IER 517: Molybdenum Critical Experiment Design

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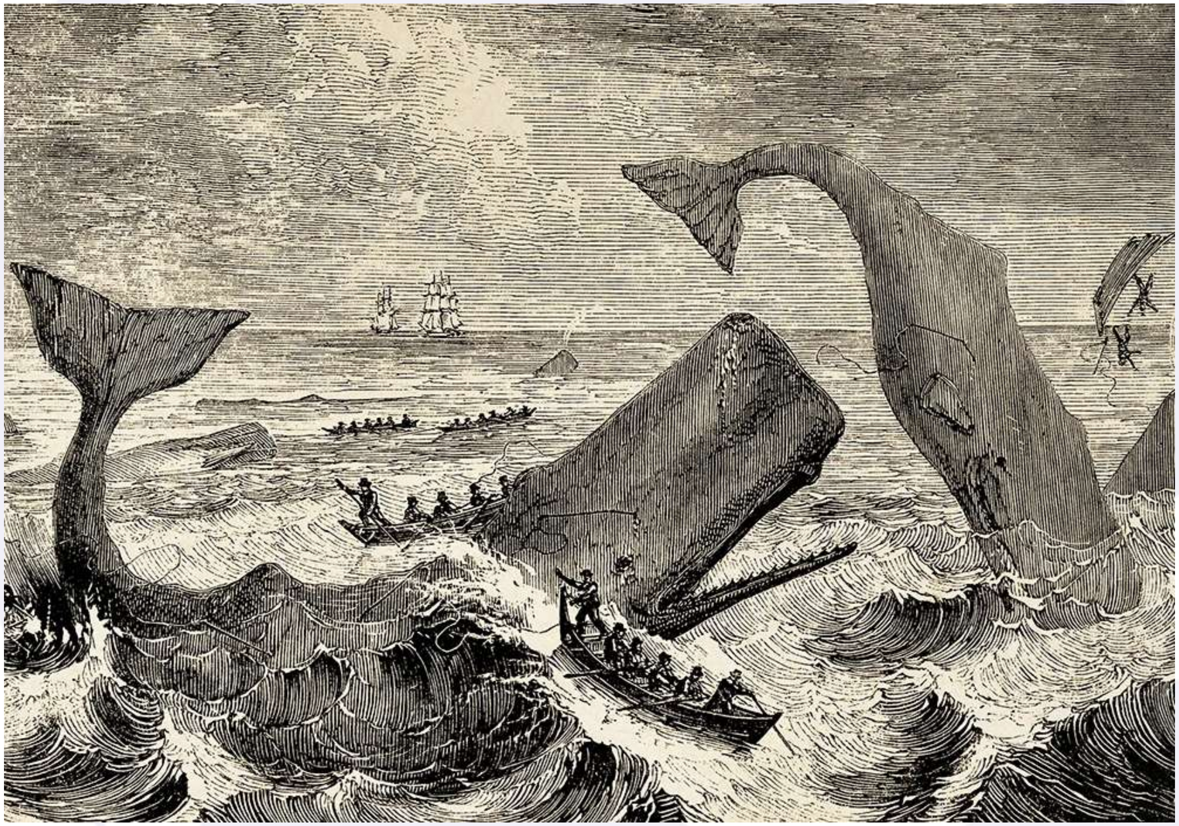
Experiment Name

Molybdenum Optimized Benchmark System Demonstrating Integral Correlations

(MOBY DICK)



Molybdenum in Nuclear

- **In Fuels:** U-Mo metallic fuels are used in new space reactor designs and new research reactor fuels. MITR, MURR, and NBSR reactors plan on converting from different HEU fuels to a U-Mo HALEU fuel [1].

- **In Spent Nuclear Fuel:** ^{95}Mo is one of the 15 main absorbing fission products in irradiated LWR fuel [2]. This makes it important for criticality safety studies in transportation and reprocessing.

- **In Structural Materials:** Molybdenum is found commonly in alloys that make up the structural materials of nuclear reactors such as type 316 SS. Molybdenum helps to improve high temperature performance and corrosion resistance [2].

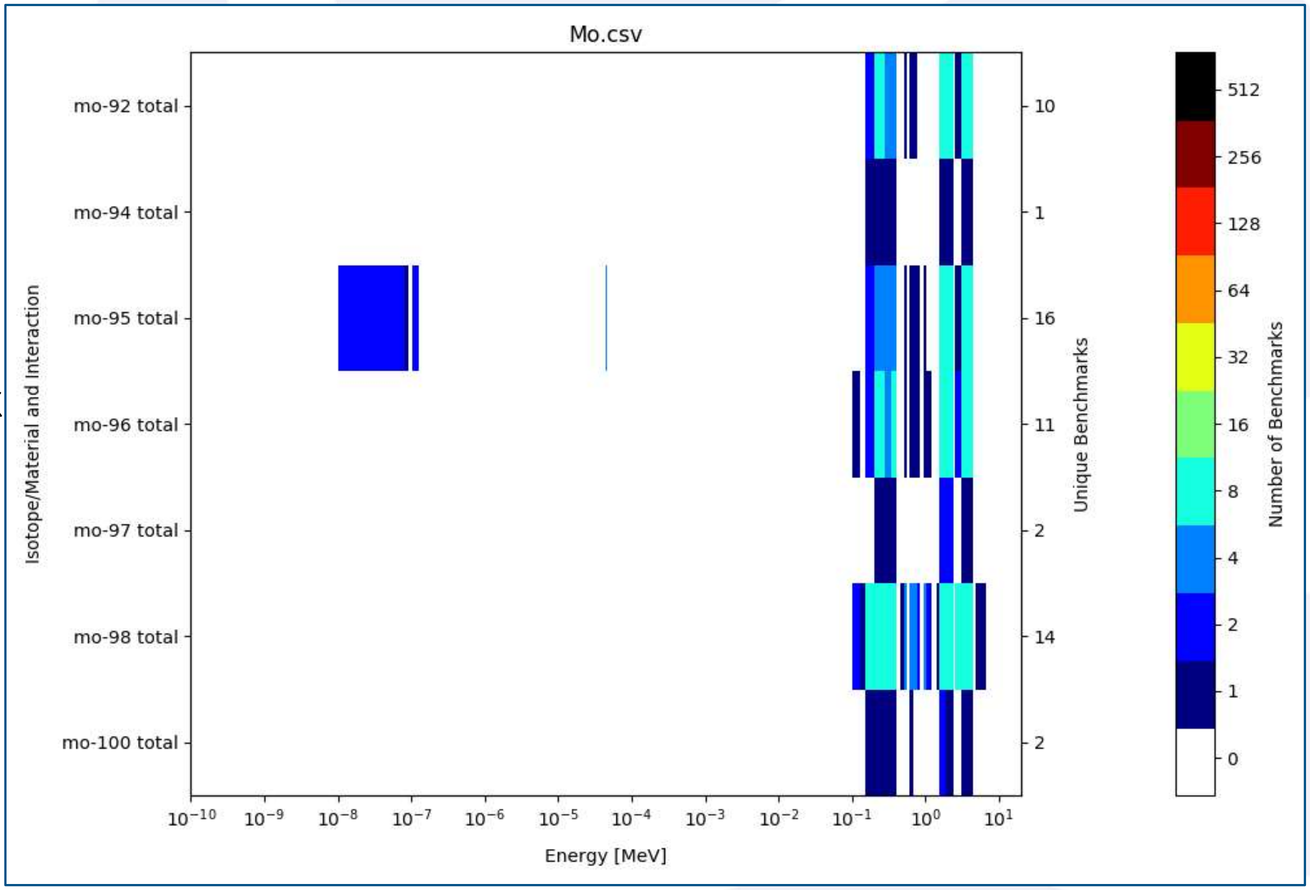
Molybdenum Nuclear Data

- Differential measurements of Molybdenum cross sections in the unresolved resonance region (URR) performed in 2015 at Rensselaer Polytechnic Institute

