16TH NUCLEAR DATA
FOR SCIENCE AND TECHNOLOGY CONFERENCE
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Integral Experiment Validation of Hafnium with TEX-HEU and TEX-Hf

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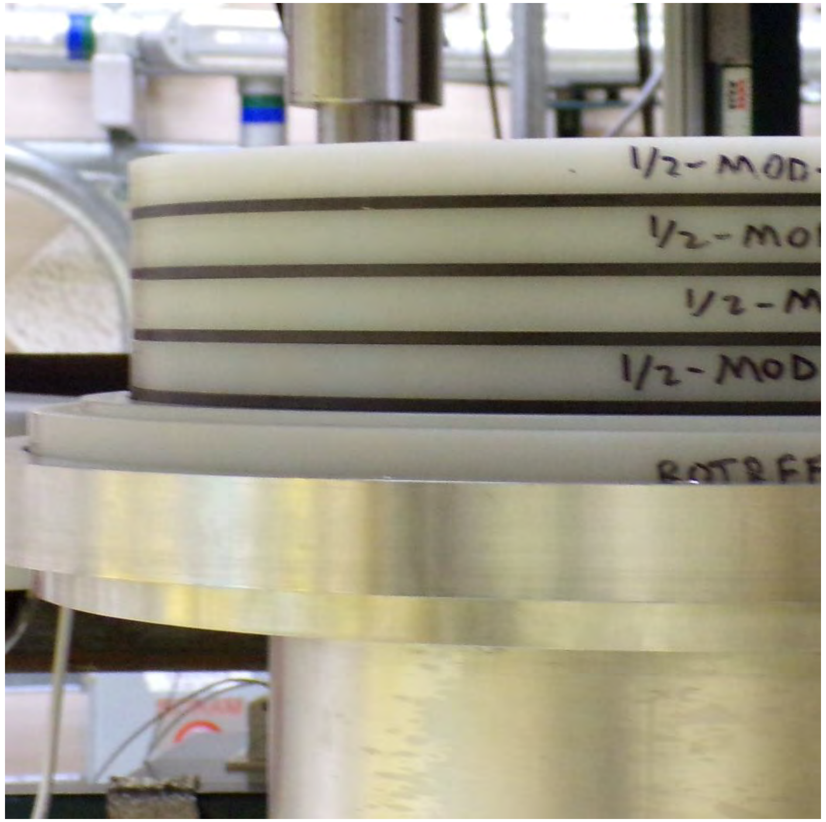
LLNL-CFPRES-2007750

Thermal/Epithermal eXperiments (TEX)

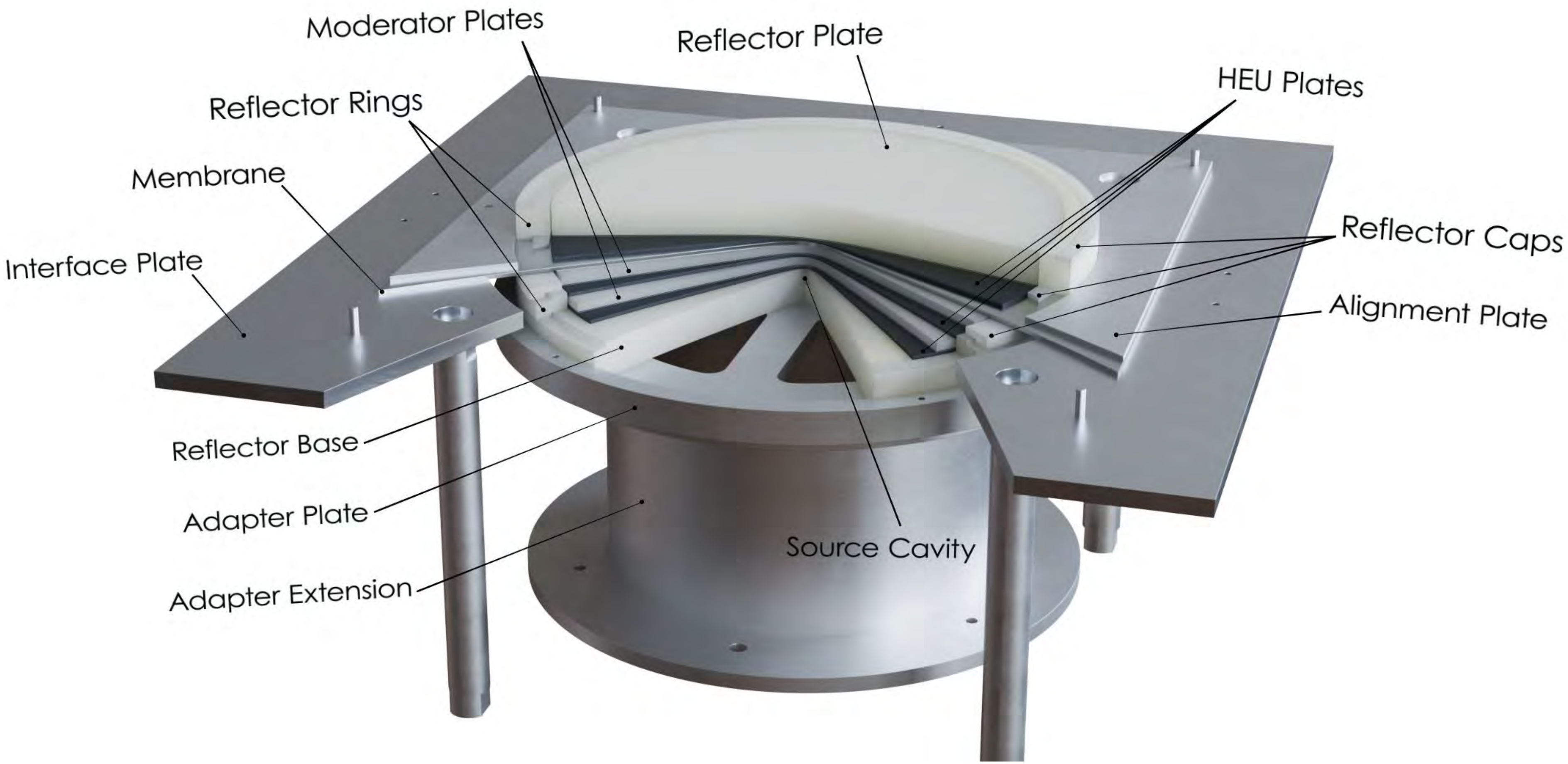
- Lead by Lawrence Livermore National Laboratory under the U.S. Department of Energy's Nuclear Criticality Safety Program
- The goal of TEX is to provide integral benchmark experiments than span the entire neutron energy spectrum and incorporate high-priority materials
- TEX includes two test bed configurations providing a baseline for comparison to better understand the contribution of additional materials
  - TEX-Pu with plutonium and TEX-HEU with highly enriched uranium
  - TEX-Pu: Tantalum (complete), Iron (in-progress), + more
  - TEX-HEU: Hafnium (complete), Chlorine (complete), Lithium (in-design), + more

TEX with Highly Enriched Uranium (TEX-HEU)

- Highly enriched uranium (HEU) fuel with high density polyethylene (HDPE) moderator and reflector
  - Published in the 2022/2023 ICSBEP as HEU-MET-MIXED-021
- Varying the thickness of the moderator plates allows the neutron spectrum to be fine-tuned to a specific energy regime
  - From fast (no moderator) to thermal (up to 1.5 in. (3.81 cm) thick moderator)



TEX-HEU Design

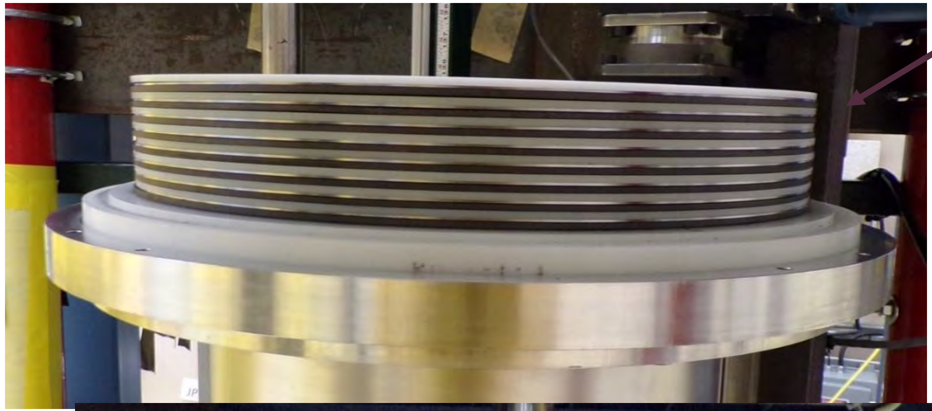


J. Norris, *et. al.*, "TEX-HEU: Baseline Assemblies Benchmark and Results, HEU-MET-MIXED-021." American Nuclear Society Winter Meeting & Technology Expo. Pheonix, AZ (2022).

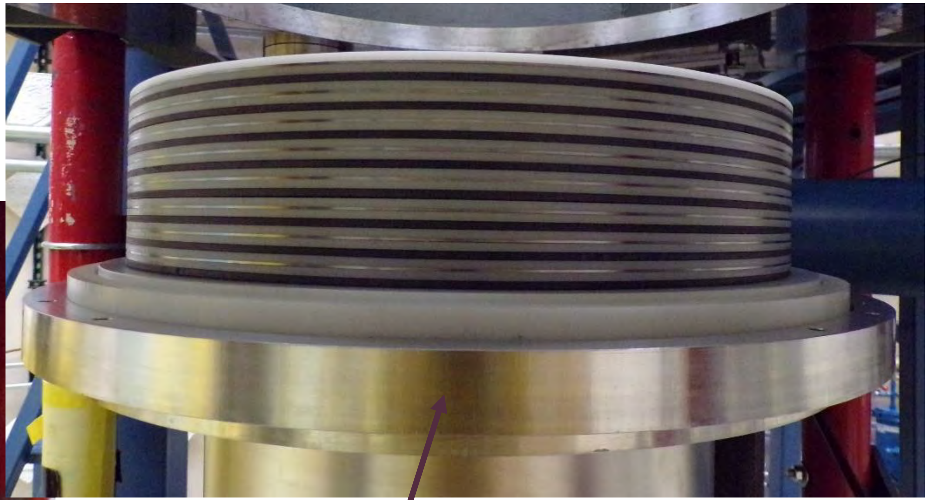
TEX-HEU with Hafnium (TEX-Hf)

- TEX-Hf is the first variation on TEX-HEU and incorporates hafnium (Hf) as the diluent material
  - Published in the 2024 ICSBEP as HEU-MET-INTER-013
- The goal of the TEX-Hf configurations is maximize the sensitivity in k_{eff} to the hafnium isotope cross sections
  - Configurations position hafnium as both an interstitial material and reflector using three stacking variations

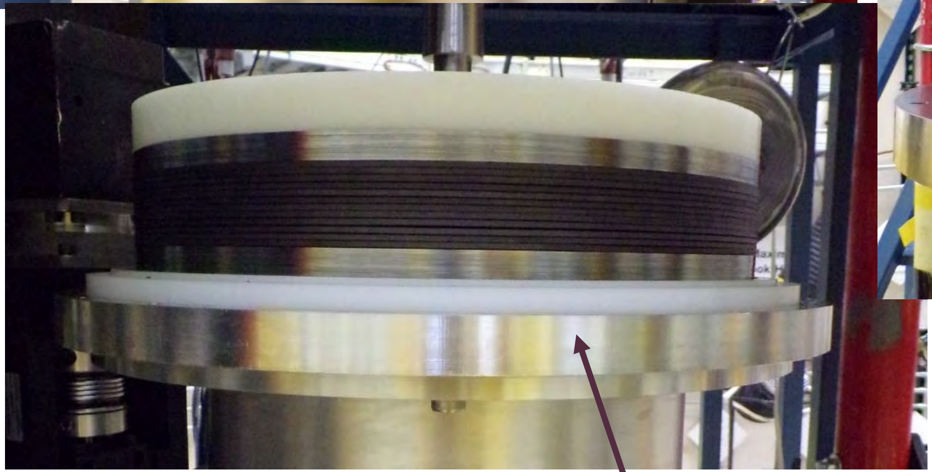
TEX-Hf Stacking Variations



Standard (Case 1-5)
Hafnium between HEU and HDPE



Sandwich (Case 6)
Hafnium between HDPE



Bunched (Case 7)
Hafnium as a reflector

J. Norris, *et. al.*, "TEX-HEU & TEX-Hf: Critical Assemblies with Highly Enriched Uranium, Polyethylene, and Hafnium." The 12th International Conference on Nuclear Criticality Safety, Sendai, Japan (2023).

