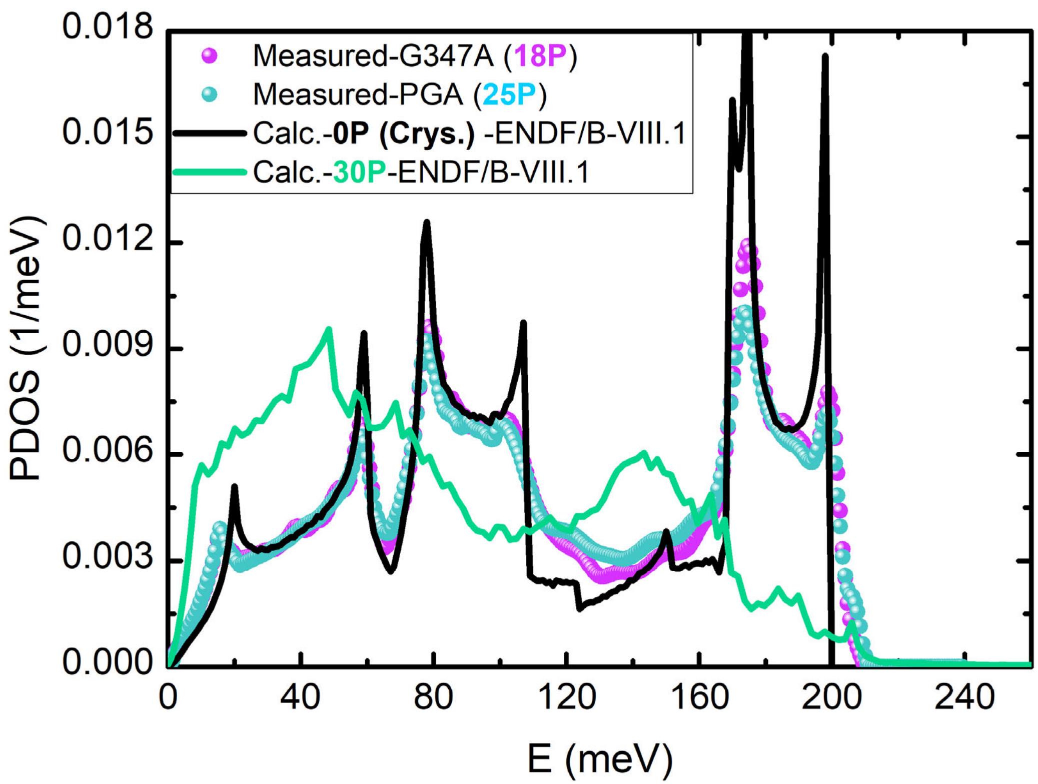
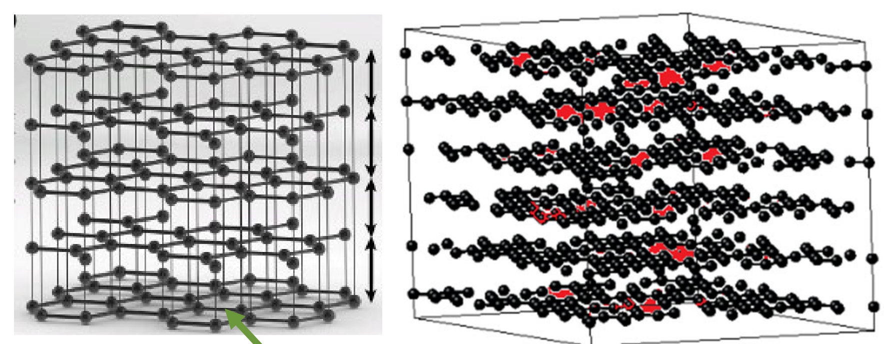
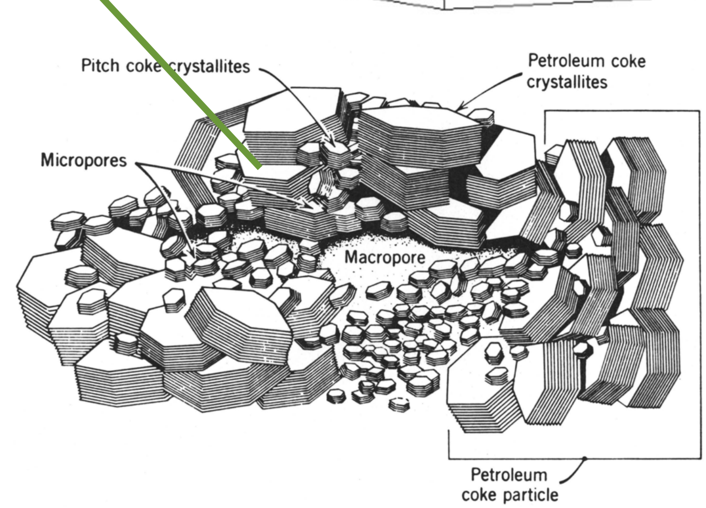
MD Porosity modeling??



Perfect Graphite SC

Defected graphite SC
Randomly removed atoms

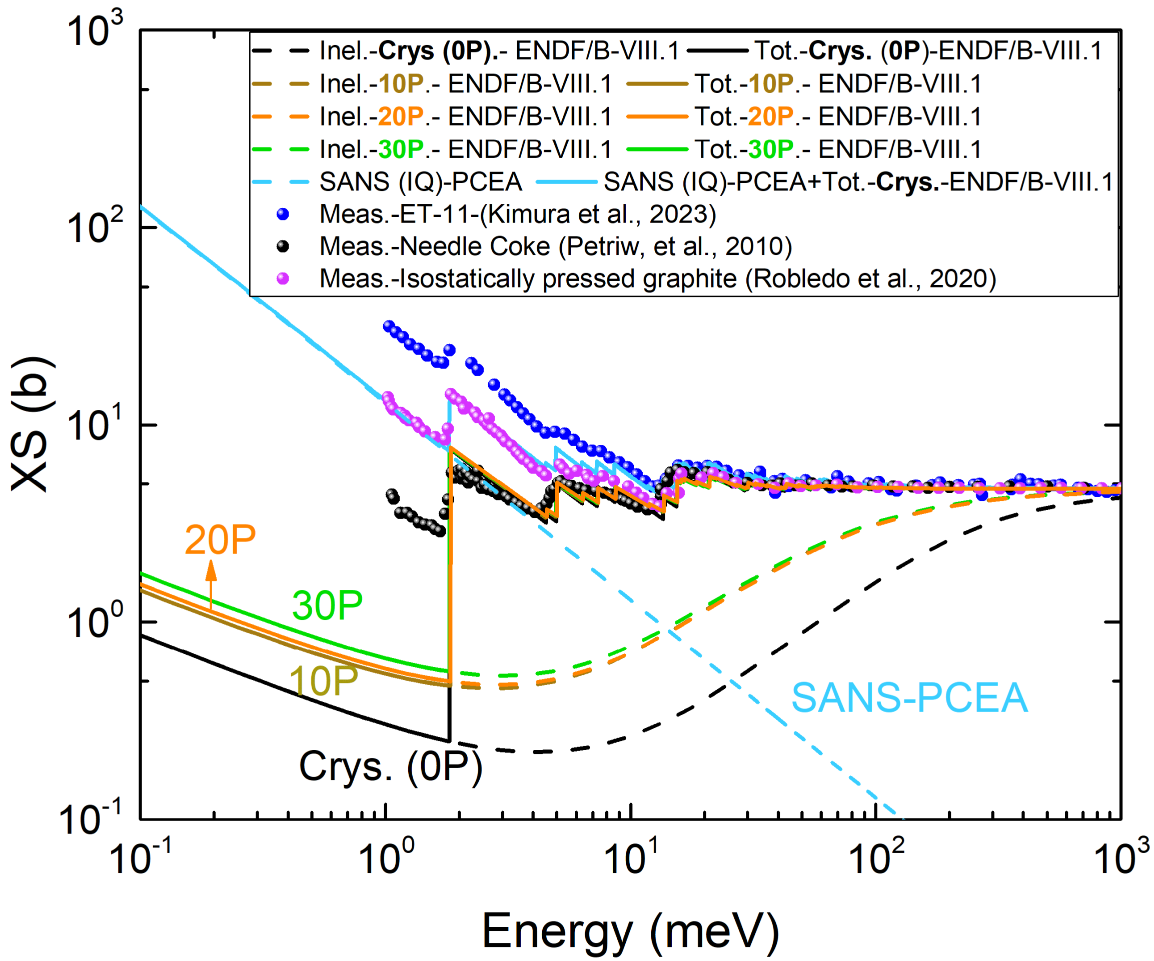




Al-Qasir et al., Neutron thermalization in nuclear graphite: A modern story of a classic moderator, Annals of Nuclear Energy **161**, 108437 (2021)