- Institut de Radioprotection et de Sûreté Nucléaire (IRSN) and the Japan Atomic Energy Agency (JAEA) are currently performing differential Molybdenum cross section measurements and the J-PARC facility in Japan

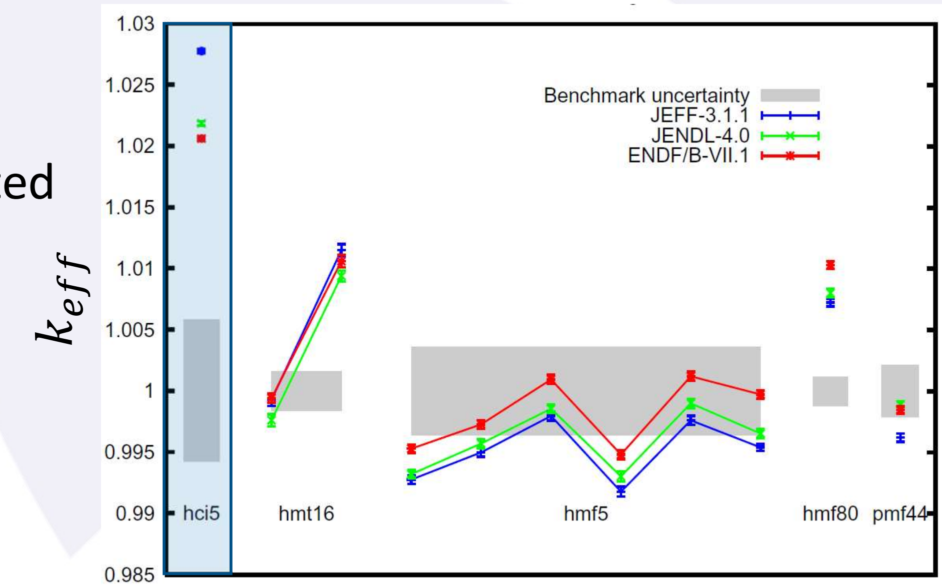
- There are few benchmarks sensitive to Molybdenum

- Only one intermediate Molybdenum benchmark in the ICSBEP Handbook

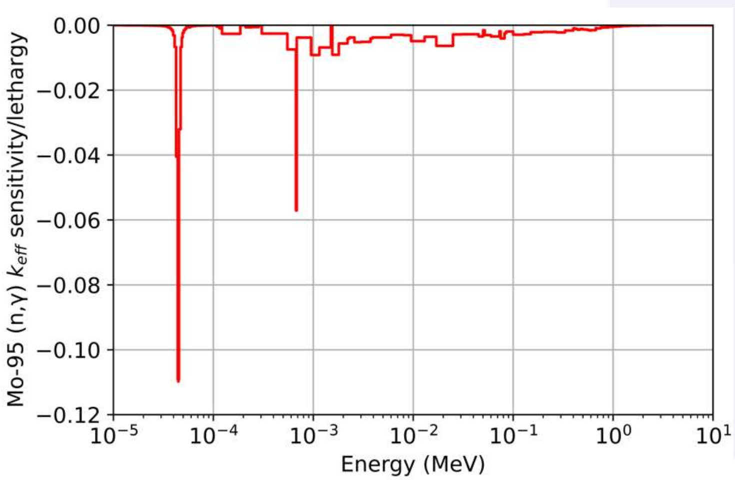


Existing Molybdenum Benchmarks

- Only one intermediate molybdenum sensitive benchmark in the ISCBEP handbook, HEU-COMP-INTER-005
- Conducted in Russia in the 1980's, accepted to handbook in 2002
- Large bias between computational and experimental results



ICSBEP benchmarks containing Mo



HEU-COMP-INTER-005 ^{95}Mo(n,γ) sensitivity

Category	N	ENDF/B-VII.1	JENDL-4.0	JEFF-3.1.1
heu-comp-inter	1	2060	2185	2774
heu-met-therm	2	503	353	541
heu-met-fast	7	-5	-227	-316
pu-met-fast	1	-152	-113	-378

Average values for C/E - 1 (in pcm) for benchmarks containing Mo using MCNP6.1. N is the number of benchmarks in the category.

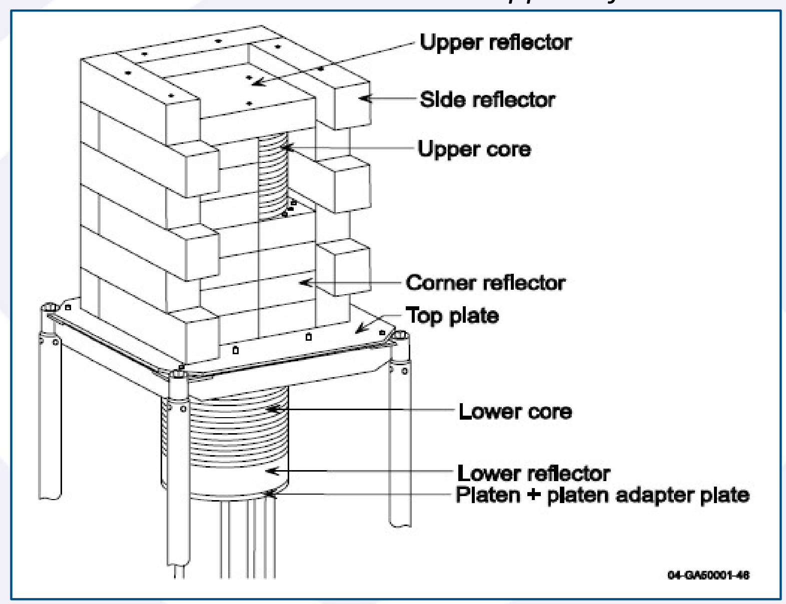
HEU/Molybdenum Experimental Design

- Comet vertical lift assembly
- Core will consist of stacking Jemima plates (HEU metal, 21” diameter), molybdenum plates, and moderator plates.
- Varying the thicknesses of the molybdenum and moderating plates will be used to shape the energy spectrum of the system
- Unit geometries repeated until criticality is reached

Unmoderated unit geometry

Moderated unit geometry

COMET with radial and axial copper reflector



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HEU Configurations

Fast (x1)

MOLYBDENUM
FUEL
MOLYBDENUM

Case 1
- "Fast Case"
- Unmoderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in fast range (>100 keV)

Intermediate (x2)

MOLYBDENUM
MODERATOR
FUEL
MODERATOR
MOLYBDENUM

Case 2
- "URR Case"
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in URR (2 keV – 200 keV)

Case 3
- "Epithermal Case"
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in epithermal range (0.625 eV – 2 keV)

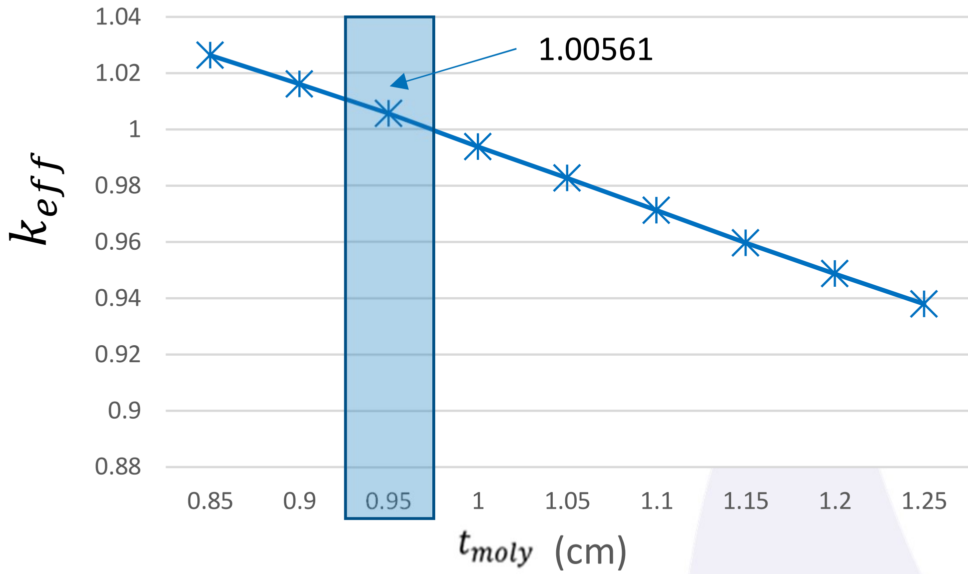
Thermal (x1)