TEX-HEU Benchmark Cases

HEU-MET-MIXED-021

- Five benchmark cases providing the baseline
  - Differ due to nominal HDPE moderator thickness used to vary the fission energy regime

TEX-HEU Case	HEU Mass (kg)	Moderator Thickness, in. (cm)	Neutron Spectrum	C/E* (ENDF/B-VIII.0)
HMM-021-01	109.1	No moderator	Fast	0.99827 ± 0.00133
HMM-021-02	70.0	0.125 (0.3175)	Mixed	0.99749 ± 0.00127
HMM-021-03	51.0	0.250 (0.6350)	Intermediate	**0.99704 ± 0.00130**
HMM-021-04	32.3	0.500 (1.2700)	Mixed	**0.99680 ± 0.00149**
HMM-021-05	29.5	1.500 (3.8100)	Thermal	0.99751 ± 0.00120

*C/E using detailed benchmark model

J. Norris, *et. al.*, "TEX-HEU & TEX-Hf: Critical Assemblies with Highly Enriched Uranium, Polyethylene, and Hafnium." The 12th International Conference on Nuclear Criticality Safety, Sendai, Japan (2023).

TEX-Hf Benchmark Cases

HEU-MET-INTER-019

- Seven benchmark cases using hafnium
  - Differ due to nominal HDPE moderator thickness and stacking variation

TEX-Hf Case	HEU Mass (kg)	Hafnium Mass (kg)	Moderator Thickness, in. (cm)	Neutron Spectrum	C/E (ENDF/B-VIII.0)
HMI-013-01	135.5	38.7	No moderator	Fast	1.00194 ± 0.00147
HMI-013-02	99.4	24.2	0.125 (0.3175)	Intermediate	1.00227 ± 0.00158
HMI-013-03	82.8	19.4	0.250 (0.6350)	Intermediate	0.99918 ± 0.00154
HMI-013-04	63.9	14.5	0.500 (1.2700)	Mixed	**0.99731 ± 0.00124**
HMI-013-05	70.4	16.1	1.500 (3.8100)	Thermal	0.99770 ± 0.00147
HMI-013-06[a]	88.4	21.0	0.250 (0.6350)	Intermediate	0.99907 ± 0.00142
HMI-013-07[b]	124.7	33.9	No moderator	Fast	**0.99662 ± 0.00137**

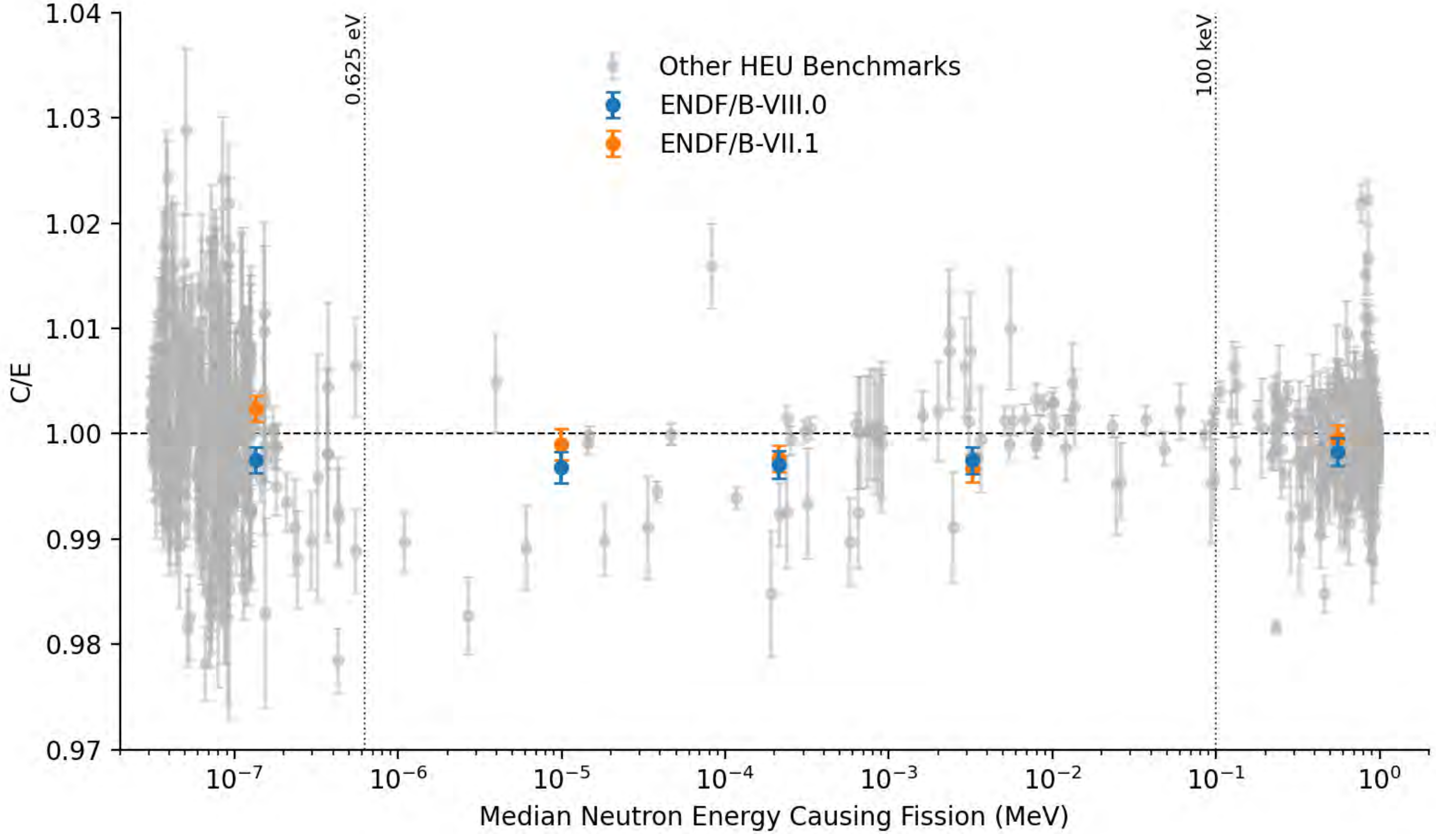
[a] Hafnium plates are sandwiched between two nominal 0.125 in. (0.635 cm) polyethylene moderator plates.
[b] Hafnium plates are bunched as 0.48 in. (1.2192 cm) top and bottom reflector surrounding the HEU plates.

J. Norris, *et. al.*, "TEX-HEU & TEX-Hf: Critical Assemblies with Highly Enriched Uranium, Polyethylene, and Hafnium." The 12th International Conference on Nuclear Criticality Safety, Sendai, Japan (2023).

TEX-HEU Benchmark Results

HEU-MET-MIXED-021 - MCNP® 6.2 with Continuous-Energy ENDF/B

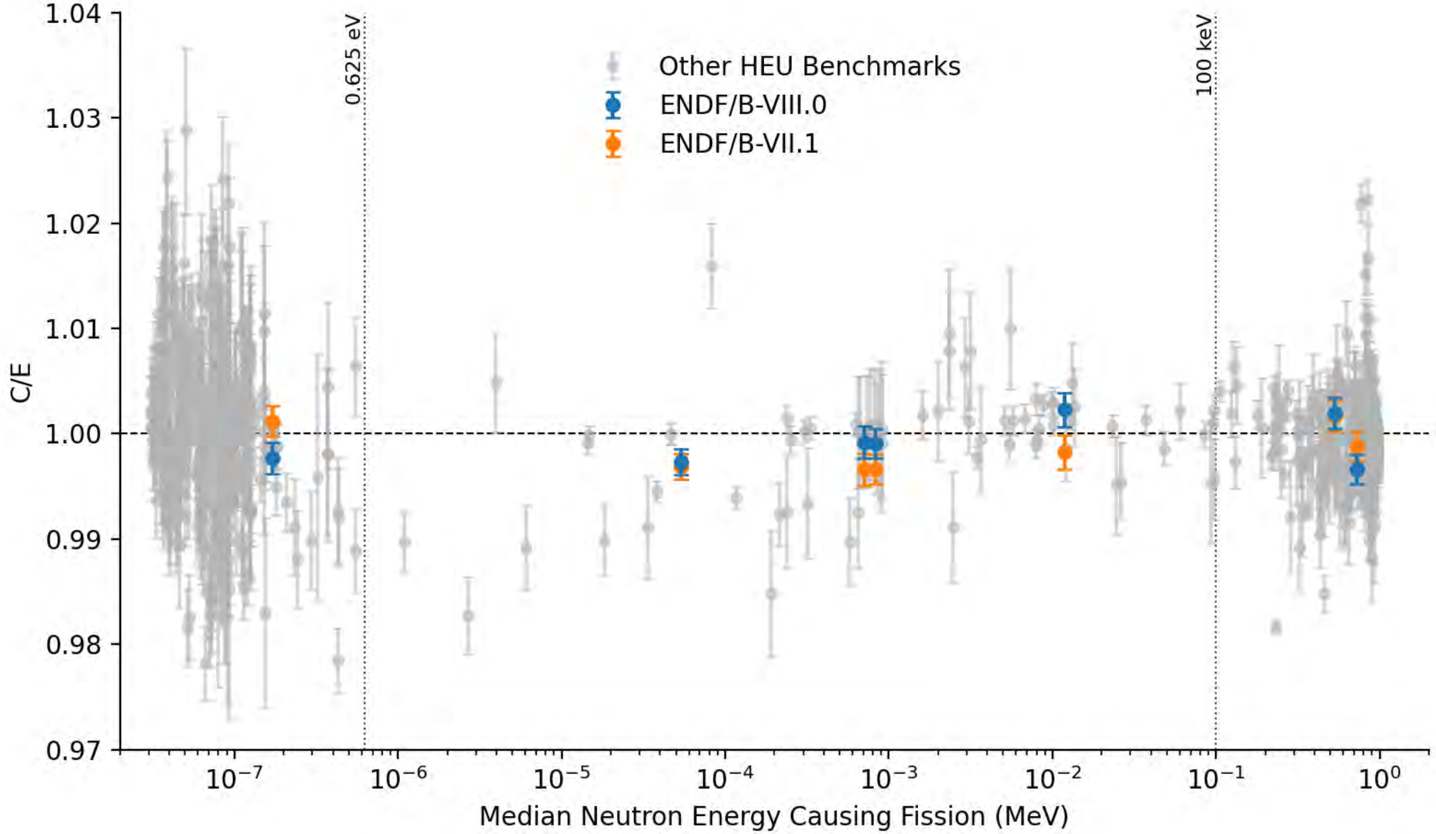
- One-sigma uncertainty between 0.12%-0.15% (120-150 pcm)