Small Angle Neutron Scattering (SANS)

- Different nuclear graphite types show different cross section due to SANS
- SANS is much higher than inelastic scattering cross section



Gaps/ Nuclear Graphite

- The following **measurements** are need for different types of nuclear grade graphite

  1- Temperature-dependent inelastic neutron scattering cross section

  2- Small angle neutron scattering

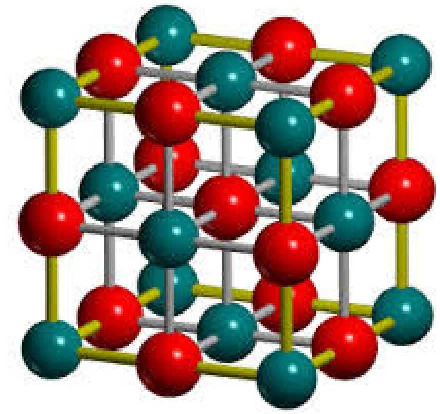
  3- Temperature-dependent benchmarking

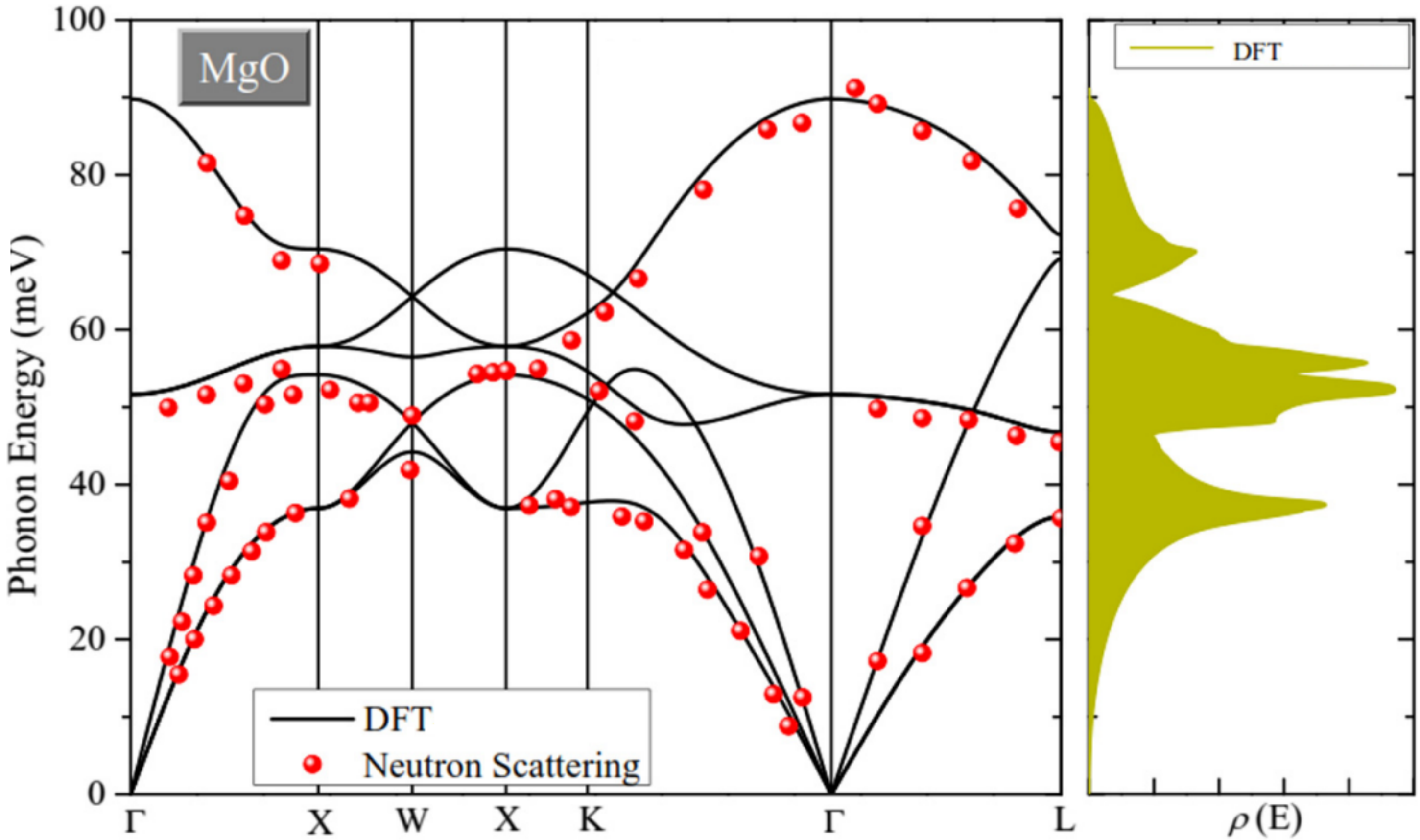
- The behavior of atomic vibrations at high temperatures (anharmonicity effects)need to be calculated.