MOLYBDENUM
MODERATOR
FUEL
MODERATOR
MOLYBDENUM

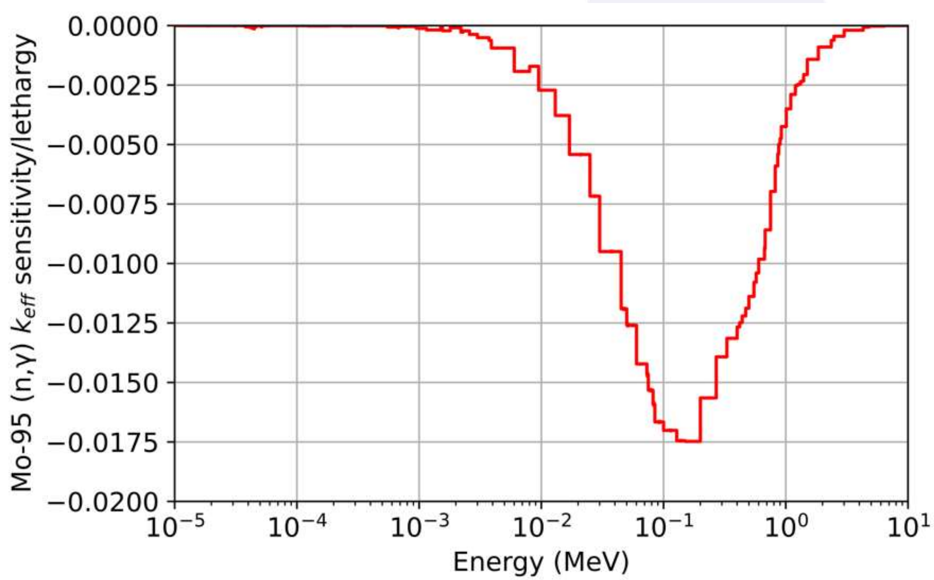
Case 4
- "Thermal Case"
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in thermal range (<0.625 eV)

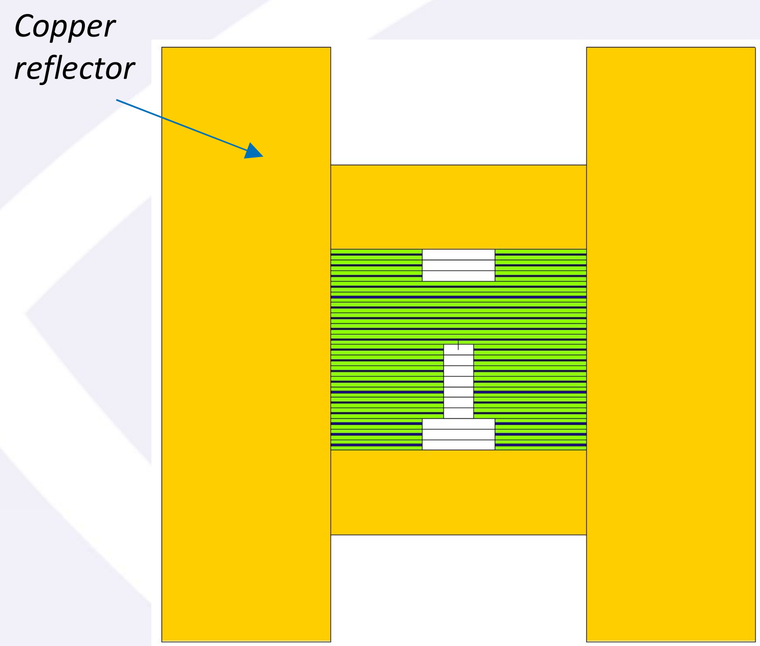
Energy

Case 1 – Fast Case (>100 keV)



Case 1 Unit Geometry





Case 1 Geometry (20 units)

k_{eff} of various configurations (2 keV – 200 keV)

Alumina

Alumina Thickness (cm) \ Molybdenum Thickness (cm)	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00	1.05
1.20	**0.9972**	0.9824	0.9683	0.9549	0.9417	0.9287	0.9162	0.9039	0.8925	0.8813
1.10	**1.0046**	**0.9901**	0.9758	0.9626	0.9496	0.9368	0.9244	0.912	0.8995	0.8884
1.00	1.0128	**0.9992**	0.9844	0.9712	0.9568	0.9444	0.932	0.9198	0.9081	0.8961
0.90	1.022	**1.0073**	**0.9929**	0.9796	0.9657	0.9532	0.9398	0.9273	0.9157	0.9036
0.80	1.0295	1.0155	**1.0015**	0.9879	0.9745	0.9612	0.9489	0.9356	0.9237	0.912
0.70	1.0389	1.025	1.0108	**0.9972**	0.9835	0.9702	0.9578	0.9452	0.9324	0.92
0.60	1.0481	1.0331	1.0201	**1.0055**	**0.9925**	0.9794	0.9665	0.9541	0.9407	0.9292
0.50	1.0553	1.0421	1.0288	1.0153	**1.0018**	0.9895	0.976	0.9633	0.9512	0.939
0.40	1.0635	1.0507	1.0372	1.0239	1.0115	**0.9979**	0.9853	0.9728	0.9601	0.9478
0.30	1.0705	1.0581	1.0455	1.0322	1.0194	**1.0067**	**0.9948**	0.9815	0.9696	0.9572

Beryllium

Beryllium Thickness (cm) \ Molybdenum Thickness (cm)	0.85	0.90	0.95	1.00	1.05	1.10	1.15	1.20	1.25	1.30
1.30	1.0511	1.0358	1.0224	**1.0089**	**0.9951**	0.9818	0.9689	0.9568	0.9442	0.9321
1.20	1.0499	1.035	1.0207	**1.0065**	**0.9932**	0.9807	0.9673	0.9547	0.9426	0.9305
1.10	1.0475	1.0333	1.0184	**1.005**	**0.9909**	0.978	0.9656	0.9532	0.9401	0.9285
1.00	1.0467	1.0316	1.0168	**1.0024**	0.9895	0.9759	0.9632	0.9496	0.9379	0.9257
0.90	1.0443	1.029	1.0153	**1.0003**	0.9862	0.9735	0.9602	0.9482	0.9359	0.9235
0.80	1.0421	1.027	1.0122	**0.9979**	0.9842	0.9709	0.9581	0.9452	0.9329	0.9207
0.70	1.0401	1.0248	1.0101	**0.9959**	0.982	0.9686	0.9549	0.9424	0.9308	0.9185
0.60	1.0369	1.0224	**1.0077**	**0.994**	0.9802	0.9665	0.9533	0.9411	0.9281	0.9157
0.50	1.0348	1.0205	**1.0055**	**0.9921**	0.9776	0.9642	0.951	0.9387	0.9263	0.9143
0.40	1.0348	1.0189	**1.0045**	0.9899	0.9762	0.963	0.9502	0.9374	0.9256	0.9137