TEX-Hf Benchmark Results

HEU-MET-INTER-013 - MCNP® 6.2 with Continuous-Energy ENDF/B

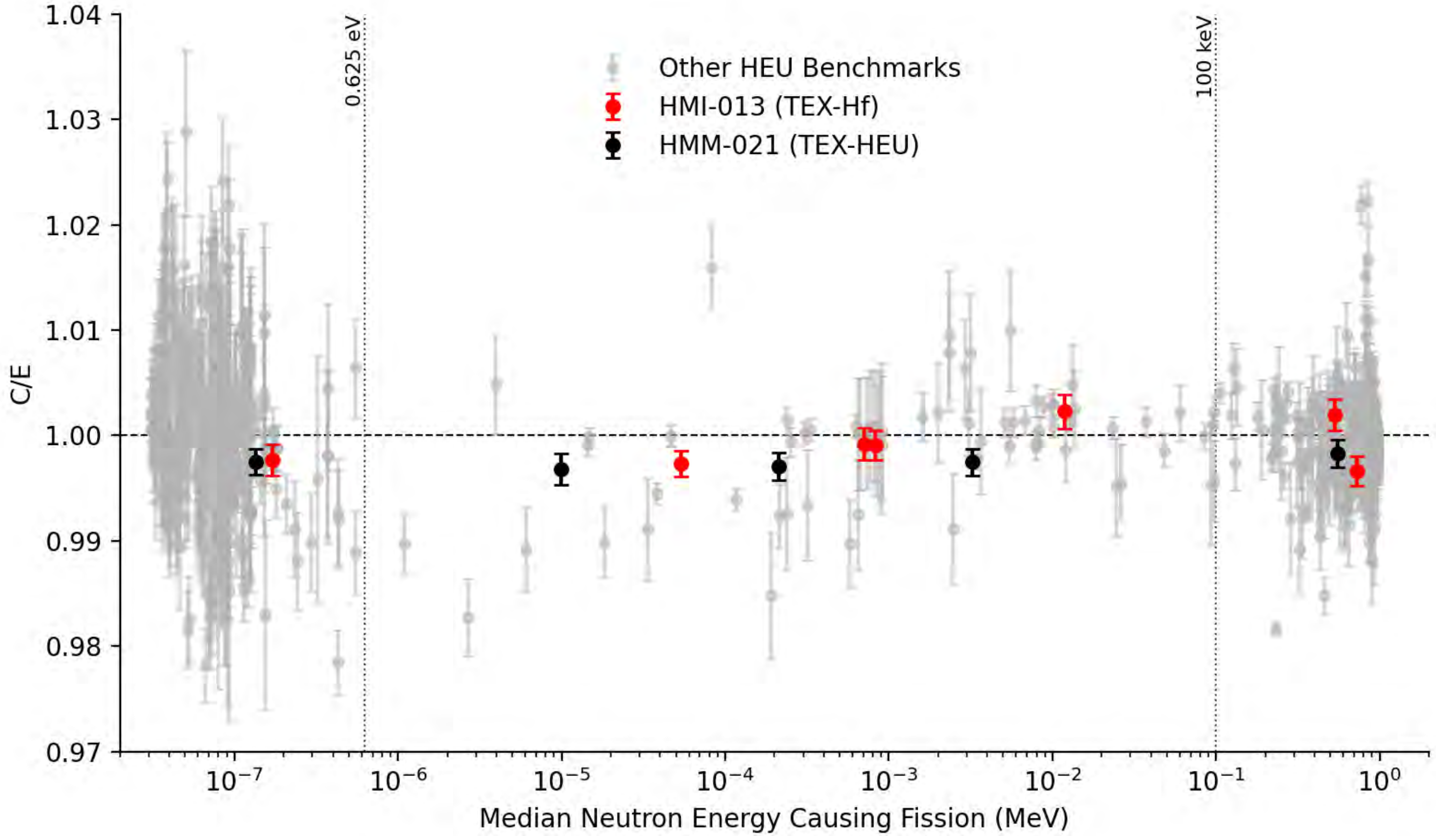
- One-sigma uncertainty between 0.12%-0.16% (120-160 pcm)



Comparison of Benchmark Results

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

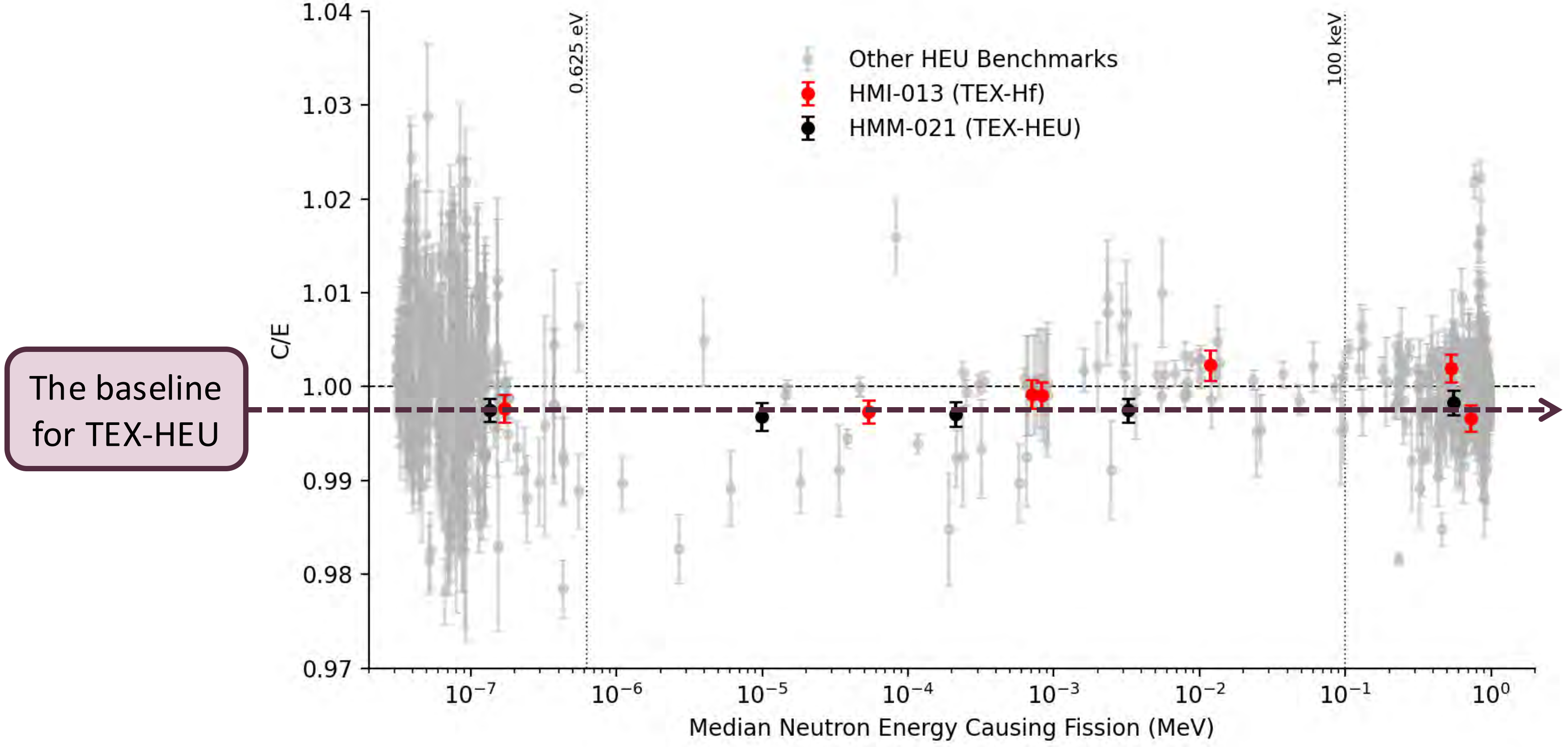
- Appears to increasingly disagree as the energy spectrum hardens



Why the Baseline Configurations Matter

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

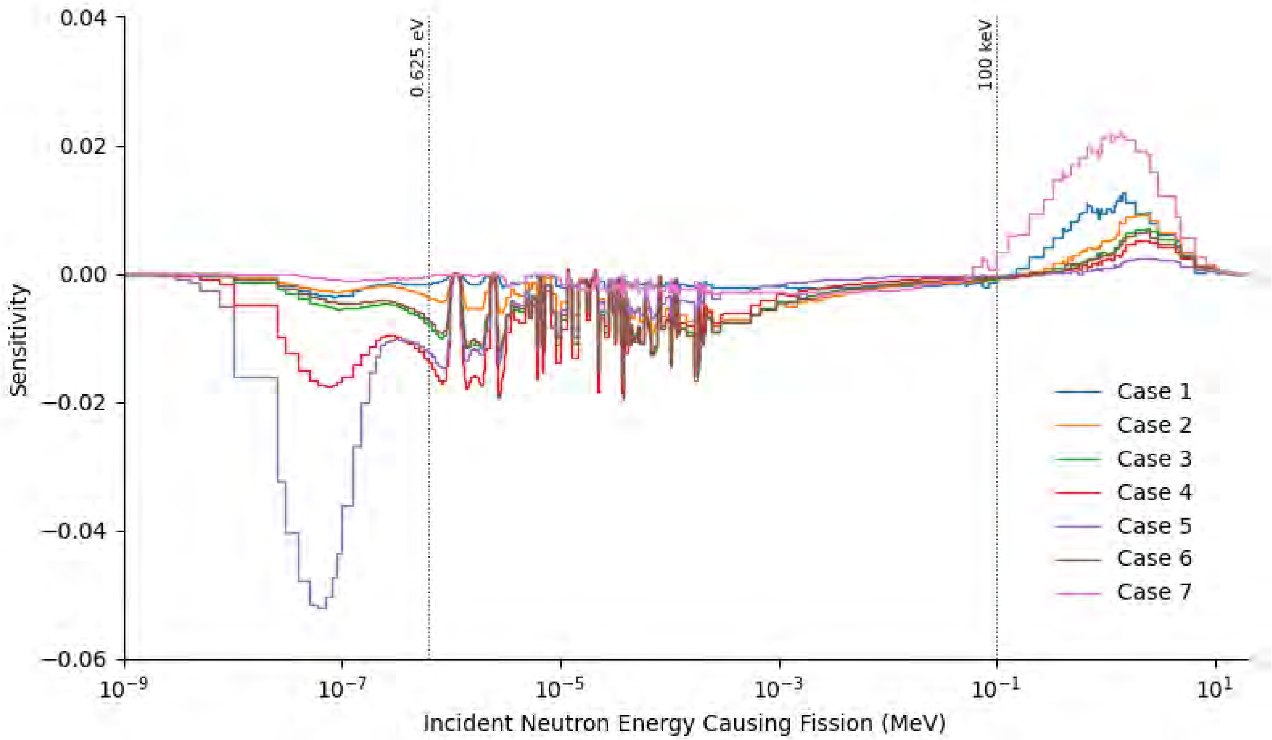
- Consistent underprediction in k_{eff} for TEX-HEU