Current Status of MgO TSL Sub-library

MgO Phonon Calculations

MgO Unit Cell
Rock Salt Structure

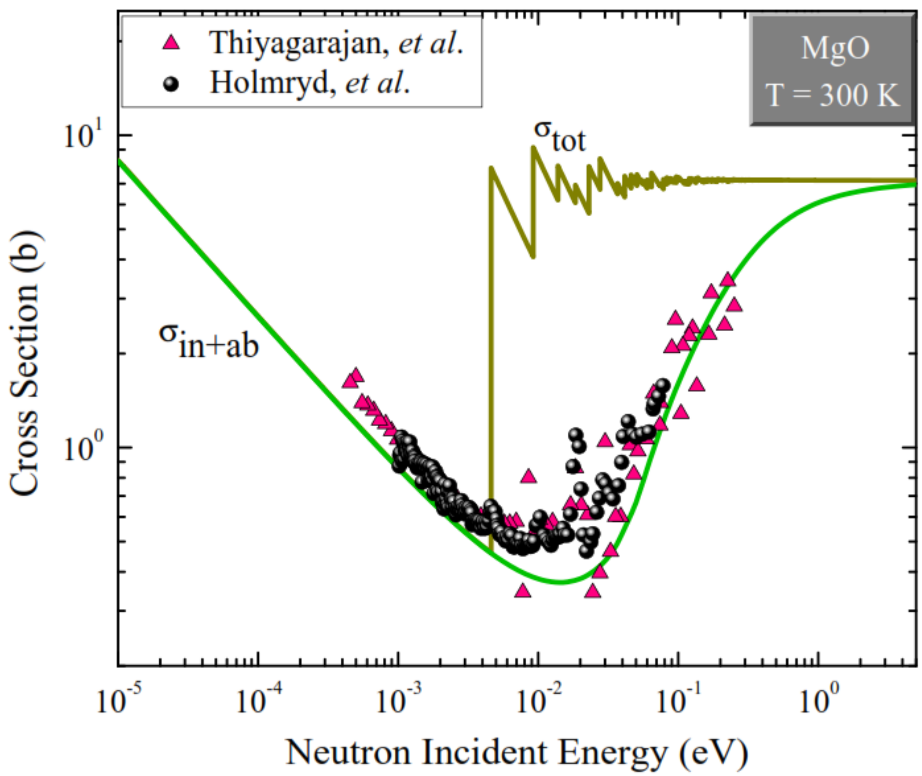


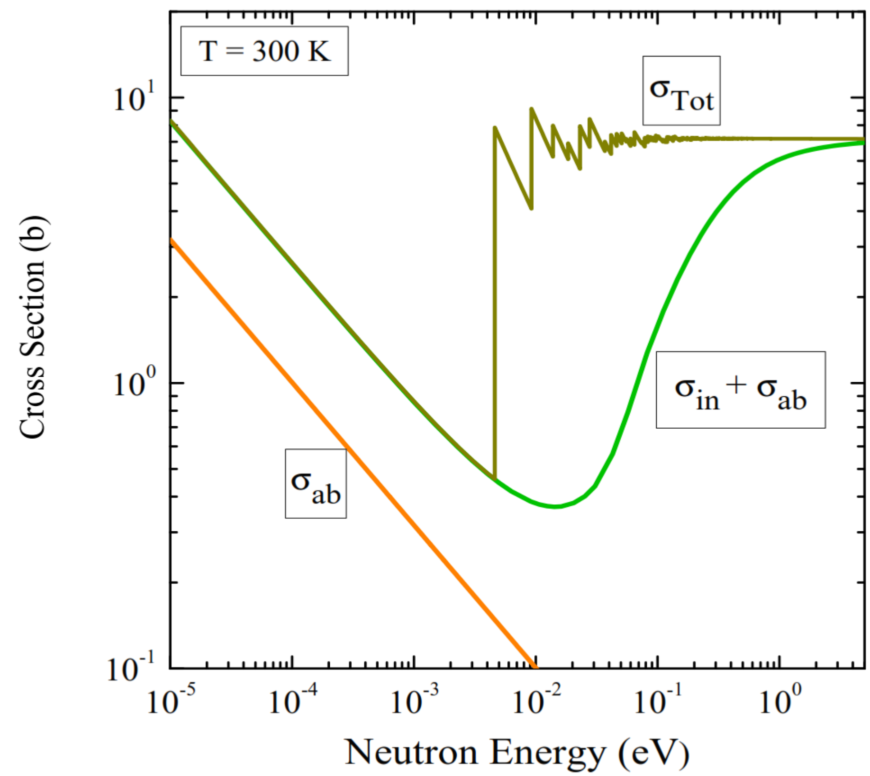


- ✓ ABINIT code
- ✓ LDA-PW
- ✓ Norm Conserving PP
- ✓ Ecut = 40 Ha
- ✓ 8 x8x8 k-mesh
- ✓ 4x4x4 –q mesh

Al-Qasir *et al.,* Thermal neutron scattering cross sections of beryllium and magnesium oxides, Annals of Nuclear Energy **87**, 242 (2016)

MgO Inelastic and Elastic Scattering Cross Section**





** The MgO TSL sub-library has been submitted to the Cross Section Evaluation Working Group (CSEWG) for approval and inclusion in the ENDF database; approval is pending.

Al-Qasir *et al.,* Thermal neutron scattering cross sections of beryllium and magnesium oxides, Annals of Nuclear Energy **87**, 242 (2016)

Gaps/MgO

- Temperature-dependent inelastic neutron scattering cross measurements of high pure MgO are required

- The behavior of atomic vibrations at high temperatures (anharmonicity effects)need to be calculated.

Nuclear Materials in Reactor Core (High Temperature)

Extreme Conditions

High Temperature Anharmonicity

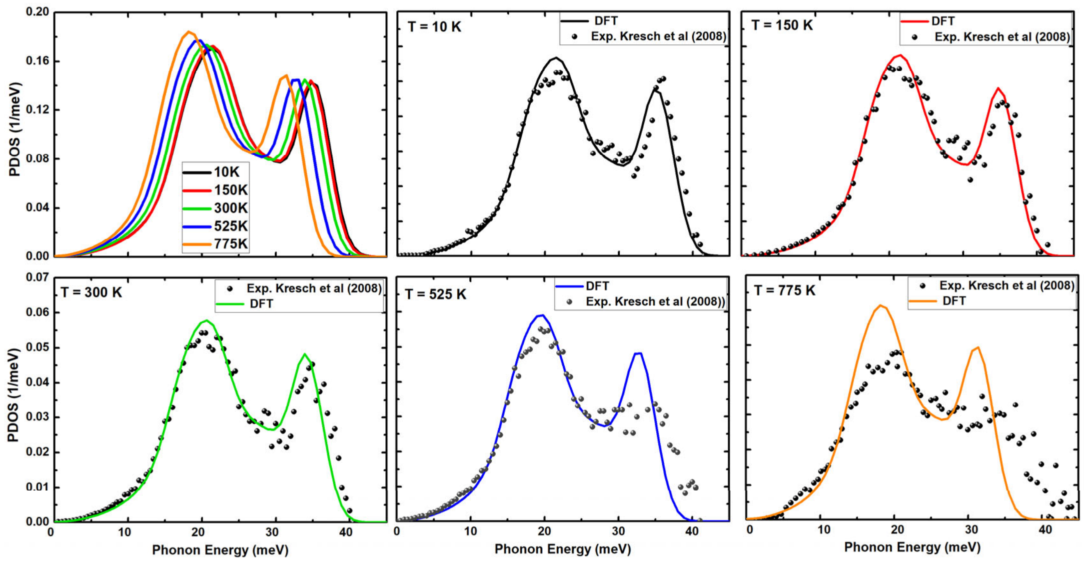
Dimensional Changes Large Atomic Displacement

Shift and Broadening

Vibrational changes

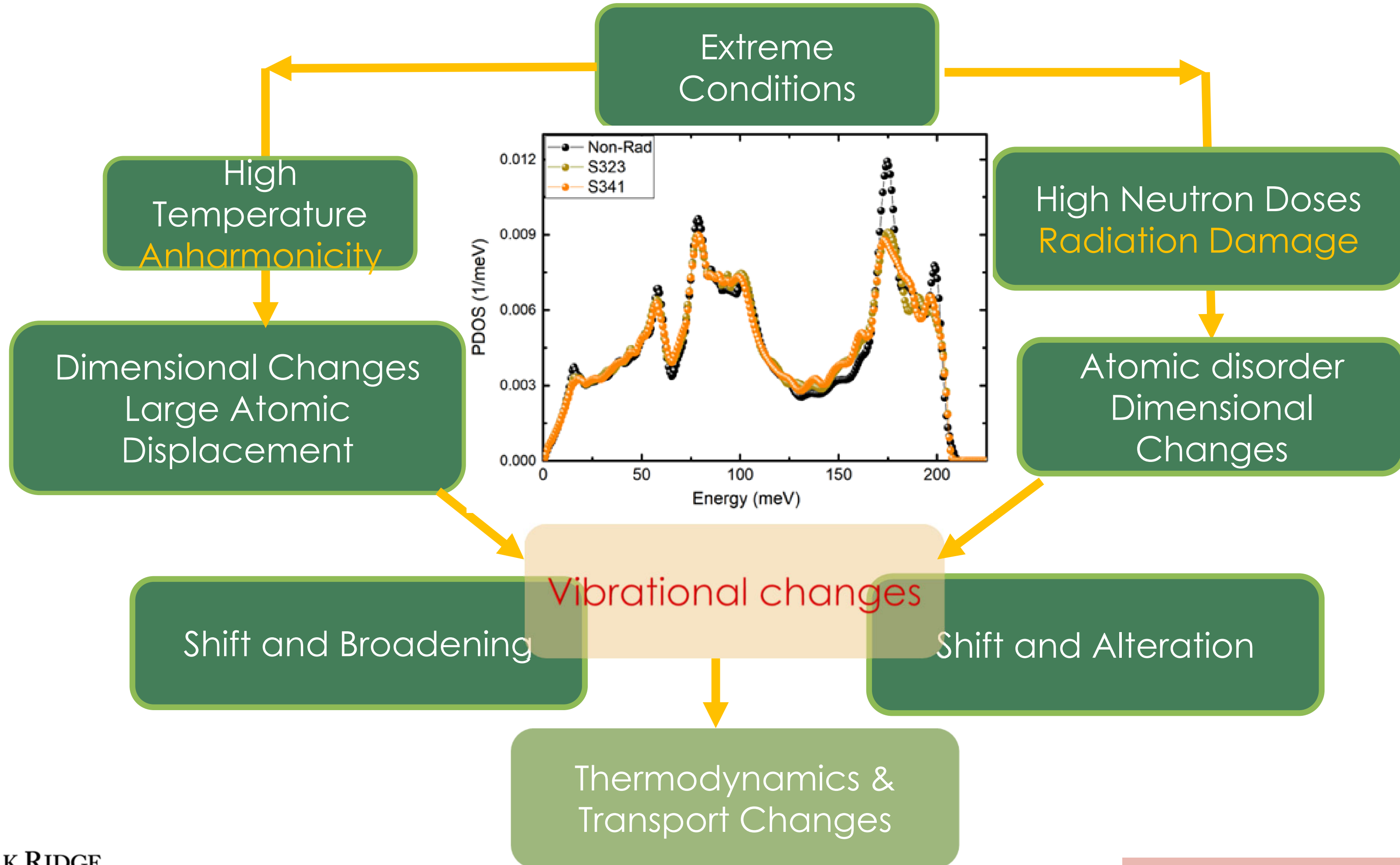
Thermodynamics & Transport Changes

Al Phonon Density of States



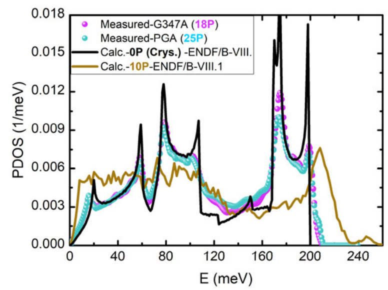
Exp. Meas.
Kresch et al, Phys. Rev. B **77**, 024301 (2008)