Polyethylene

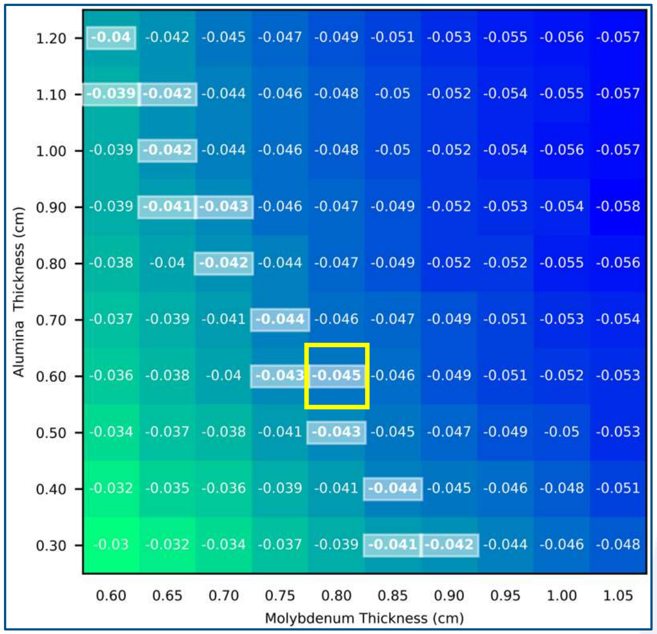
Polyethylene Thickness (cm) \ Molybdenum Thickness (cm)	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40	2.60	2.80
1.00	1.2348	1.1939	1.156	1.1216	1.0888	1.0594	1.0324	**1.0064**	0.9834	0.962
0.90	1.234	1.1917	1.1535	1.1179	1.0845	1.0543	1.0256	**0.9986**	0.9752	0.9525
0.80	1.2285	1.1855	1.1467	1.1109	1.0772	1.0453	1.0158	0.9891	0.9636	0.9406
0.70	1.2193	1.1756	1.136	1.099	1.0651	1.0329	**1.002**	0.9744	0.9485	0.9239
0.60	1.2055	1.1612	1.1204	1.0834	1.0485	1.0153	0.985	0.9553	0.9283	0.904
0.50	1.1855	1.1409	1.0998	1.0621	1.0262	**0.9922**	0.9618	0.932	0.9032	0.8775
0.40	1.1588	1.1134	1.0717	1.0332	**0.9967**	0.9635	0.9315	0.9008	0.8726	0.8454
0.30	1.1241	1.0784	1.0364	**0.997**	0.9592	0.9251	0.8933	0.8622	0.8326	0.8066
0.20	1.0813	1.0347	**0.9915**	0.9514	0.914	0.8789	0.8465	0.8153	0.7861	0.7585
0.10	1.0311	0.9839	0.9394	0.8983	0.8602	0.8254	0.7925	0.7612	0.7323	0.7052

Teflon

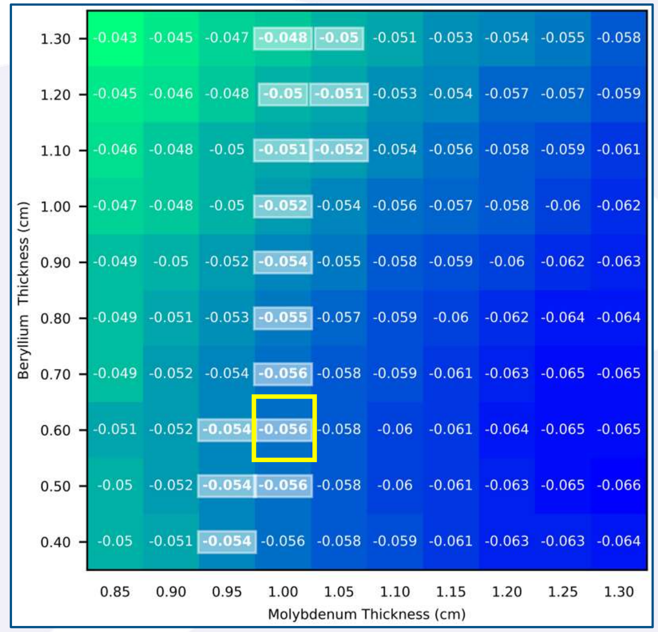
Teflon Thickness (cm) \ Molybdenum Thickness (cm)	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
2.50	0.9774	0.9461	0.9167	0.8897	0.8639	0.8408	0.8183	0.7968	0.7776	0.7608
2.25	**1.0002**	0.9697	0.9406	0.9123	0.8868	0.8617	0.8383	0.8166	0.7958	0.7767
2.00	1.0222	**0.9916**	0.9635	0.9364	0.9098	0.8849	0.8608	0.8382	0.8165	0.7955
1.75	1.0426	1.0126	0.9842	0.958	0.9326	0.9075	0.884	0.8605	0.838	0.8166
1.50	1.063	1.0345	**1.0061**	0.9803	0.9545	0.9295	0.9058	0.883	0.861	0.8383
1.25	1.0844	1.0565	1.0303	**1.0032**	0.9773	0.9526	0.9284	0.906	0.8834	0.8615
1.00	1.1036	1.0796	1.0542	1.0282	**1.0028**	0.9775	0.9533	0.9296	0.9069	0.8844
0.75	1.119	1.1004	1.0777	1.0538	1.0292	**1.0048**	0.9803	0.9554	0.9322	0.9094
0.50	1.1257	1.1144	1.0984	1.0779	1.0554	1.032	**1.0079**	0.9839	0.96	0.937
0.25	1.1257	1.1158	1.1088	1.0961	1.0781	1.0583	1.0357	1.0124	0.9896	0.9658

$S_{k_{eff},\sigma_{URR}}$ of various configurations (2 keV – 200 keV)