Hafnium Nuclear Data Sensitivities in TEX-Hf

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

- Calculated using KSEN with the SCALE 252-group energy structure



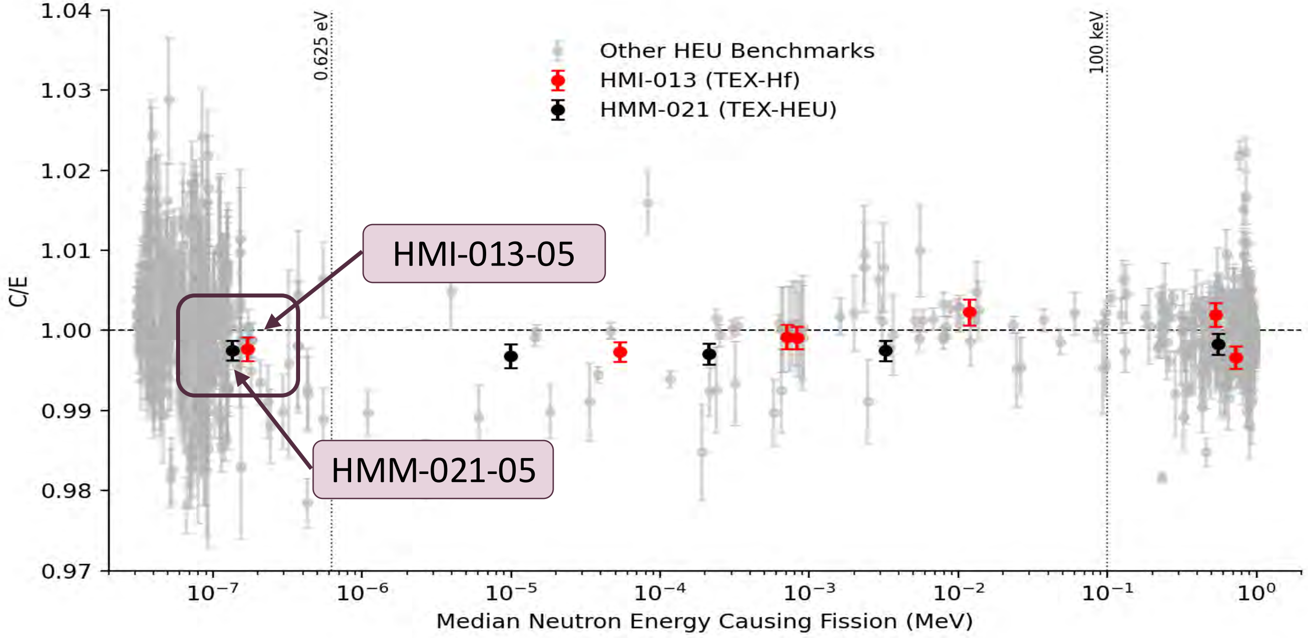
TEX-Hf Case	Sensitivity			
	Capture	Inelastic	Elastic	Total
HMI-013-01	-0.032	0.020	0.011	-0.001
HMI-013-02	-0.062	0.015	0.011	-0.036
HMI-013-03	-0.083	0.011	0.007	-0.065
HMI-013-04	-0.116	0.008	0.004	-0.104
HMI-013-05	-0.148	0.004	-0.003	-0.148
HMI-013-06	-0.083	0.010	0.010	-0.063
HMI-013-07	-0.017	0.031	0.021	0.035

*Sensitivities are normalized per unit lethargy

Comparison of Thermal Configurations

HEU-MET-MIXED-021 Case 5 & HEU-MET-INTER-013 Case 5

- Thermal configurations agree, but both underpredict experiment
  - There is a significant simplification bias from correcting the temperature of the benchmark models to 20°C due to the ^{1}H in CH_2 TSL

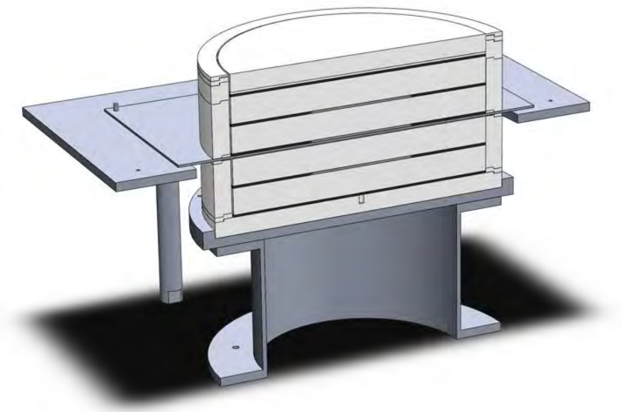


Comparison of Thermal Configurations

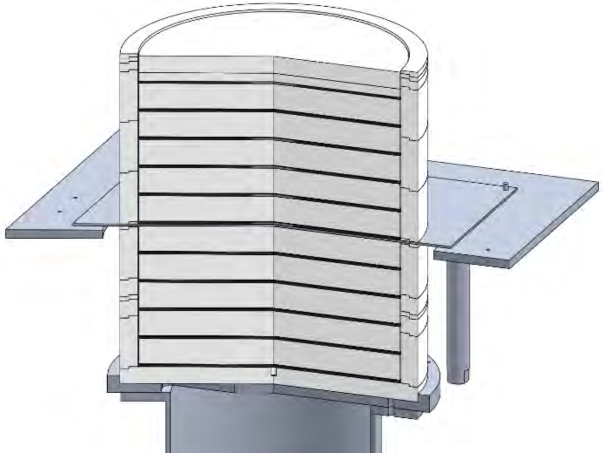
HEU-MET-MIXED-021 Case 5 & HEU-MET-INTER-013 Case 5

Baseline →

Case	HEU Mass (kg)	Hf Mass (kg)	Moderator Thickness, in. (cm)	Fission Fractions*	C/E (ENDF/B-VIII.0)
HMM-021-05	29.5	-	1.500 (3.8100)	0.63 / 0.26 / 0.11	0.99751 ± 0.00120
HMI-013-05	70.4	16.1	1.500 (3.8100)	0.60 / 0.28 / 0.12	0.99770 ± 0.00147



HEU-MET-MIXED-021-01
Baseline without hafnium,
1.5 in. moderator



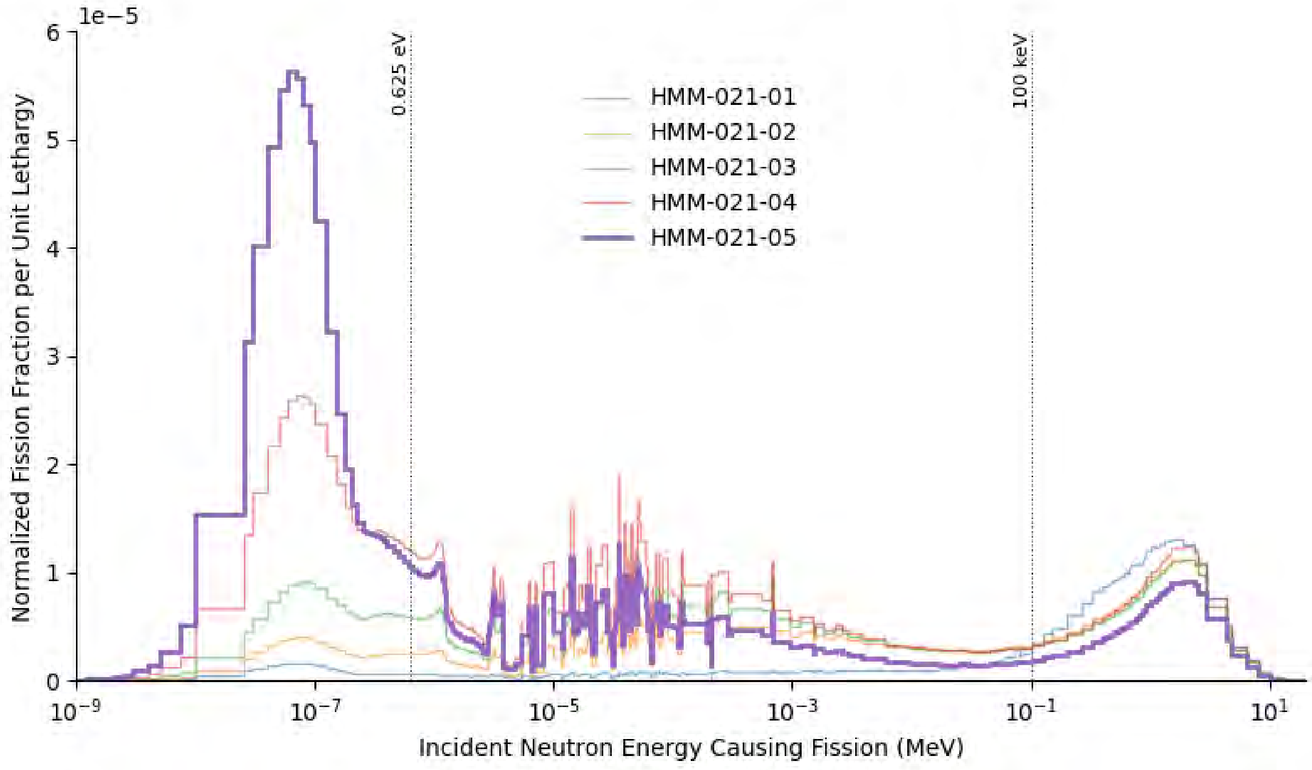
HEU-MET-INTER-013-05
Interstitial hafnium,
1.5 in moderator

*Thermal (<0.625 eV) / Intermediate (0.625 eV – 100 keV) / Fast (>100 keV)

TEX-HEU Thermal Fission Spectra

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

TEX-HEU Case	Neutron Spectrum
HMM-021-01	Fast
HMM-021-02	Mixed
HMM-021-03	Intermediate
HMM-021-04	Mixed
HMM-021-05	**Thermal**