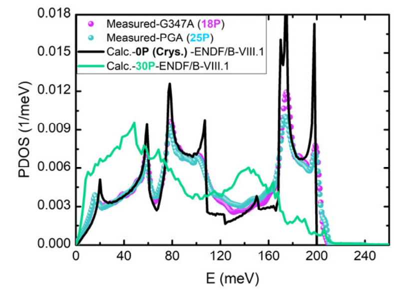
Nuclear Graphite in Reactor Core (High Doses of Radiation)

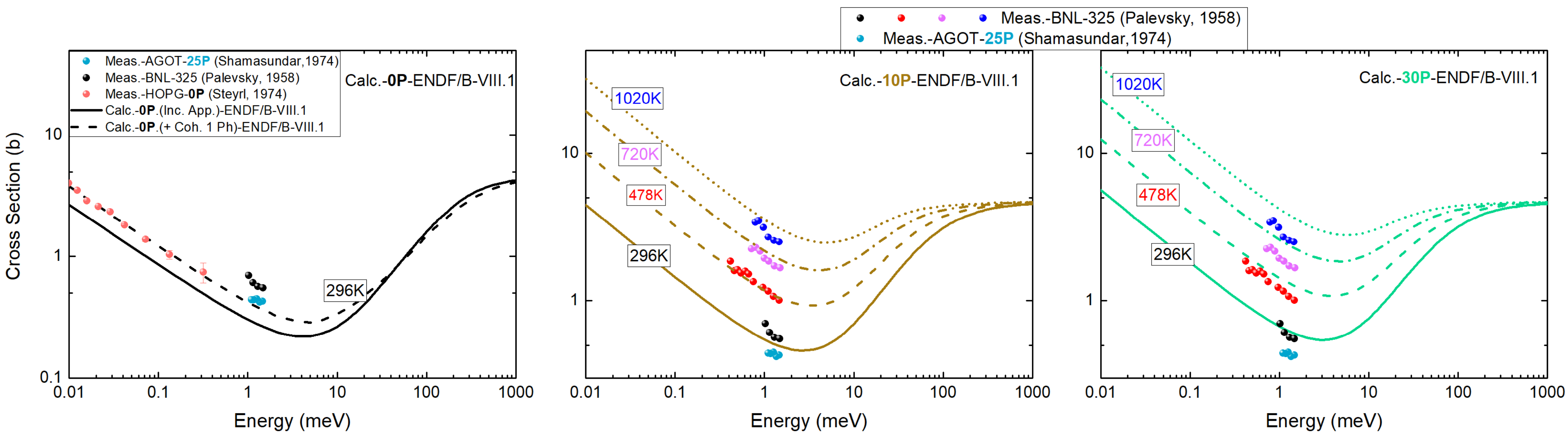


Al-Qasir et al, Carbon **168**, 42-54 (2020)

Inelastic Scattering XS



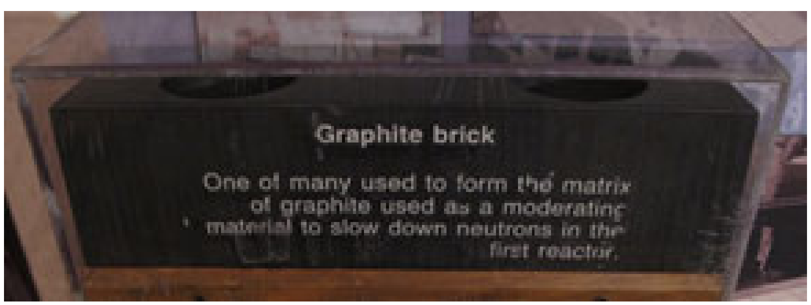


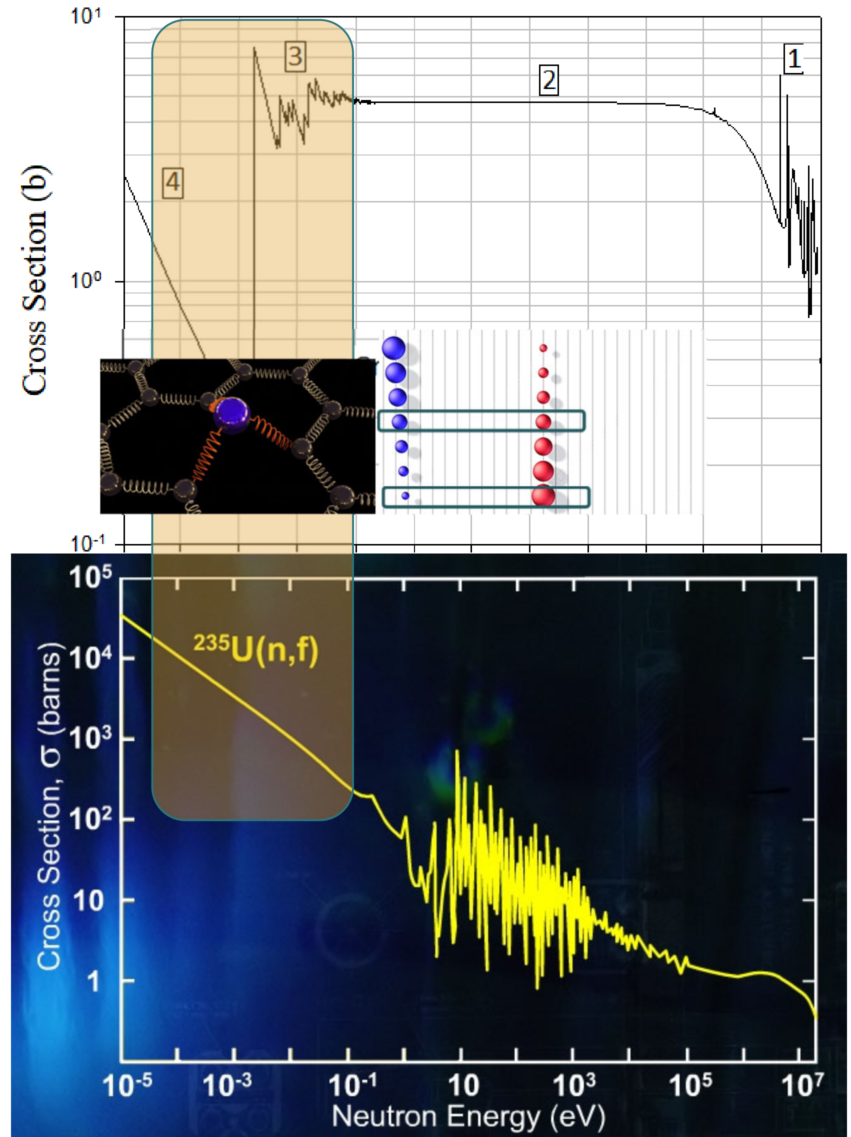


- ✓ As the temperature increases, both the 10P & 20P ENDF/B-VIII.1cross sections overestimate the measured cross sections of Palevsky.
- ✓ The higher the temperature, the higher overestimation. This is due to the phono excess in the low energy part of the PDOSs

Neutron Moderation

- *Slowing Down: Region 2*
- $Thermalization \begin{cases} Region\ 3 & Elastic\ Scattering \\ Region\ 4 & Inelastic\ Scattering \end{cases}$
- High Purity (low boron content)
- High Thermal Conductivity
- High Strength
- Good stability under irradiation
- High oxidation Resistivity
- Low anisotropy
- Low Cost





Nuclear Criticality Safety Validation & Similarity Assessment

B.J. Marshall

DNCSH Workshop
Germantown, MD
February 29, 2024

Outline

- Verification and validation
- Validation overview
- Brief introduction to sensitivity coefficients
- Sensitivity/uncertainty basis for similarity assessment
- Uncertainty propagation and correlation coefficients
- Similarity assessment via integral index c_k
- Summary

Verification and validation

- "All models are wrong, some models are useful."
  - George E.P. Box, FRS
- There are two separate yet equally important processes to confirm the usefulness of a model:
  - Verification: Was the intended model implemented?
  - Validation: Does that model accurately predict real world measurements of the phenomena being modeled?
- This talk focuses on validation because in the United States each organization is responsible for its own validation