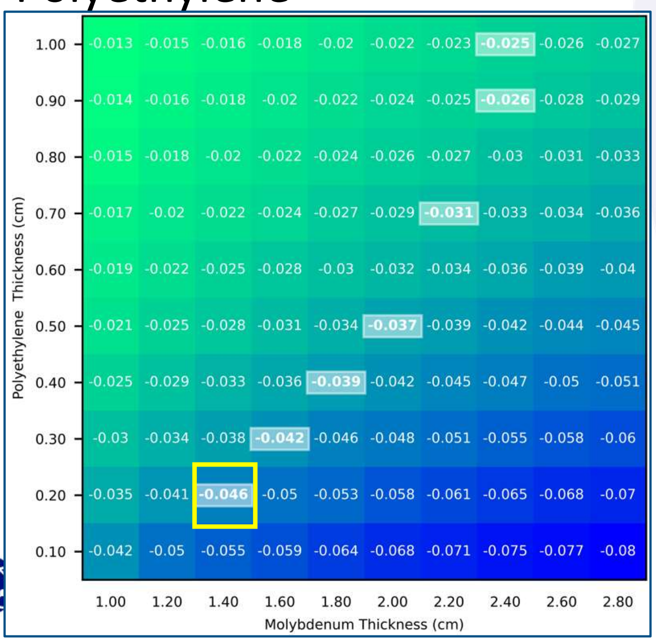
Alumina



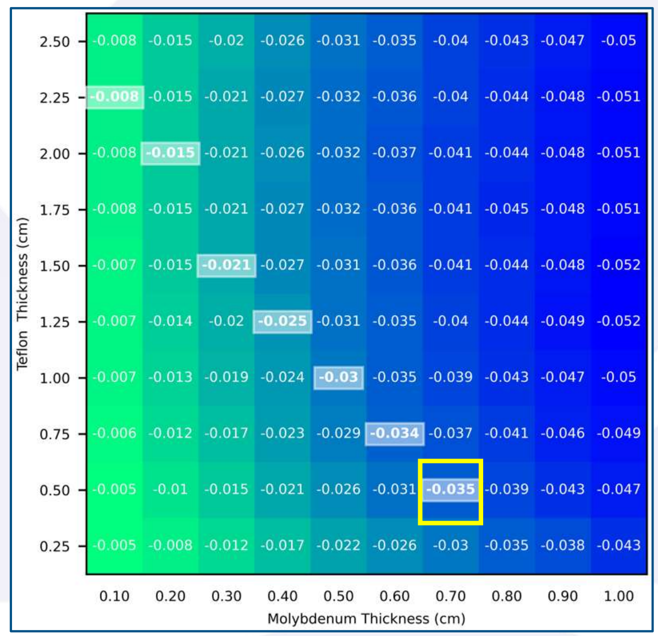
Beryllium



Polyethylene

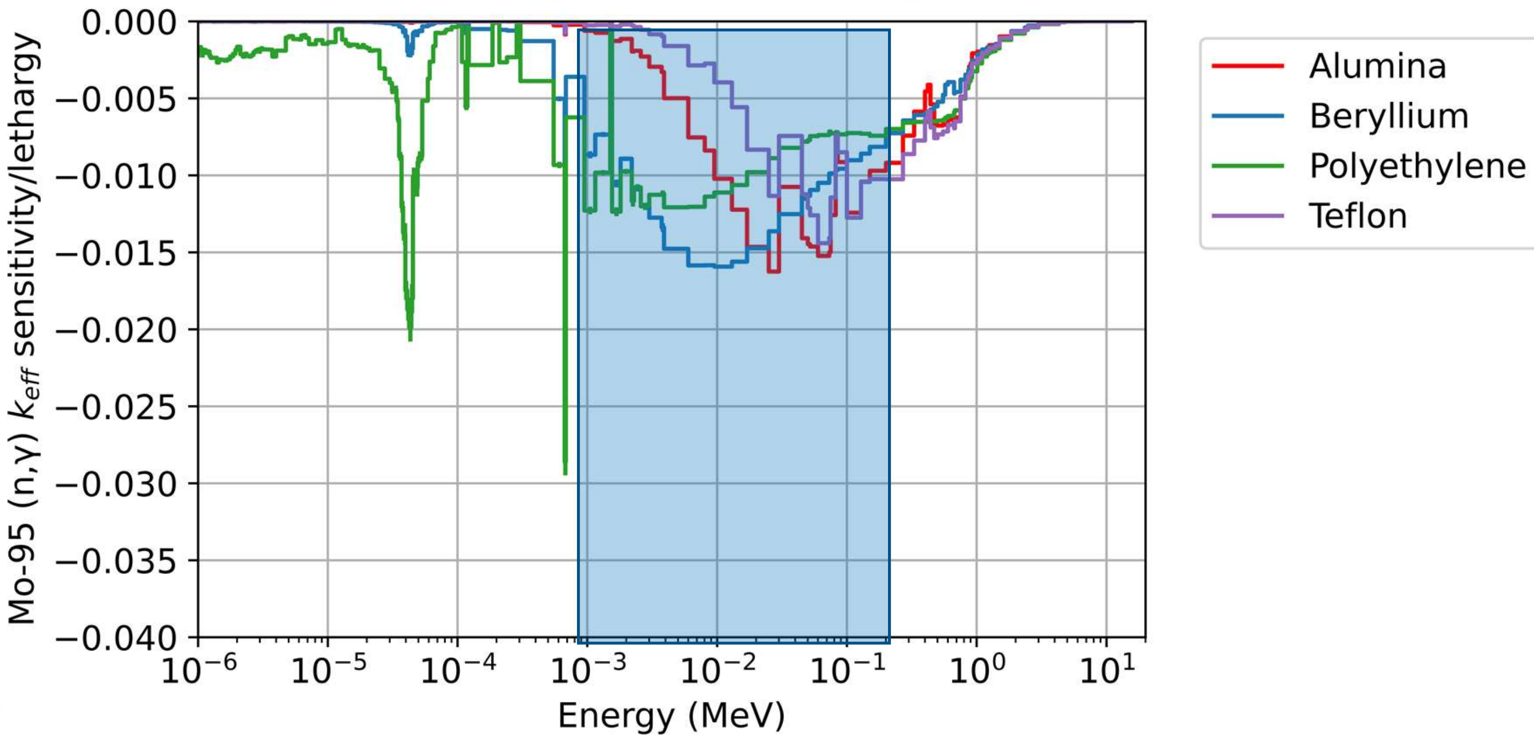


Teflon

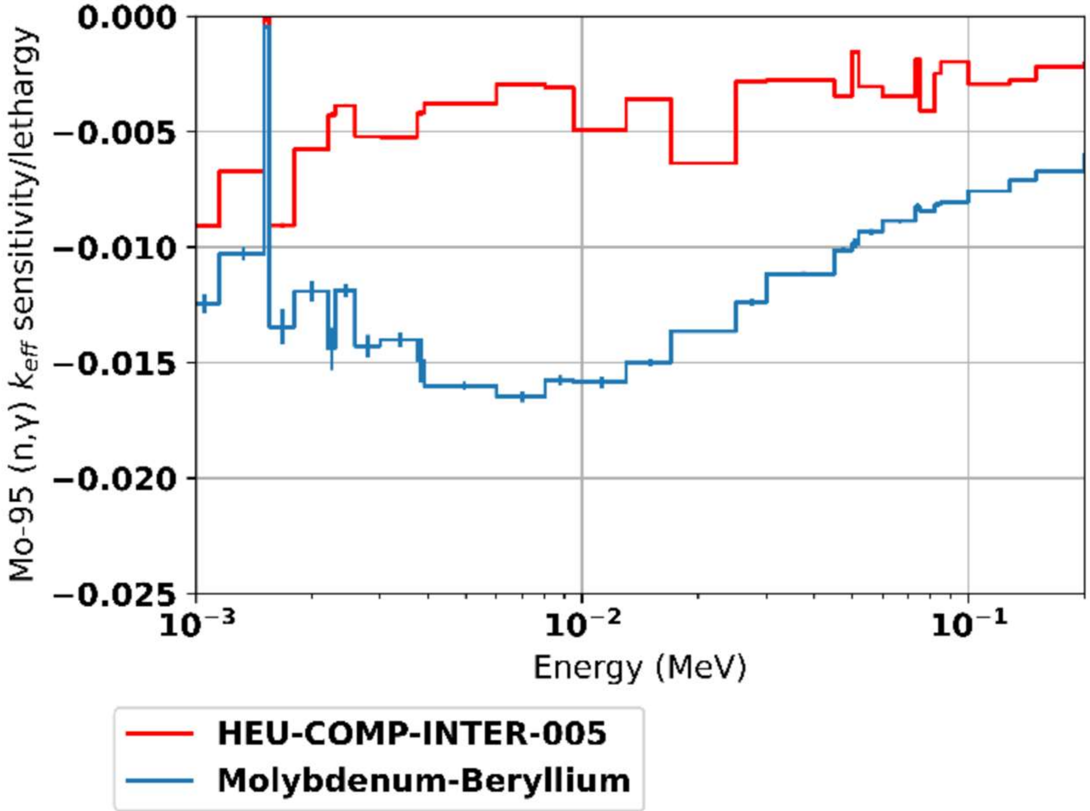


Investigated URR Moderators (2 keV – 200 keV)