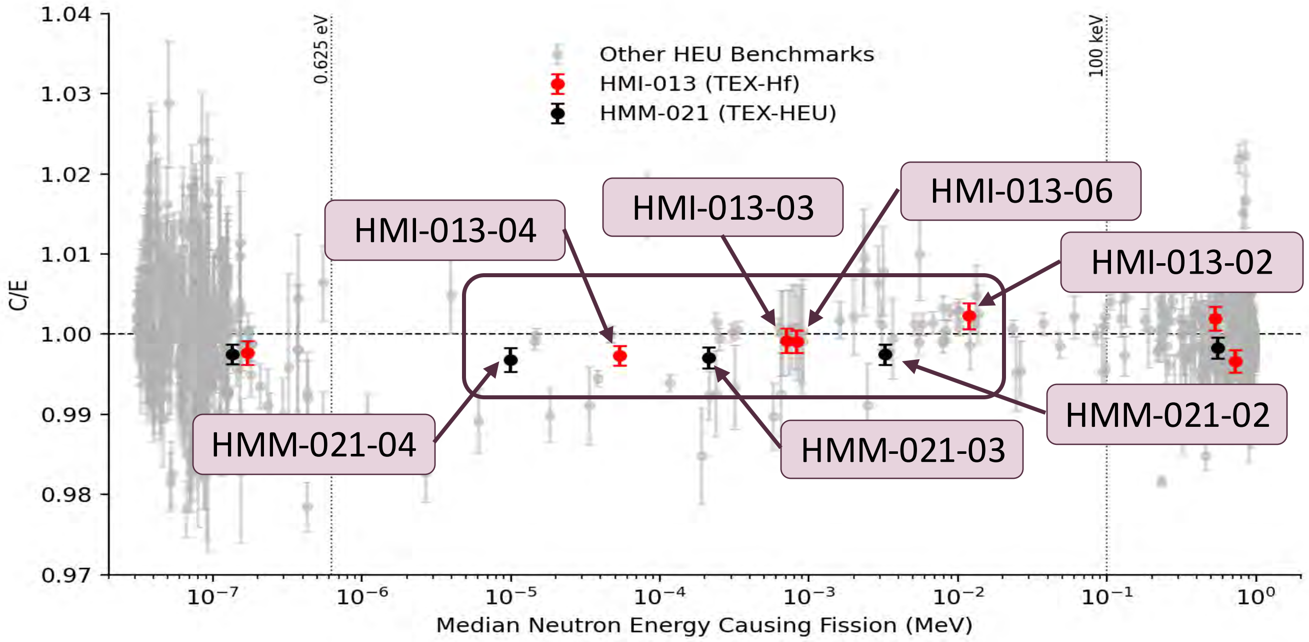
*Fission fractions are normalized per unit lethargy

*Thermal (<0.625 eV) / Intermediate (0.625 eV – 100 keV) / Fast (>100 keV)

Comparison of Mixed & Inter. Configurations

HEU-MET-MIXED-021 Cases 2-4 & HEU-MET-INTER-013 Cases 2-4 and 6

- As the neutron energy spectrum hardens there appears to be increasing disagreement between the baseline configurations (TEX-HEU) and the configurations with hafnium (TEX-Hf)

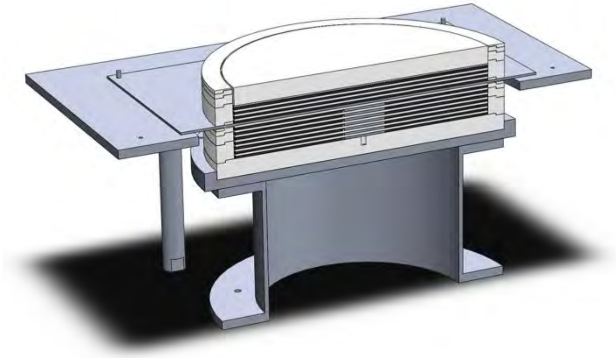


Comparison of Mixed Configurations

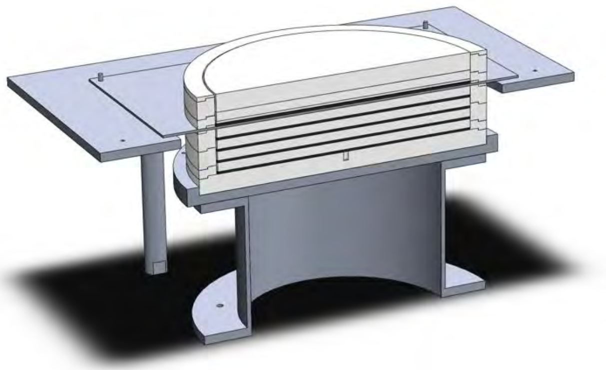
HEU-MET-MIXED-021 Cases 2 and 4 & HEU-MET-INTER-013 Case 4

Baseline

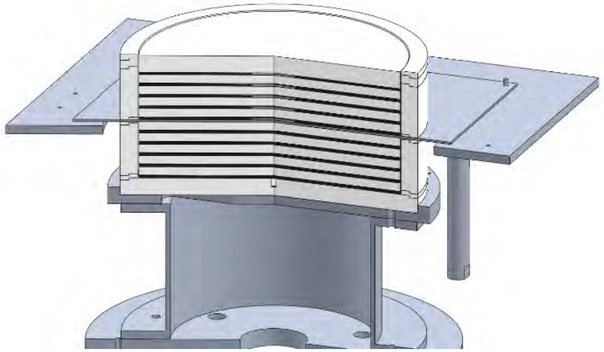
Case	HEU Mass (kg)	Hf Mass (kg)	Moderator Thickness, in. (cm)	Fission Fractions*	C/E (ENDF/B-VIII.0)
HMM-021-02	70.0	-	0.125 (0.3175)	0.14 / 0.50 / 0.36	0.99749 ± 0.00127
HMM-021-04	32.3	-	0.500 (1.2700)	0.39 / 0.44 / 0.17	0.99680 ± 0.00149
HMI-013-04	63.9	14.5	0.500 (1.2700)	0.31 / 0.49 / 0.20	0.99731 ± 0.00124



HEU-MET-MIXED-021-02
Baseline without hafnium,
0.125 in. moderator



HEU-MET-MIXED-021-04
Baseline without hafnium,
0.5 in. moderator



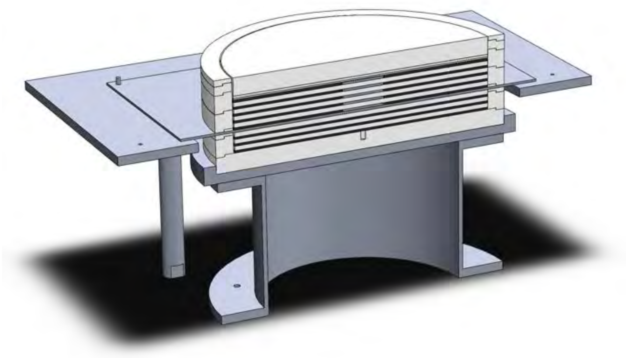
HEU-MET-INTER-013-04
Interstitial hafnium,
0.5 in. moderator

*Thermal (<0.625 eV) / Intermediate (0.625 eV – 100 keV) / Fast (>100 keV)

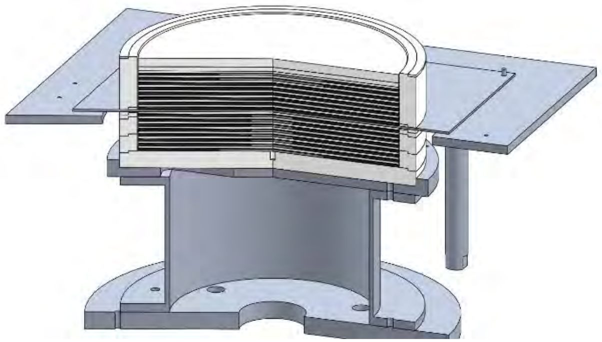
Comparison of Intermediate Configurations

HEU-MET-MIXED-021 Case 3 & HEU-MET-INTER-013 Cases 2, 3, and 6

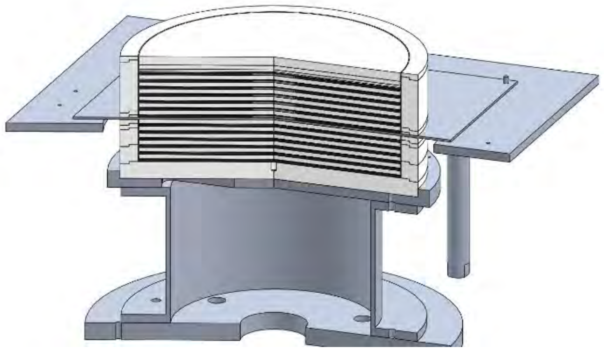
	Case	HEU Mass (kg)	Hf Mass (kg)	Moderator Thickness, in. (cm)	Fission Fractions*	C/E (ENDF/B-VIII.0)
Baseline →	HMM-021-03	51.0	-	0.250 (0.6350)	0.23 / 0.51 / 0.26	0.99704 ± 0.00130
	HMI-013-02	99.4	24.2	0.125 (0.3175)	0.09 / 0.51 / 0.40	1.00227 ± 0.00158
	HMI-013-03	82.8	19.4	0.250 (0.6350)	0.16 / 0.55 / 0.29	0.99918 ± 0.00154
	HMI-013-06	88.4	21.0	0.250 (0.6350)	0.13 / 0.57 / 0.30	0.99907 ± 0.00142



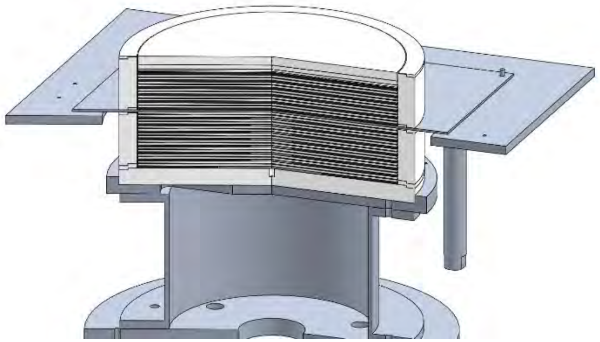
HEU-MET-MIXED-021-03
Baseline without hafnium,
0.25 in. moderator