Validation overview

- Validation is necessary to understand how calculated model results apply to the real world
- Criticality safety validation is required to be performed by comparison to measured critical benchmark experiments
- Experiments must be neutronically similar to the safety application or applications being evaluated
- A large number of independent experiments should be used to determine the *bias* and *bias uncertainty* for the computational method being used

Introduction to sensitivity coefficients

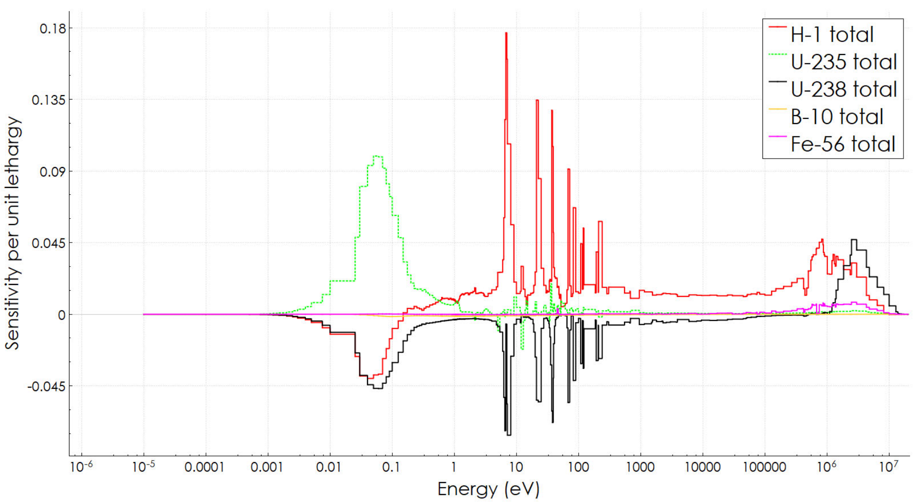
- Sensitivity coefficients represent the expected change in k_{eff} due to a change in nuclear data
- The sensitivity coefficients are dimensionless ratios
- What would happen to the system k_{eff} if some piece of data were changed by some amount?

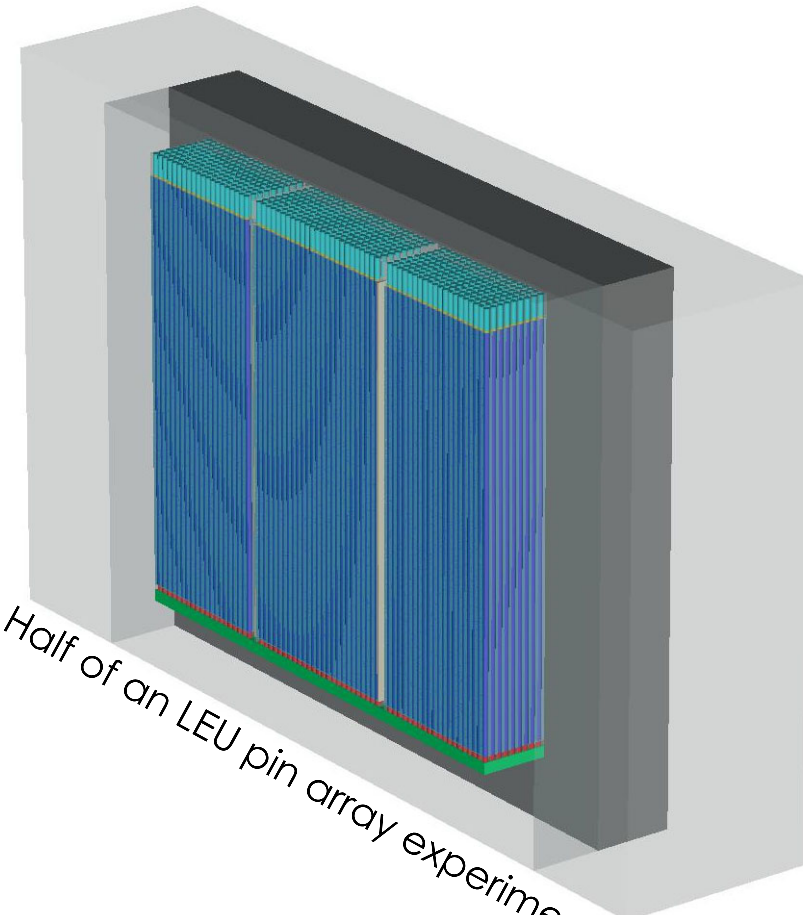
$$S_{k,\Sigma} = \frac{\frac{\partial k}{k}}{\frac{\partial \Sigma}{\Sigma}} \Longleftrightarrow \Delta k_{eff} = \left(S_{k,\Sigma}\right)\left(\frac{\delta\Sigma}{\Sigma}\right)$$

OAK RIDGE National Laboratory

k_{eff} sensitivities for a critical experiment

Nuclide	Material	Sensitivity
H-1	Moderator	0.240
U-235	Fuel	0.242
U-238	Fuel	-0.140
B-10	Absorber	-0.010
Fe-56	Reflector	0.020





Half of an LEU pin array experiment

S/U basis for similarity assessment

- Principle: bias is caused by errors in nuclear data, which are bounded by their uncertainties
- Systems will have similar computational biases if they have similar sensitivities to the same nuclear data errors
- System sensitivity combined with nuclear data uncertainties estimate potential for bias in each system
- Comparison examines nuclide-, reaction-, and energy-dependent data

Propagation of nuclear data uncertainties

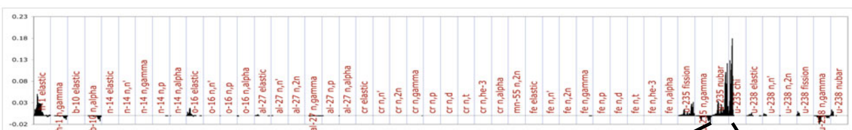
- Nuclear data uncertainty (i.e., covariances) can be propagated to quantify the data-induced uncertainty in k_{eff}

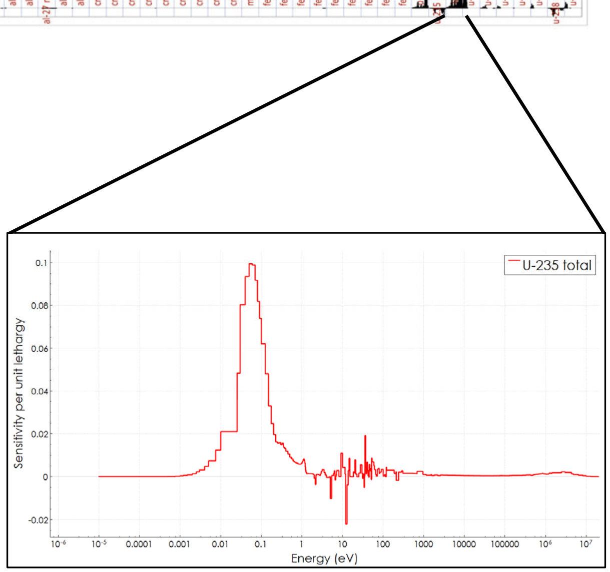
$$\sigma_k^2 = SC_{aa}S^T$$

- Where:
  - S is a matrix of all energy-dependent sensitivity data for all systems considered (S^T is transpose)
  - C_{aa} is a matrix containing energy-dependent covariance information evaluated for all nuclear data

Uncertainty propagation: single system uncertainty

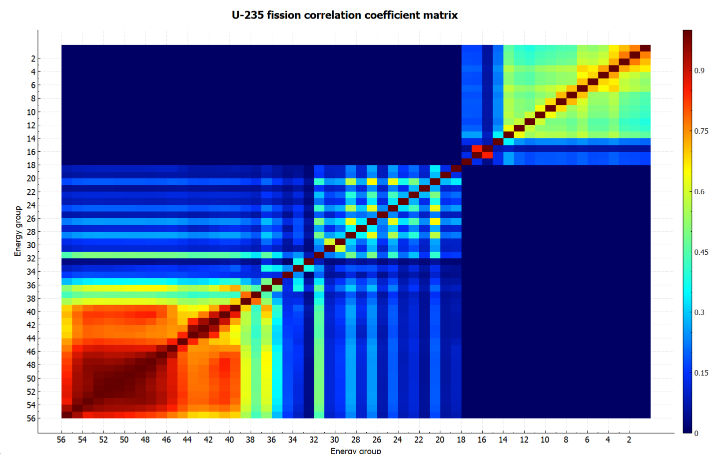
- Uncertainty in k_{eff} of a single system