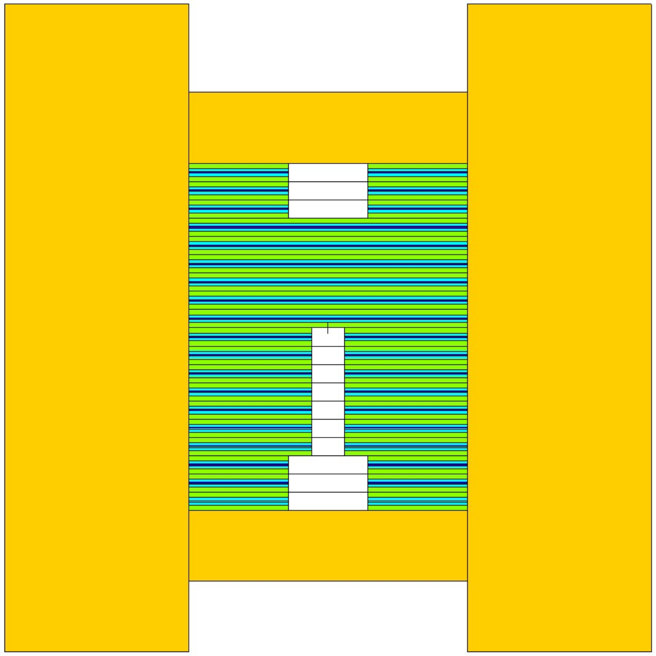
Moderator	Alumina	Beryllium	Polyethylene	Teflon
Formula	Al_2O_3	Be	C_2H_4	C_2F_4
Density $[\frac{g}{cm^3}]$	3.97	1.848	0.93	2.25
$S_{k_{eff},\sigma_{URR}}$	-0.045	-0.056	-0.046	-0.035
$t_{moly}[cm]$	0.8	1.0	1.4	0.7
$t_{mod}[cm]$	0.6	0.6	0.2	0.5



Proposed Case 2 – URR Case (2 keV – 200 keV)



Moderator	Beryllium
Formula	Be
Density $[\frac{g}{cm^3}]$	1.848
$S_{k_{eff},\sigma_{URR}}$	-0.056
$t_{moly}[cm]$	1.0
$t_{mod}[cm]$	0.6



k_{eff} of various configurations (0.625 eV – 2 keV)

Alumina

Alumina Thickness (cm) \ Molybdenum Thickness (cm)	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
3.10	1.0297	**0.9911**	0.9569	0.9267	0.8988	0.8726	0.8487	0.8263	0.8056	0.7857
2.80	1.0515	1.0116	0.9771	0.9459	0.9162	0.8898	0.8649	0.8417	0.8201	0.7995
2.50	1.0732	1.0323	**0.9972**	0.9649	0.9353	0.908	0.8817	0.8576	0.8349	0.8139
2.20	1.0945	1.0535	1.0178	0.9852	0.9546	0.9267	0.9002	0.8756	0.8522	0.8305
1.90	1.1163	1.0752	1.0395	**1.0058**	0.9746	0.9459	0.9193	0.8936	0.87	0.8474
1.60	1.1386	1.0977	1.0611	1.0275	**0.9957**	0.9663	0.9393	0.9136	0.8889	0.8654
1.30	1.159	1.1195	1.0839	1.0501	1.0186	0.9883	0.9605	0.9347	0.9093	0.8858
1.00	1.178	1.1414	1.1077	1.0748	1.0426	1.0128	0.9844	0.9568	0.932	0.9081
0.70	1.1886	1.1586	1.1283	1.0985	1.0679	1.0389	1.0108	0.9835	0.9578	0.9324
0.40	1.1765	1.1604	1.1401	1.1155	1.0903	1.0635	1.0372	1.0115	0.9853	0.9601

Beryllium

Beryllium Thickness (cm) \ Molybdenum Thickness (cm)	0.80	0.85	0.90	0.95	1.00	1.05	1.10	1.15	1.20	1.25
1.75	1.0707	1.056	1.041	1.0283	1.0154	**1.0028**	0.9896	0.9777	0.9658	0.9546
1.65	1.0695	1.0544	1.0404	1.027	1.014	**1.0007**	0.9888	0.9771	0.9647	0.9533
1.55	1.0692	1.054	1.0404	1.0257	1.0126	**0.9992**	0.9868	0.9742	0.9625	0.9509
1.45	1.0674	1.0527	1.0388	1.025	1.0107	**0.9979**	0.9851	0.9724	0.9602	0.9486
1.35	1.0667	1.0519	1.037	1.0231	**1.0095**	**0.9962**	0.9827	0.9706	0.9586	0.9466
1.25	1.0657	1.051	1.0363	1.0215	**1.0078**	**0.9943**	0.9811	0.9692	0.9564	0.9444
1.15	1.0642	1.0485	1.034	1.0197	**1.0049**	**0.9922**	0.9792	0.9661	0.9531	0.9415
1.05	1.0624	1.0474	1.0327	1.0176	**1.0041**	**0.9902**	0.9771	0.9641	0.9517	0.9397
0.95	1.0607	1.0449	1.0304	1.0156	**1.0012**	0.9881	0.975	0.9622	0.9491	0.9369
0.85	1.0587	1.0436	1.0287	1.0136	**0.9989**	0.9858	0.9723	0.9598	0.9464	0.9343

Polyethylene

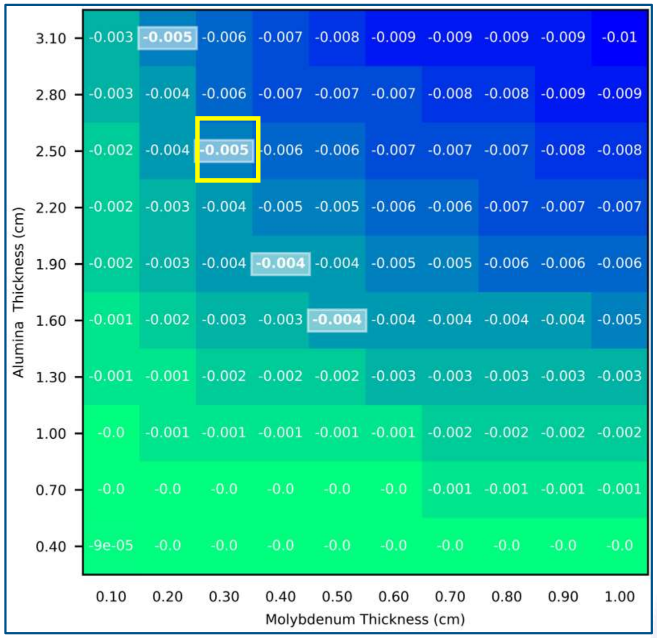
Polyethylene Thickness (cm) \ Molybdenum Thickness (cm)	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40	2.60	2.80
1.00	1.2348	1.1939	1.156	1.1216	1.0888	1.0594	1.0324	**1.0064**	0.9834	0.962
0.90	1.234	1.1917	1.1535	1.1179	1.0845	1.0543	1.0256	**0.9986**	0.9752	0.9525
0.80	1.2285	1.1855	1.1467	1.1109	1.0772	1.0453	1.0158	0.9891	0.9636	0.9406
0.70	1.2193	1.1756	1.136	1.099	1.0651	1.0329	**1.002**	0.9744	0.9485	0.9239
0.60	1.2055	1.1612	1.1204	1.0834	1.0485	1.0153	0.985	0.9553	0.9283	0.904
0.50	1.1855	1.1409	1.0998	1.0621	1.0262	**0.9922**	0.9618	0.932	0.9032	0.8775
0.40	1.1588	1.1134	1.0717	1.0332	**0.9967**	0.9635	0.9315	0.9008	0.8726	0.8454
0.30	1.1141	1.0784	1.0364	**0.997**	0.9592	0.9251	0.8933	0.8622	0.8326	0.8066
0.20	1.0813	1.0347	**0.9915**	0.9514	0.914	0.8789	0.8465	0.8153	0.7861	0.7585
0.10	1.0311	0.9839	0.9394	0.8983	0.8602	0.8254	0.7925	0.7612	0.7323	0.7052