HEU-MET-INTER-013-02
Interstitial hafnium,
0.125 in. moderator



HEU-MET-INTER-013-03
Interstitial hafnium,
0.25 in. moderator

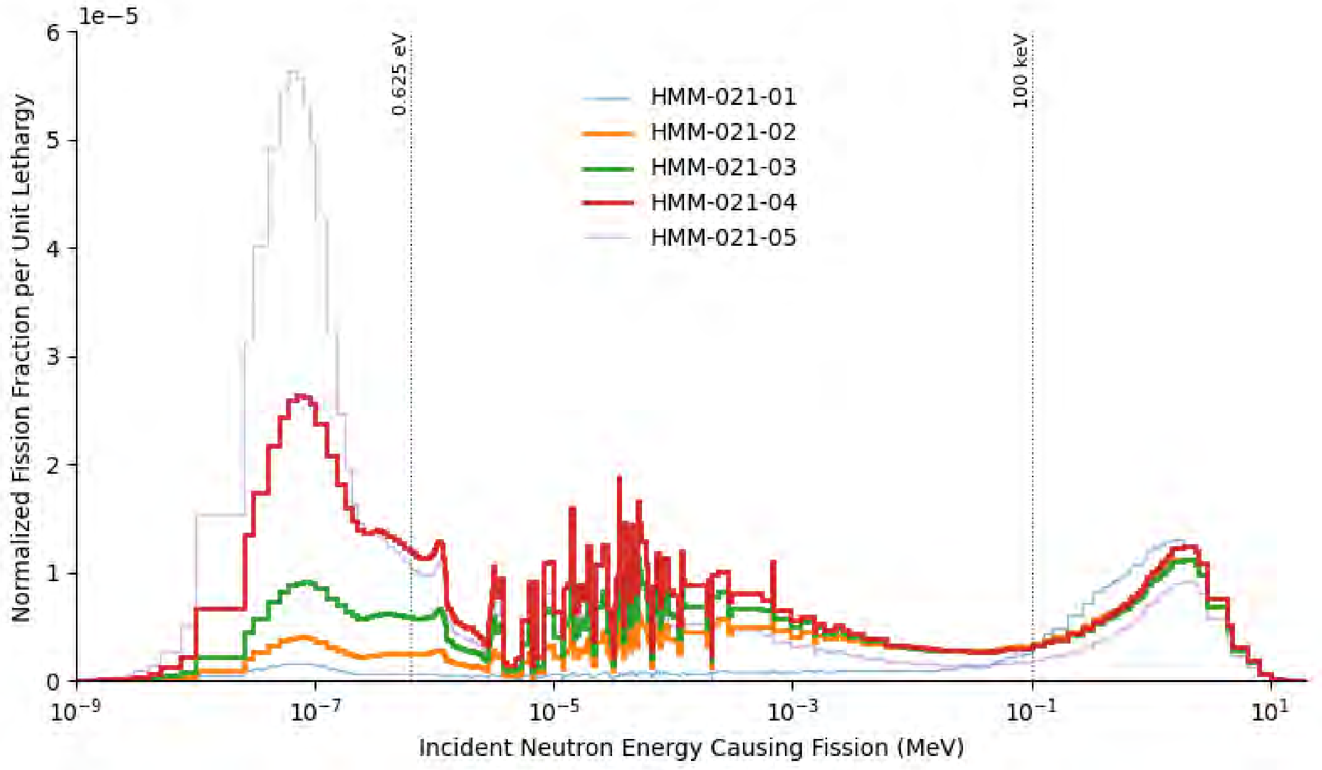


HEU-MET-INTER-013-06
Sandwiched hafnium,
nominal 0.25 in. moderator

TEX-HEU Mixed & Intermediate Fission Spectra

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

TEX-HEU Case	Neutron Spectrum
HMM-021-01	Fast
HMM-021-02	Mixed
HMM-021-03	Intermediate
HMM-021-04	Mixed
HMM-021-05	Thermal



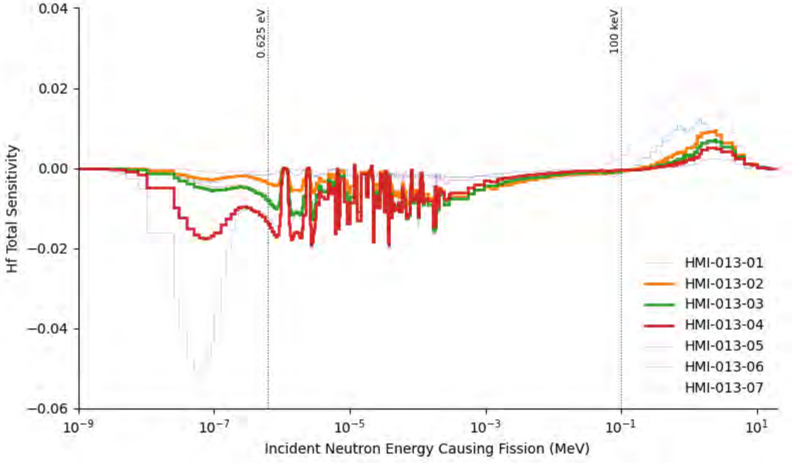
*Fission fractions are normalized per unit lethargy

*Thermal (<0.625 eV) / Intermediate (0.625 eV – 100 keV) / Fast (>100 keV)

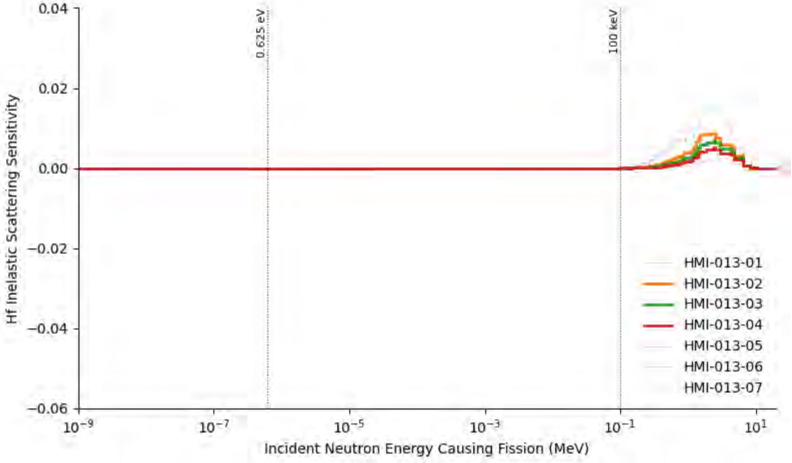
Nuclear Data Sensitivities – Inter. Configurations

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

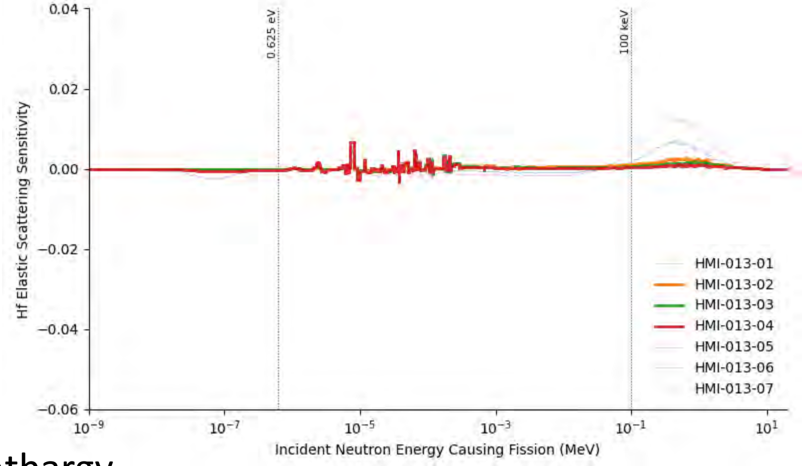
Hafnium Total



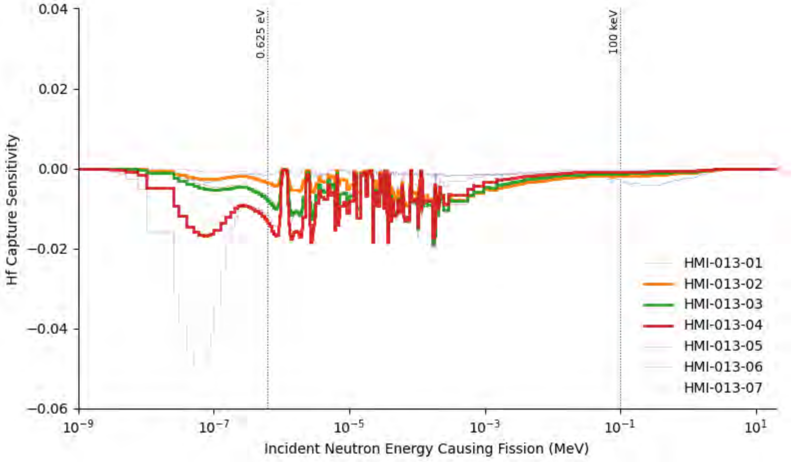
Hafnium Inelastic



Hafnium Elastic



Hafnium Capture

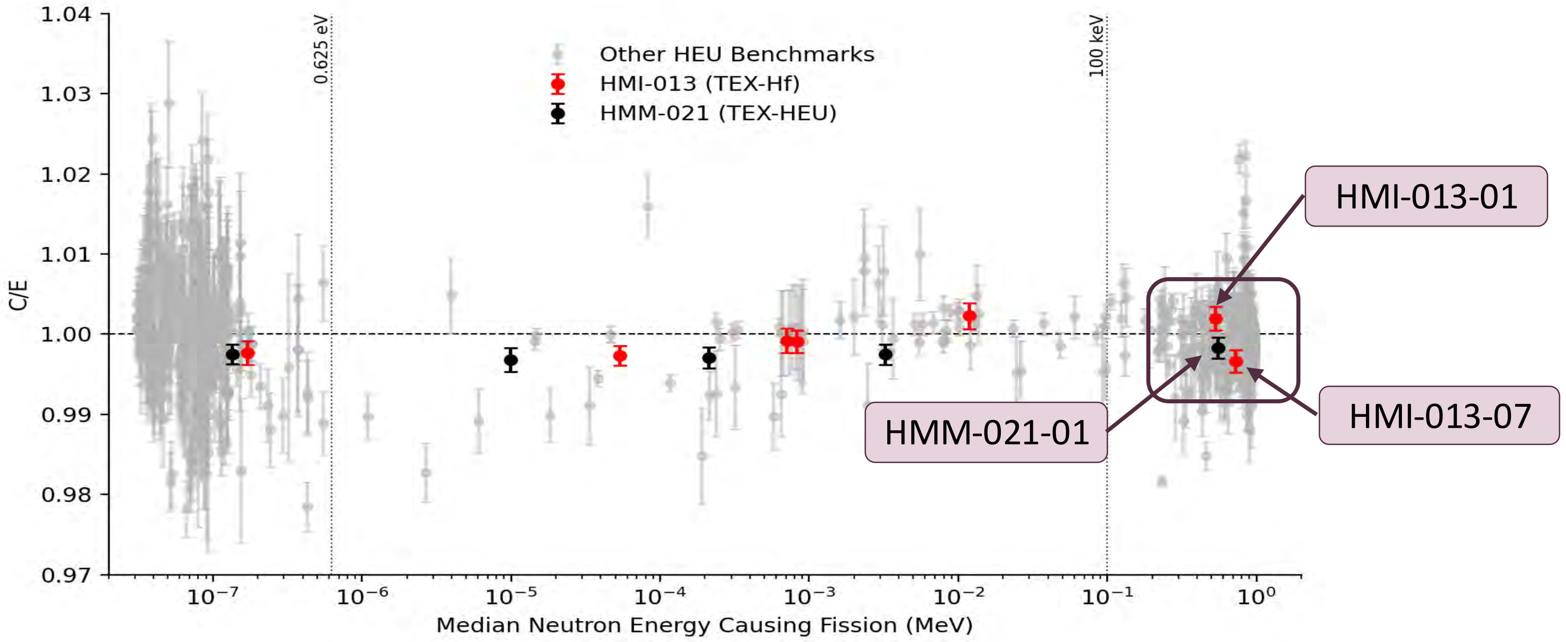


*Normalized per unit lethargy

Comparison of Fast Configurations

HEU-MET-MIXED-021 Case 1 & HEU-MET-INTER-013 Cases 1 and 7

- The addition of hafnium significantly impacts the fast calculations
  - Further disagreement depending on the location of the hafnium, either interstitially (HMI-013-01) or as a reflector (HMI-013-07)