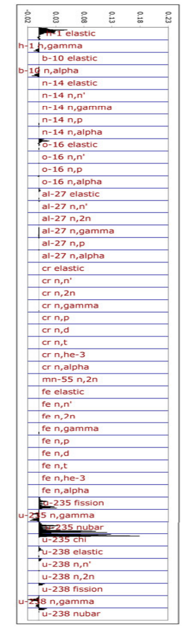
S

$$\left(\frac{\frac{\partial k}{k}}{\frac{\partial \Sigma}{\Sigma}}\right)$$



$C_{\alpha\alpha}$

$$\left(\frac{d\Sigma}{\Sigma}\right)^2$$



S^T

$$\left(\frac{\frac{\partial k}{k}}{\frac{\partial \Sigma}{\Sigma}}\right)$$

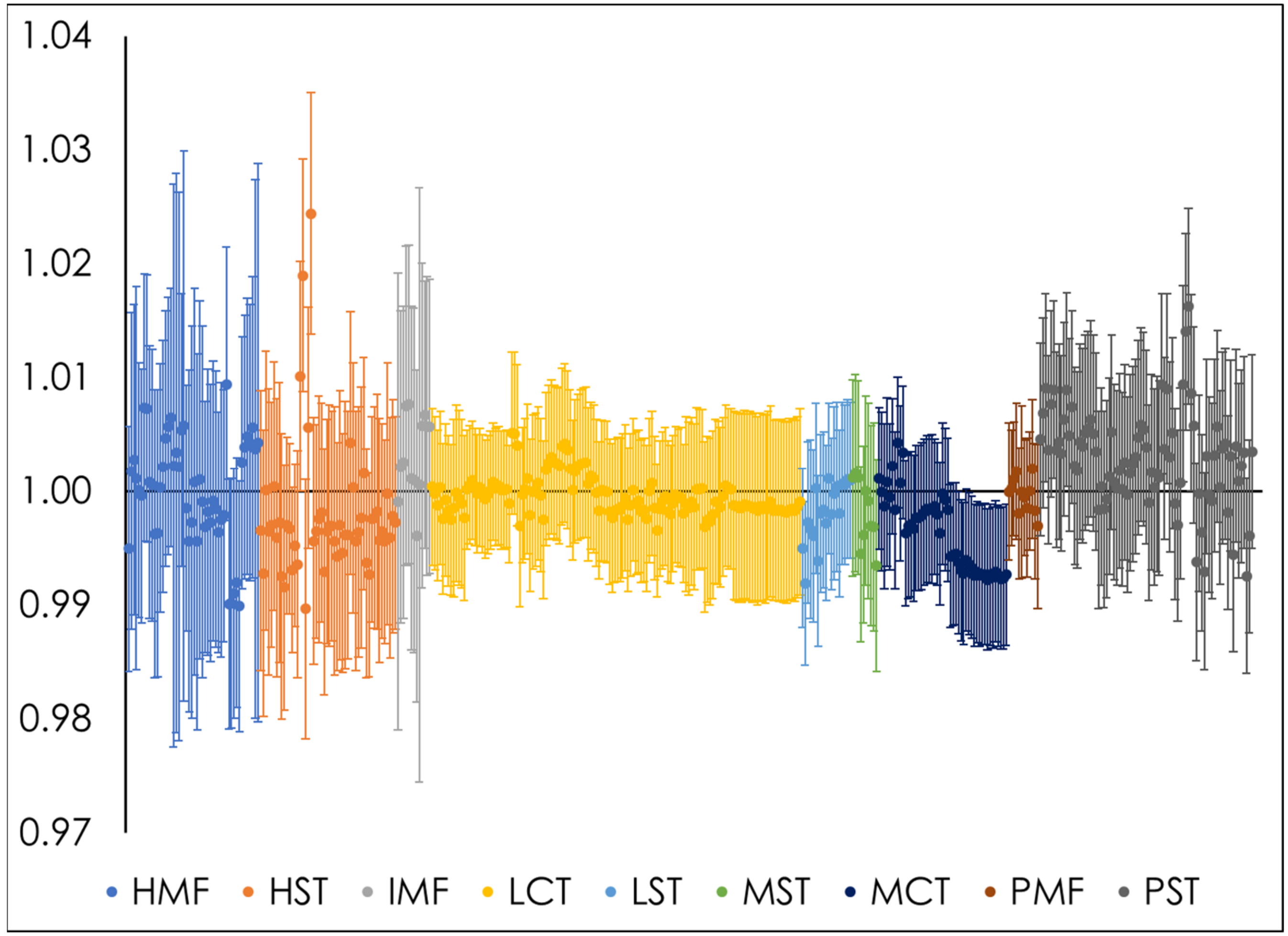
$$= \sigma^2$$

C_{kk}

$$\left(\frac{dk}{k}\right)^2$$

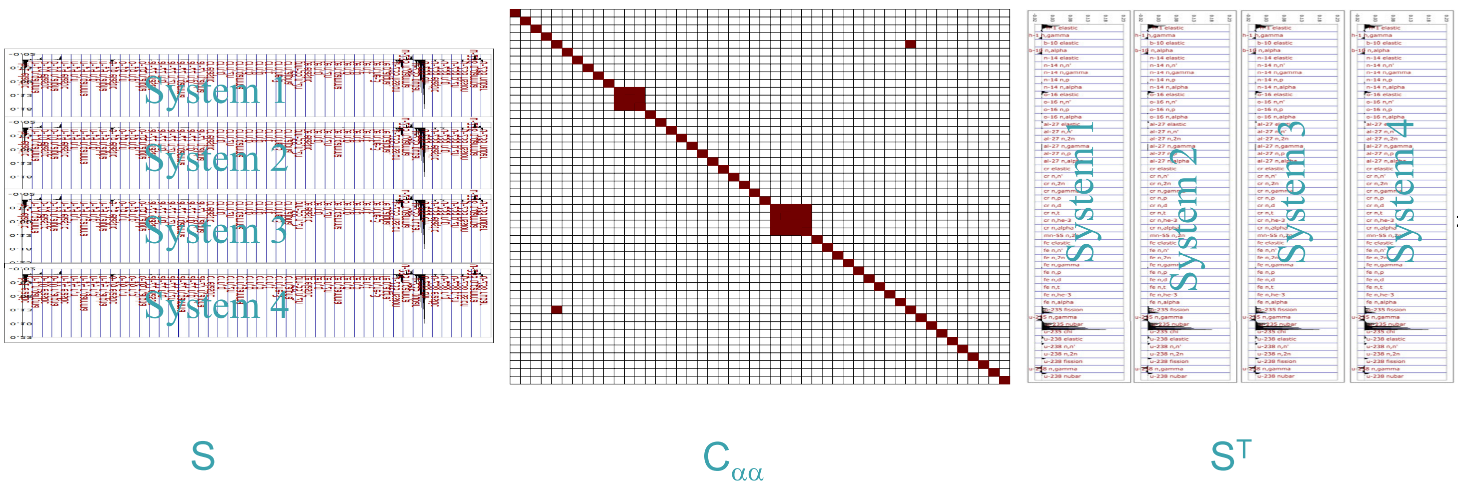
Uncertainties for critical benchmarks experiments

- Results from SCALE 6.2.2 Validation Report
  (ORNL/TM-2018/884)
- ~96.5% of C/E values within 1σ of unity
- **Uncertainty bounds bias!**



Uncertainty propagation: multiple system uncertainties

- Suppose we have sensitivity information for multiple systems:

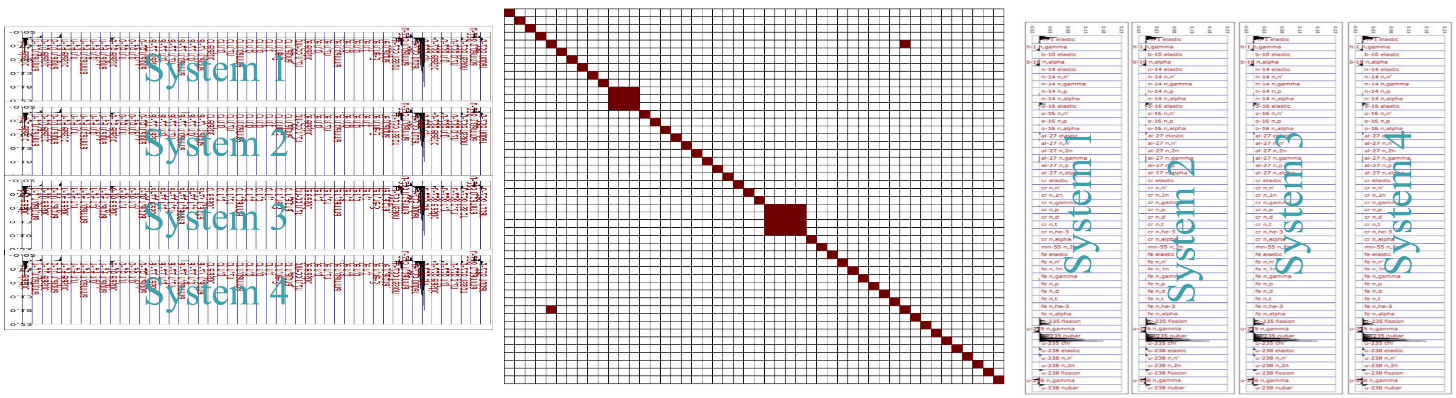


$$= \begin{bmatrix} \sigma_{11}^2 & & & \\ & \sigma_{22}^2 & & \\ & & \sigma_{33}^2 & \\ & & & \sigma_{44}^2 \end{bmatrix}$$