Teflon

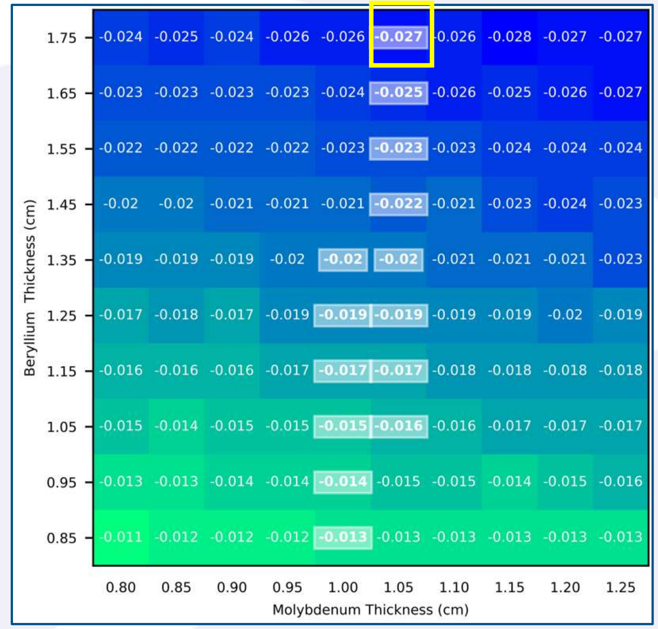
Teflon Thickness (cm) \ Molybdenum Thickness (cm)	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
2.50	0.9774	0.9461	0.9167	0.8897	0.8639	0.8408	0.8183	0.7968	0.7776	0.7608
2.25	**1.0002**	0.9697	0.9406	0.9123	0.8868	0.8617	0.8383	0.8166	0.7958	0.7767
2.00	1.0222	**0.9916**	0.9635	0.9364	0.9098	0.8849	0.8608	0.8382	0.8165	0.7955
1.75	1.0426	1.0126	0.9842	0.958	0.9326	0.9075	0.884	0.8605	0.838	0.8166
1.50	1.063	1.0345	**1.0061**	0.9803	0.9545	0.9295	0.9058	0.883	0.861	0.8383
1.25	1.0844	1.0565	1.0303	**1.0032**	0.9773	0.9526	0.9284	0.906	0.8834	0.8615
1.00	1.1036	1.0796	1.0542	1.0282	**1.0028**	0.9775	0.9533	0.9296	0.9069	0.8844
0.75	1.119	1.1004	1.0777	1.0538	1.0292	**1.0048**	0.9803	0.9554	0.9322	0.9094
0.50	1.1257	1.1144	1.0984	1.0779	1.0554	1.032	**1.0079**	0.9839	0.96	0.937
0.25	1.1257	1.1158	1.1088	1.0961	1.0781	1.0583	1.0357	1.0124	0.9896	0.9658

$S_{k_{eff},\sigma_{Epithermal}}$ of various configurations (0.625 eV – 2 keV)