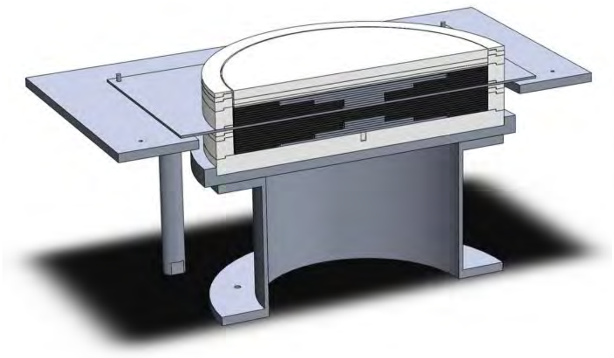


Comparison of Fast Configurations

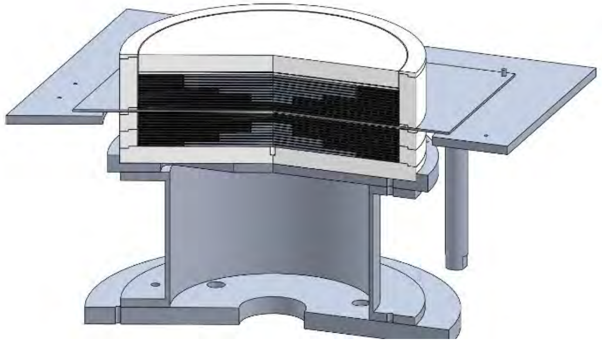
HEU-MET-MIXED-021 Case 1 & HEU-MET-INTER-013 Cases 1 and 7

Baseline

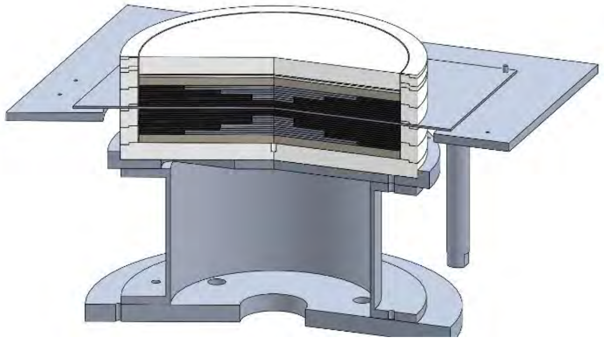
Case	HEU Mass (kg)	Hf Mass (kg)	Moderator Thickness, in. (cm)	Fission Fractions*	C/E (ENDF/B-VIII.0)
HMM-021-01	109.1	-	No moderator.	0.08 / 0.20 / 0.72	0.99827 ± 0.00133
HMI-013-01	135.5	38.7	No moderator.	0.06 / 0.18 / 0.76	1.00194 ± 0.00147
HMI-013-07	124.7	33.9	No moderator.	0.01 / 0.14 / 0.85	0.99662 ± 0.00137



<u>HEU-MET-MIXED-021-01</u>
Baseline without hafnium, no moderator



<u>HEU-MET-INTER-013-01</u>
Hafnium as interstitial between HEU layers



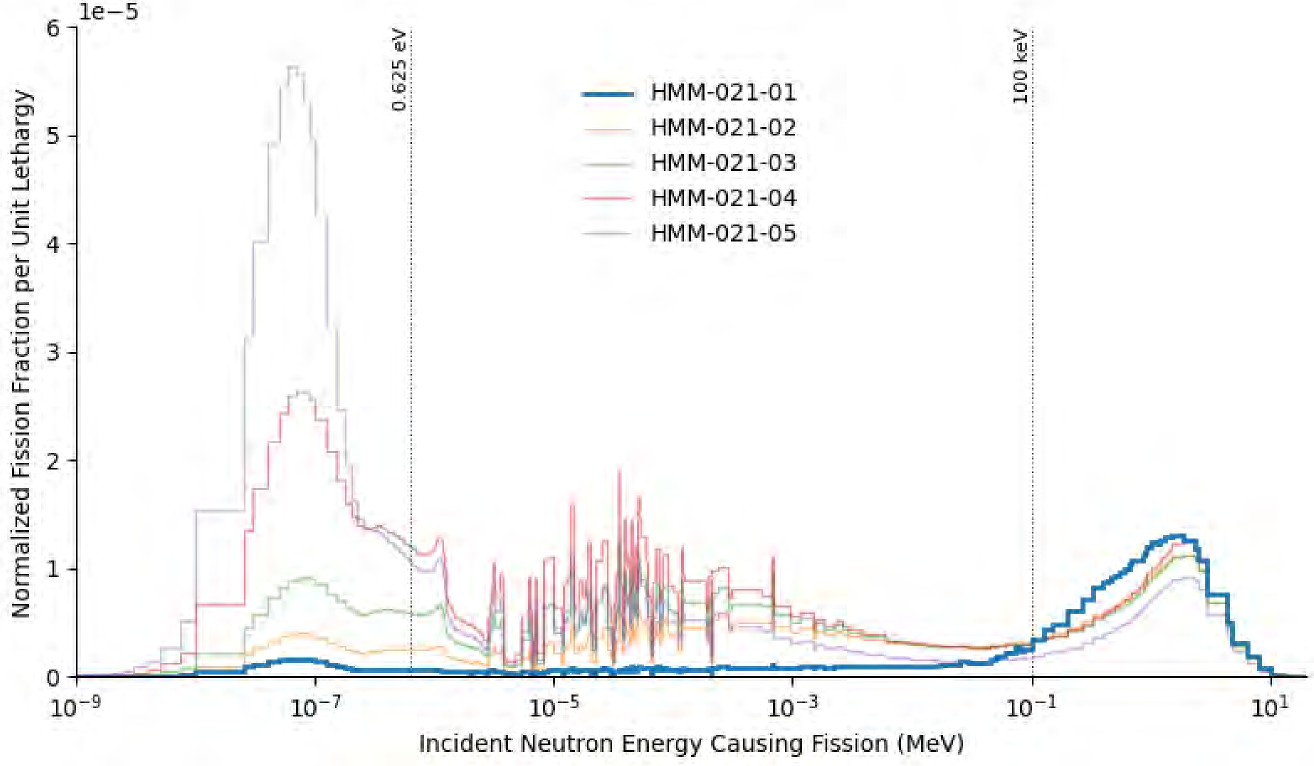
<u>HEU-MET-INTER-013-07</u>
Hafnium as reflector on top and bottom of HEU core

*Thermal (<0.625 eV) / Intermediate (0.625 eV – 100 keV) / Fast (>100 keV)

TEX-HEU Fast Fission Spectra

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

TEX-HEU Case	Neutron Spectrum
HMM-021-01	Fast
HMM-021-02	Mixed
HMM-021-03	Intermediate
HMM-021-04	Mixed
HMM-021-05	Thermal

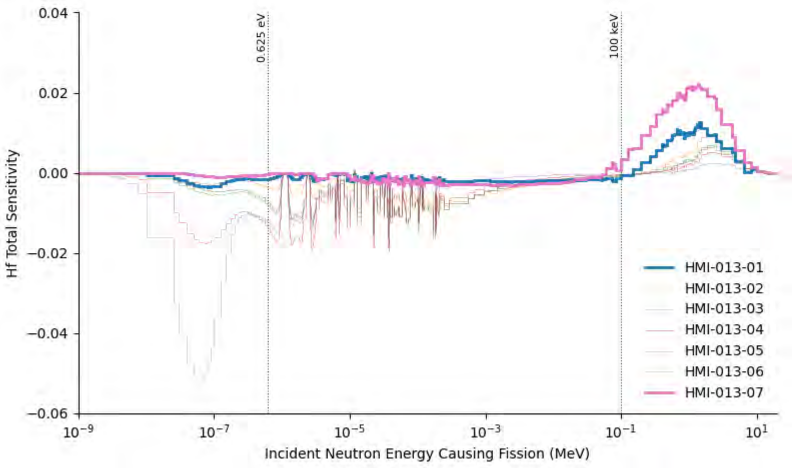


*Fission fractions are normalized per unit lethargy
*Thermal (<0.625 eV) / Intermediate (0.625 eV – 100 keV) / Fast (>100 keV)

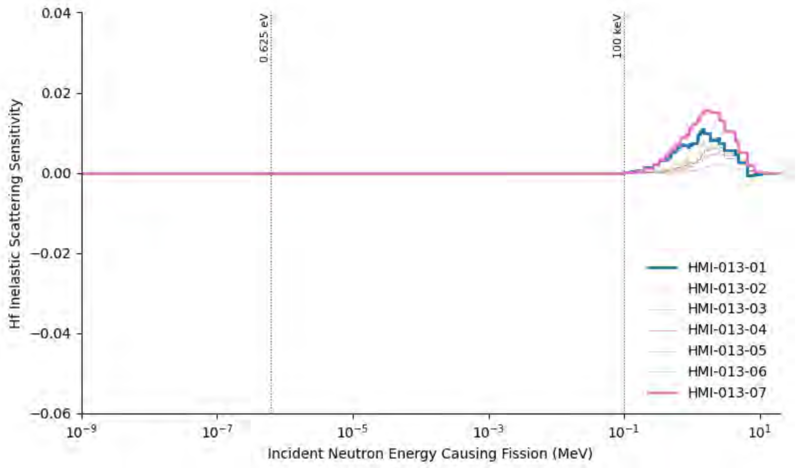
Nuclear Data Sensitivities – Fast Configurations