Diagonal elements are variance in each system

Uncertainty propagation: multiple systems covariances

- Suppose we have sensitivity information for multiple systems:



$$= \begin{bmatrix} & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \end{bmatrix}$$

S $\quad C_{\alpha\alpha} \quad S^T$

Off-diagonal elements are covariance between two systems

Correlation coefficient (c_k) for System 1 and System 4

- Integral index c_k based on definition of Pearson correlation coefficient

$$c_{kk} = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & \sigma_{33}^2 & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \sigma_{44}^2 \end{bmatrix}$$

$$c_k = \frac{\sigma_{41}^2}{\sqrt{\sigma_{11}^2}\sqrt{\sigma_{44}^2}}$$

Integral index c_k

- c_k is an integral index used to assess similarity
  - Uncertainty weighted comparison of sensitivity profiles between an application and a critical benchmark experiment
  - Measure of data-induced uncertainty shared by systems and thus a measure of the shared bias
  - Correlation coefficient, so normalized from -1.0 to +1.0
    - All caveats about use of linear correlation coefficients apply
- Current guidance:
  - c_k of 0.9 or higher indicates a highly similar system
  - c_k between 0.8 and 0.9 are “marginally” similar

Summary

- S/U-based parameters should be useful in identifying similar benchmark systems
  - Basis for similarity is both sensitivity information and nuclear data uncertainties
  - c_k can be used to filter benchmarks used in any validation approach
  - c_k values can be used in trending analyses to determine subcritical limits
- ORNL recommends c_k values greater than 0.8 for inclusion in validation

Recent ORNL-Developed Models

B.J. Marshall, Veronica Karriem, Alex Shaw

DNCSH Workshop
Germantown, MD
February 29, 2024

Outline

- TRISO pebbles in notional high-volume package
  - Model development
  - Similarity assessment
- SFR fuel in ES-3100
  - Container and fuel description
  - k_{eff} results
  - Similarity assessment
- Summary

OAK RIDGE National Laboratory

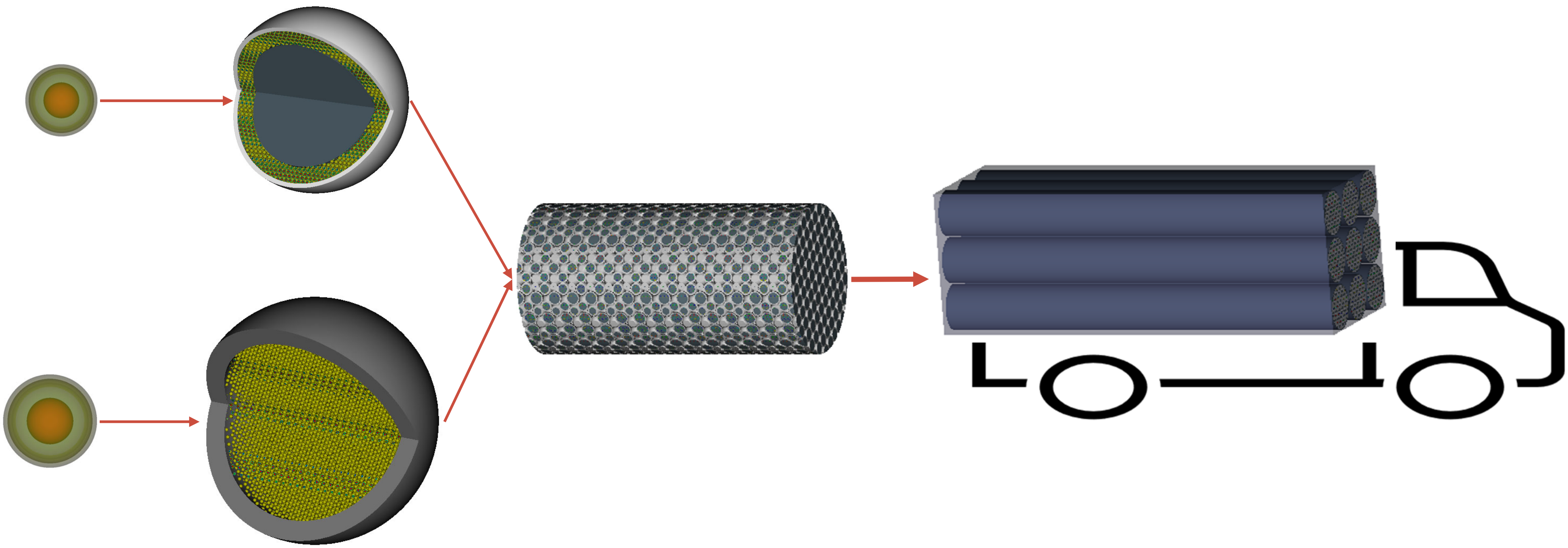
PBMR-type and Kairos-type TRISO Pebbles in Notional High-Volume Package

"Pebble Tanker"

Goals for "Pebble Tanker" design

- Create notional, high-volume transportation package for TRISO pebbles: PBMR-type pebble and Kairos-type pebble
- Concept is an array of metal tubes filled with pebbles inside a "dry van" semi trailer
- Size and spacing of tubes meets a k_{eff} limit of 0.94 to generate a representative system
- No analysis outside of k_{eff} dry/flooded and sensitivity coefficients calculations for both conditions

The “pebble tanker” concept



- Kairos-type pebble (top): 4×4 array of 22 cm radius tubes
- PBMR-type pebble (bottom): 3×3 array of 28 cm radius tubes

Pebble tanker model specifications

Parameter	PBMR-type pebble	Kairos-type pebble
Volume fraction (grain)	50.4 %	36.8 %
U mass/pebble	9.50 g	5.93 g
Total mass/pebble	204.1 g	54.37 g
Tube array size	3×3	4×4
Pebbles/tube	~12,000	~25,700
Enrichment	19.75 wt% ^{235}U	19.95 wt% ^{235}U
k_{eff} dry	0.44260 ± 0.00020	0.44993 ± 0.00020
k_{eff} flooded	0.94012 ± 0.00020	0.93144 ± 0.00020

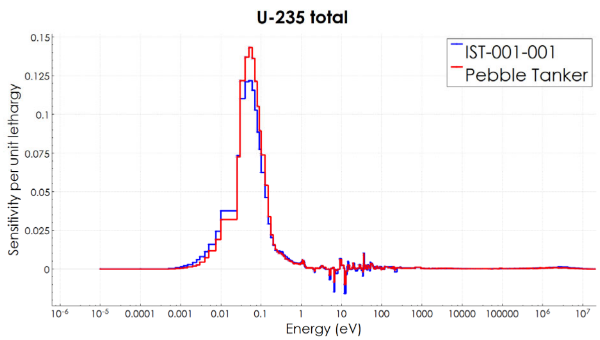
Similarity assessment

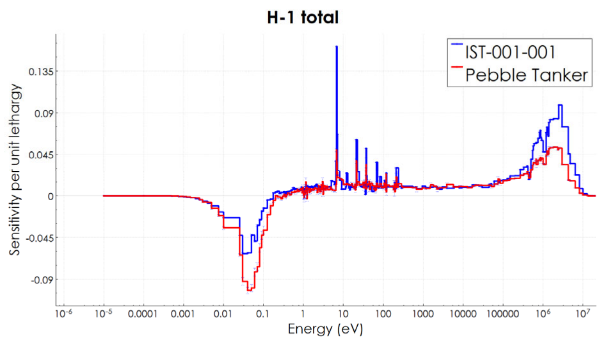
- TSUNAMI-3D used to calculate sensitivity coefficients for flooded arrays
- c_k calculated for each tanker compared to 3936 experiments
- PBMR-type application has 285 experiments with $c_k > 0.9$
- Kairos-type application has 85 experiments with $c_k > 0.9$
- Sufficient experiments to perform validation
- Applicable experiments are largely solutions with enrichments ranging from 4.31 to 93 wt% ^{235}U

Similarity assessment details

Uncertainty contributions for flooded PBMR-type tanker model (pcm)			
Nuclide	**Uncertainty**	**Running**	**Percentage**
^{235}U	678	678	88.2
^{1}H	263	727	94.6
^{56}Fe	187	751	97.7
graphite	142	764	99.5
^{16}O	69	767	99.9
Total		768	100

c_k contribution for flooded PBMR-type tanker model and IEU-SOL-THERM-001-001		
Nuclide	**c_k contribution**	**Running Total**
^{235}U	0.8029	0.8029
^{1}H	0.0855	0.8884
^{56}Fe	0.0652	0.9536
graphite	0.0112	0.9648
^{16}O	0.0087	0.9735
Total		0.9774





SFR Fuel in ES-3100

ES-3100

- 30 gal. drum with inner containment vessel (CV) for fissile material
  - Drum: Appx. 110 cm tall, 25 cm radius
  - CV: Appx. 80 cm tall, 6.5 cm radius
- Designed for transport of HEU metal and oxides, research reactor fuel
- Steel CV and casing
- Kaolite (concrete+vermiculite) fill

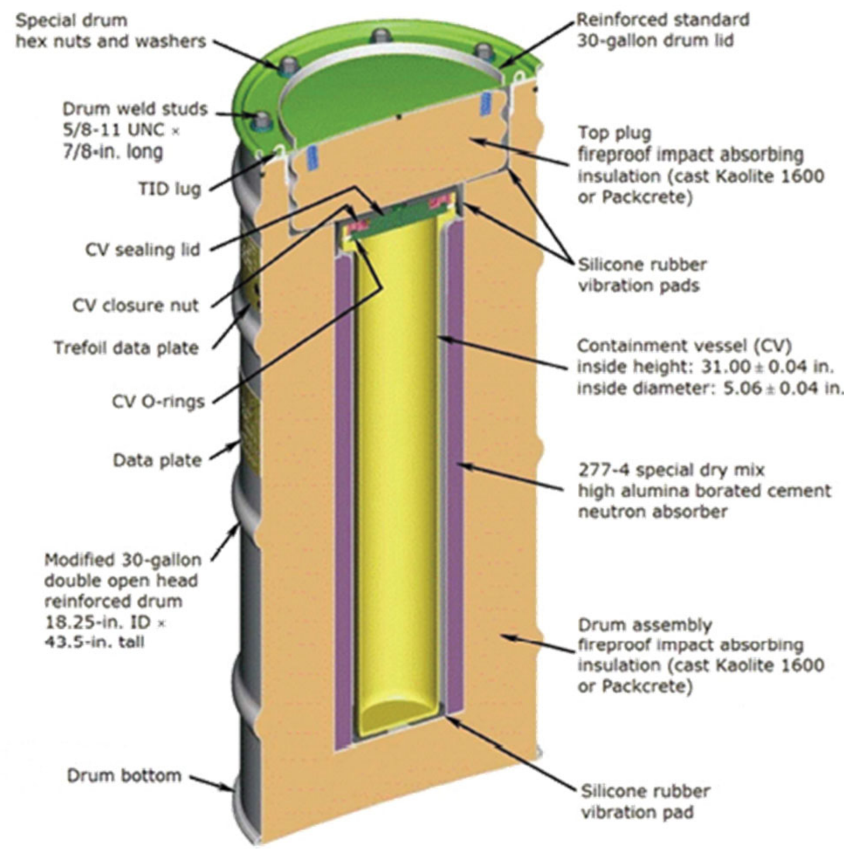


Figure from CoC 9315 Rev. 19 (USA/9315/B(U)F-96)

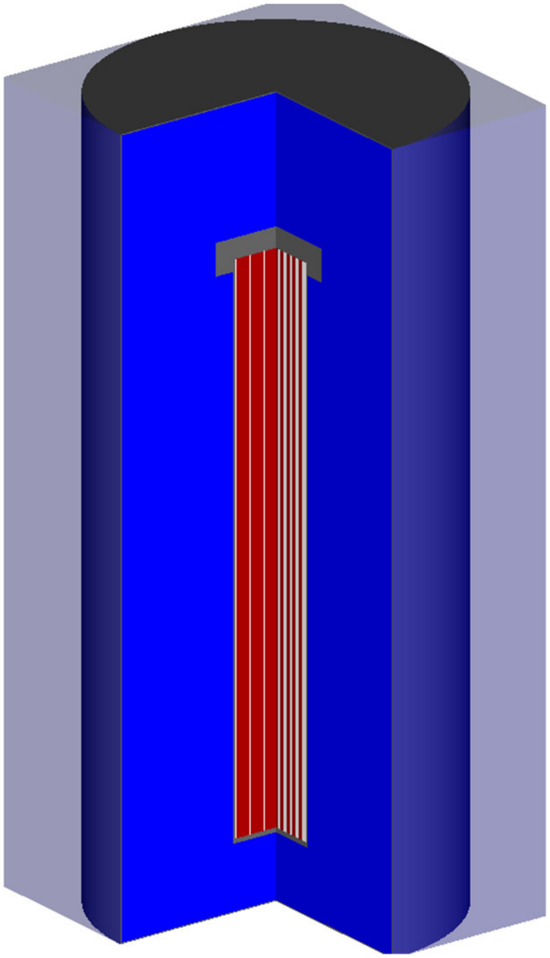
SFR Fuel Summary

- SFR fuel is expected to consist of stacked metal slugs or full-length rods
  - Example SFRs: EBR-I, EBR-II, FFTF, Fermi 1
- ORNL/TM-2022/2758 used ABTR (advanced burner test reactor) as a representative SFR design
  - Simplified composition to U/Zr alloy metallic fuel (20 wt% ^{235}U)
- ABTR uses 60 fuel assemblies for 250 MWth
- Each fuel assembly has 217 fuel slugs/rods

k_{eff} results

- 217 slugs modeled inside a single ES-3100
  - Enough fuel for a single assembly
- Modeled an infinite array of packages
  - Water flooded
  - Dry with kaolite fill
  - Polyethylene bounding of water or kaolite

Case	k_{eff}	σ
Dry	0.62301	0.00010
Water flooded	0.69196	0.00010
Polyethylene	0.70079	0.00010



Similarity assessment

- TSUNAMI-3D used to calculate sensitivity coefficients for water- and polyethylene-filled ES-3100 package arrays
- c_k calculated for each package compared to a set of 4011 experiments

Model	$0.8 < c_k < 0.9$	$0.9 < c_k$
Water	41	1
Poly	85	2

- Sufficient experiments for validation
- Further analysis needed for gap assessment

Summary

Summary

- Notional high-volume package model developed
  - Similar experiments identified for flooded case
  - No glaring data gaps for this system
  - ^{56}Fe may be a useful target given its uncertainty contribution
- ES-3100 model with simplified SFR fuel developed
  - Similar experiments identified for flooded case
  - Additional work needed to determine if gaps exist
- Additional work needed for MSR fuel forms

Summary of Workshop 1

- Demonstrate our strategy for prioritizing benchmarks
  1. Survey the field
  2. Prioritize a target application
  3. Develop an application model (today: **fresh fuel pebble transport**)
  4. Assess the validation basis
  5. Host a workshop
  6. Develop Experiment Support Opportunity (ESO) to address gaps in validation bases
  7. Rinse and repeat
- ESOs are the main vehicle for critical benchmark awards
- We are hungry for information
  – **Long lead-time on nuclear data and experiments!**
  – Existing measurements that could become benchmarks
  – From reactor designers: what are your intended transportation packages, front-end/back-end storage systems
  – Any ideas where you may need additional nuclear data or benchmarks for safe, commercial-scale operations
- Feedback methods
  – ~~Use the chat ☺~~
  – **Respond to feedback form (following the workshop)**
  – **Email DNCSH@ornl.gov**
- What next?
  – Prepare short workshop summary document and send to participants
  – Prepare ESO #1
    - April 1 2024 **Announce**
    - June 7, 2024 **Award**

Final Notes:

- Thank you for coming!
- A feedback summary will be coming to your email box. Please fill it out to provide us the needed information to make the workshop's summary report and future workshops better.
- In addition, information about the upcoming ESO will be coming to your email on or about April 1.
- Questions? Have technical information to share?

Email us at DNCSH@ornl.gov