MCNP® 6.2 with Continuous-Energy ENDF/B-VIII.0

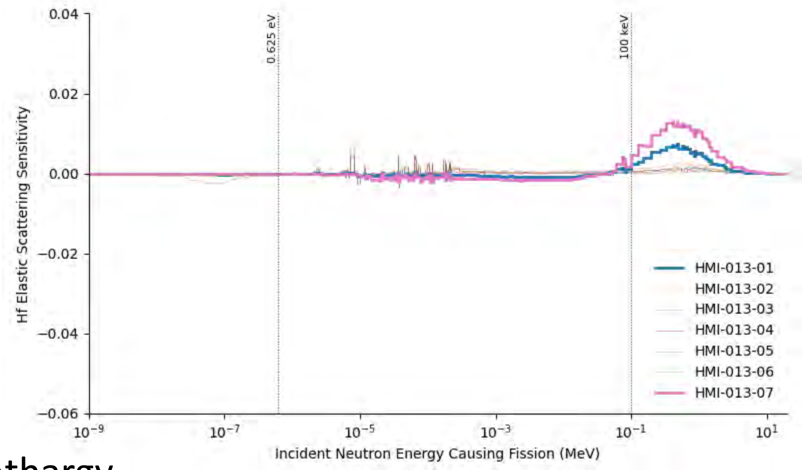
Hafnium Total



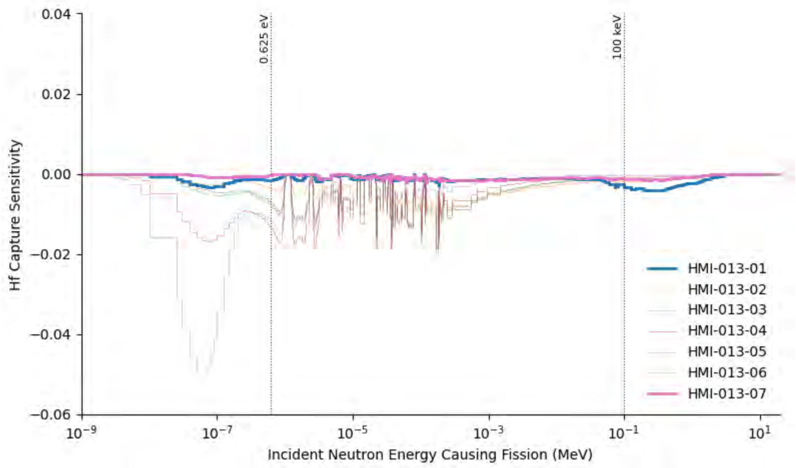
Hafnium Inelastic



Hafnium Elastic



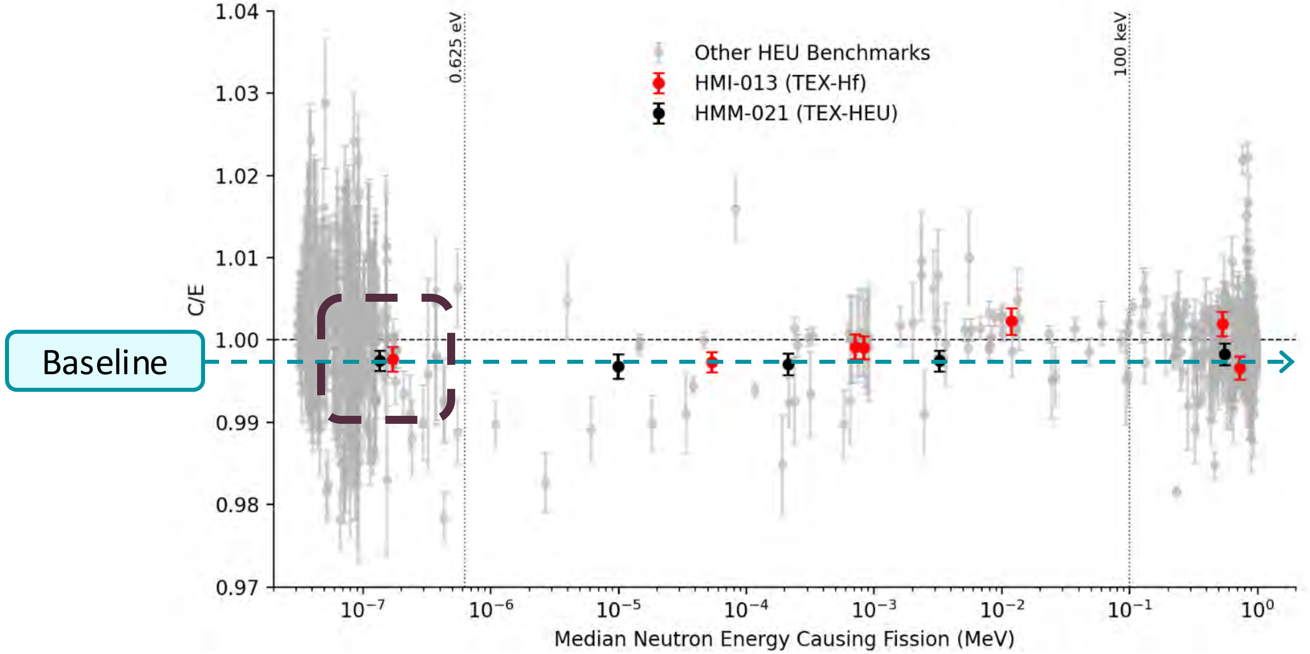
Hafnium Capture



*Normalized per unit lethargy

Results – Thermal Configurations

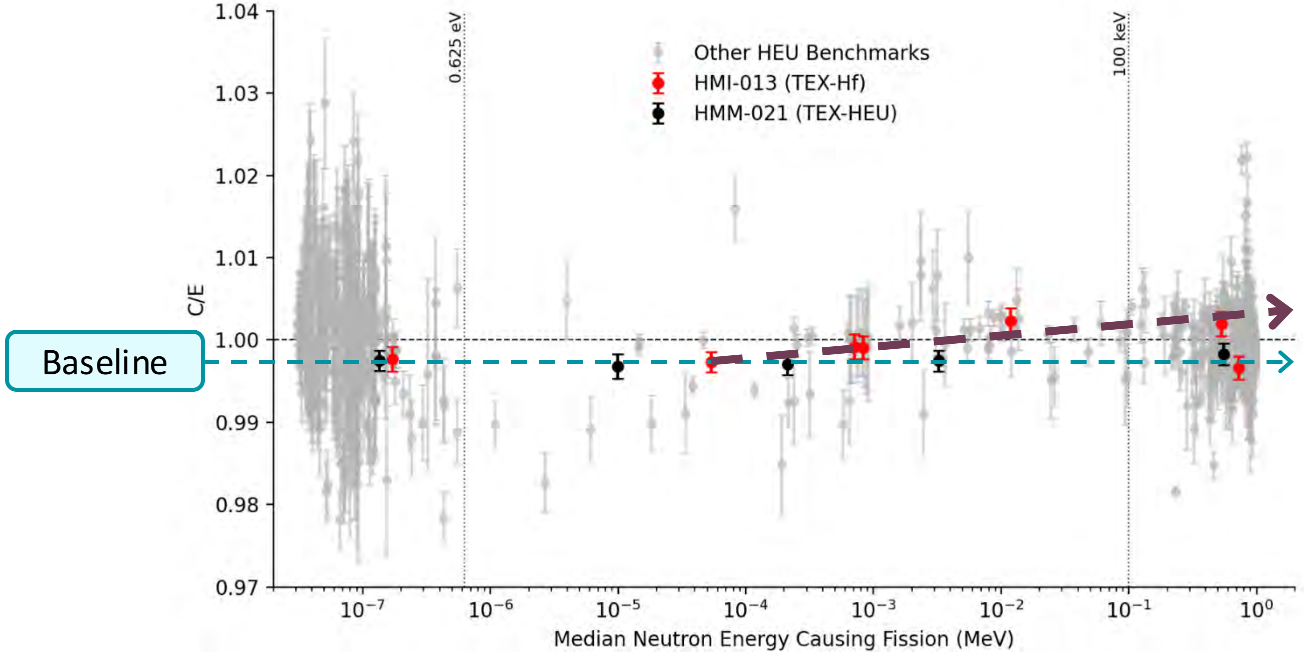
- There is good agreement in the thermal configurations, even for a large sensitivity to hafnium capture



TEX-Hf Case	Sensitivity			
	Capture	Inelastic	Elastic	Total
HMI-013-01	-0.032	0.020	0.011	-0.001
HMI-013-02	-0.062	0.015	0.011	-0.036
HMI-013-03	-0.083	0.011	0.007	-0.065
HMI-013-04	-0.116	0.008	0.004	-0.104
HMI-013-05	-0.148	0.004	-0.003	-0.148
HMI-013-06	-0.083	0.010	0.010	-0.063
HMI-013-07	-0.017	0.031	0.021	0.035

Results – Mixed, Inter., & Fast Configurations

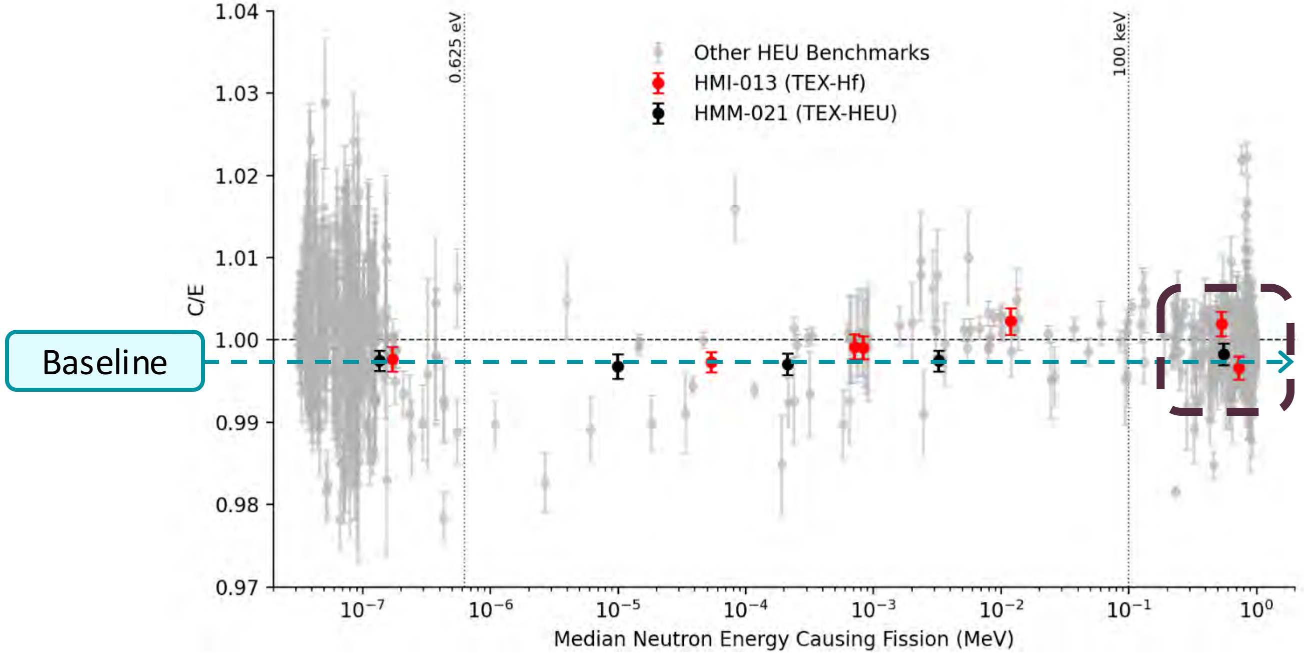
- As sensitivity to inelastic scattering in TEX-Hf increases, there is increasing disagreement with the TEX-HEU baselines



TEX-Hf Case	Sensitivity			
	Capture	Inelastic	Elastic	Total
HMI-013-01	-0.032	0.020	0.011	-0.001
HMI-013-02	-0.062	0.015	0.011	-0.036
HMI-013-03	-0.083	0.011	0.007	-0.065
HMI-013-04	-0.116	0.008	0.004	-0.104
HMI-013-05	-0.148	0.004	-0.003	-0.148
HMI-013-06	-0.083	0.010	0.010	-0.063
HMI-013-07	-0.017	0.031	0.021	0.035

Results – Fast Configurations

- In the fast configurations, there may be compensating effects between the capture, inelastic, and elastic cross sections



TEX-Hf Case	Sensitivity			
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HMI-013-07	-0.017	0.031	0.021	0.035

Conclusions

- TEX-HEU (HEU-MET-MIXED-021) and TEX-Hf (HEU-MET-INTER-013) include twelve benchmark cases now published in the ICSBEP
  - TEX-HEU provides a test bed for future materials (e.g., chlorine)
  - TEX-Hf provides integral experiment validation cases for hafnium which can be interpreted relative to the TEX-HEU baseline cases
- TEX-HEU shows a consistent underprediction in k_{eff} for ENDF/B-VIII.0
- Baseline experiments like TEX-HEU and TEX-Pu are useful when validating materials (e.g., hafnium) as they allow the effects of the material to be interpreted relative to an unperturbed system instead of in isolation

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