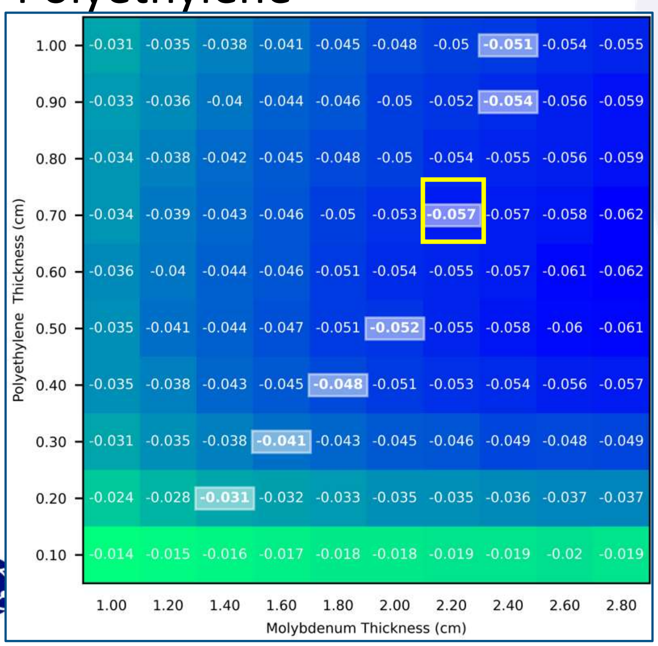
Alumina



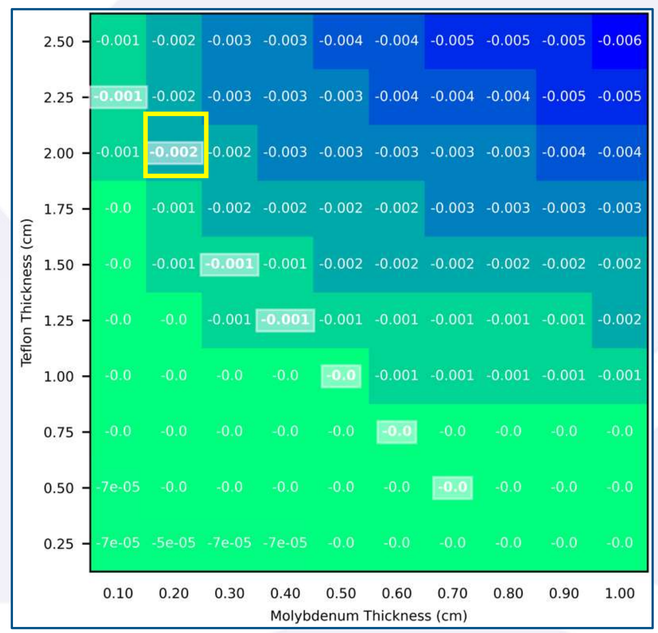
Beryllium



Polyethylene

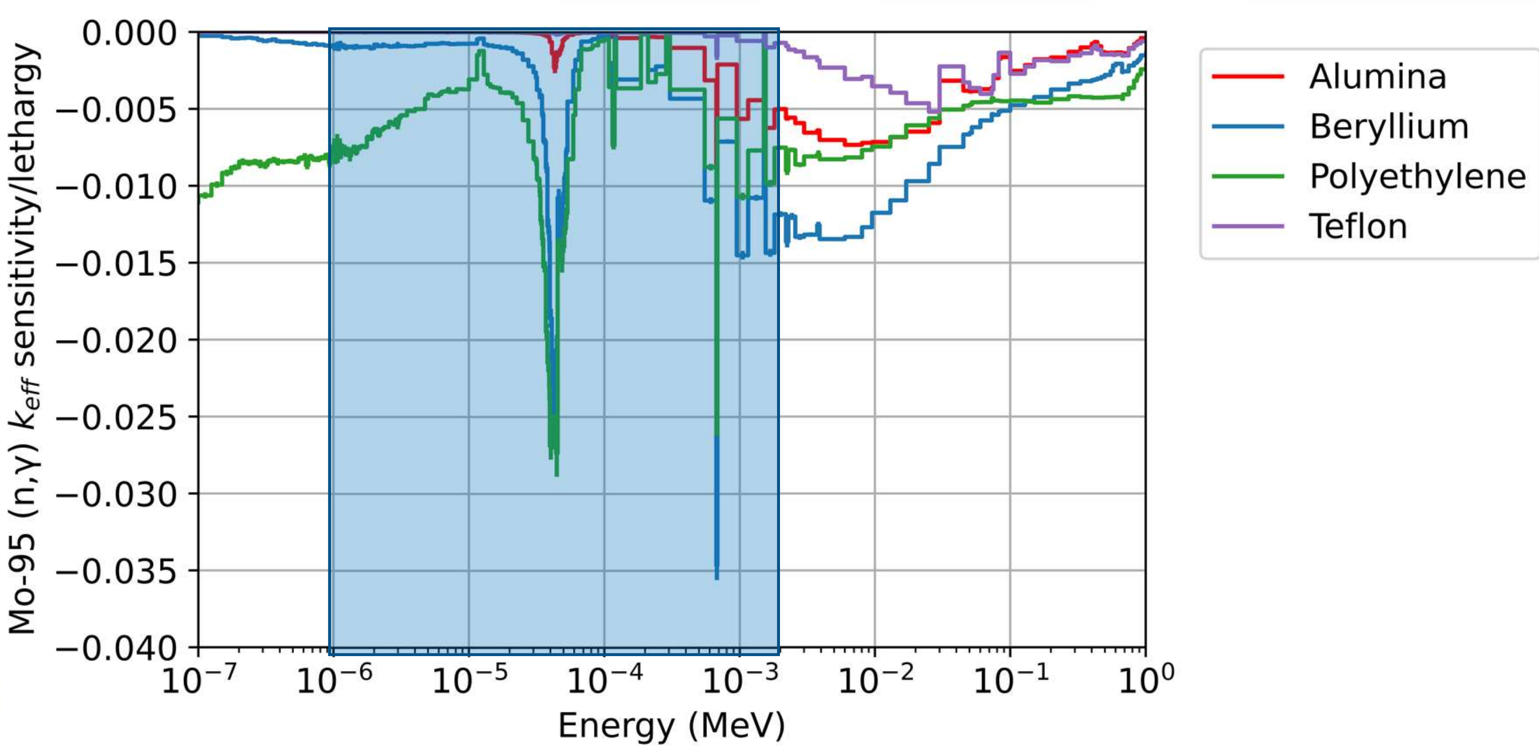


Teflon

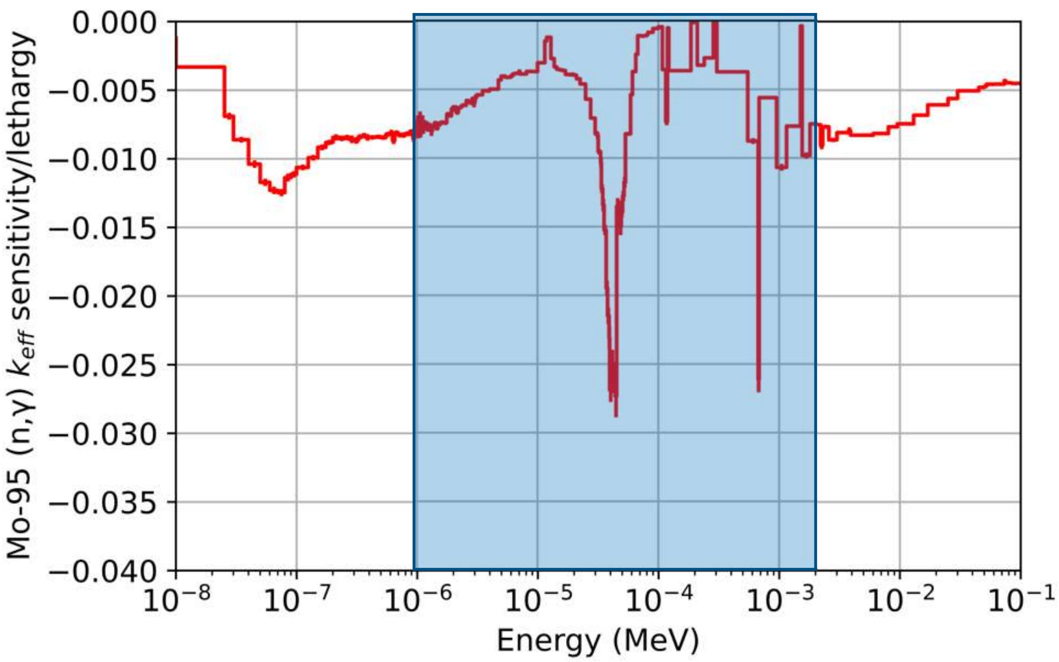


Investigated Epithermal Moderators (0.625 eV – 2 keV)

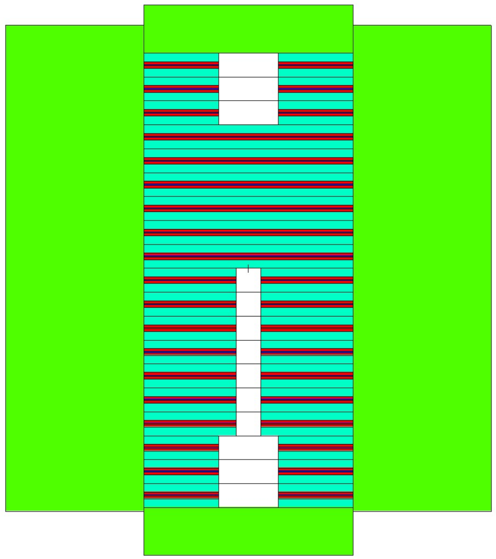
Moderator	Alumina	Beryllium	Polyethylene	Teflon
Formula	Al_2O_3	Be	C_2H_4	C_2F_4
Density $[\frac{g}{cm^3}]$	3.97	1.848	0.93	2.25
$S_{k_{eff},\sigma_{Epithermal}}$	-0.005	-0.027	-0.057	-0.002
$t_{moly}[cm]$	0.3	1.05	2.2	0.2
$t_{mod}[cm]$	2.5	1.75	0.7	2.0



Proposed Case 3 – Epithermal Case (0.625 eV – 2 keV)



Moderator	Polyethylene
Formula	C_2H_4
Density $[\frac{g}{cm^3}]$	0.93
$S_{k_{eff},\sigma_{Epithermal}}$	-0.057
$t_{moly}[cm]$	2.2
$t_{mod}[cm]$	0.7



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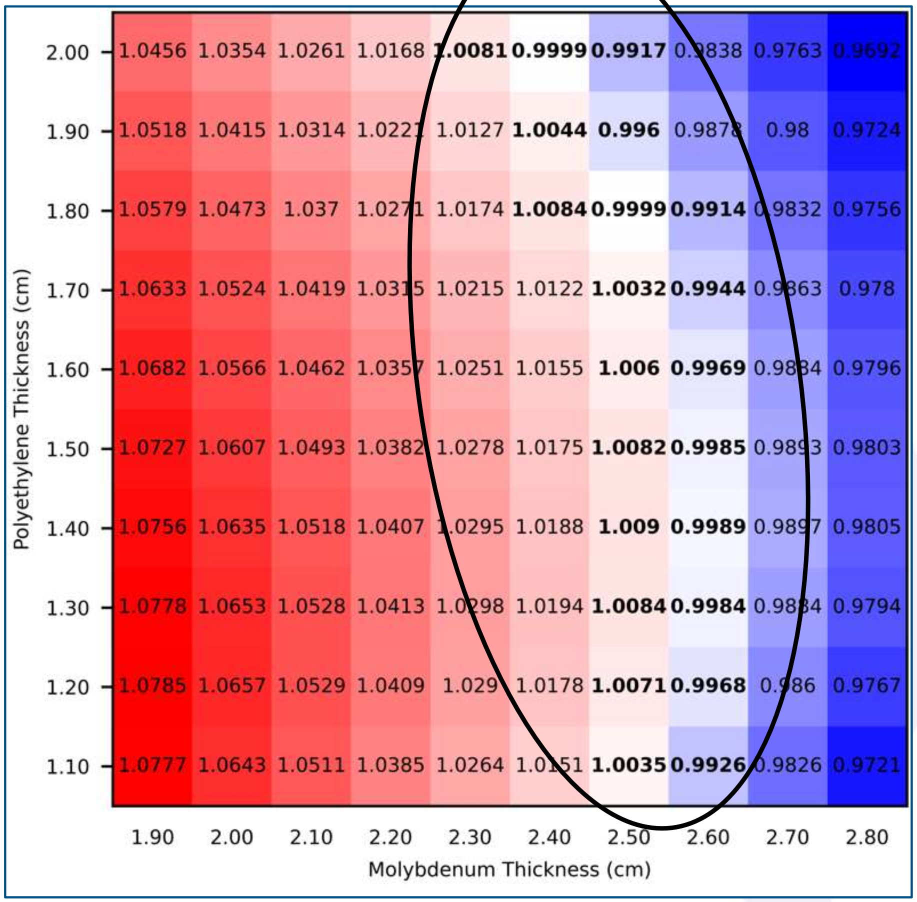
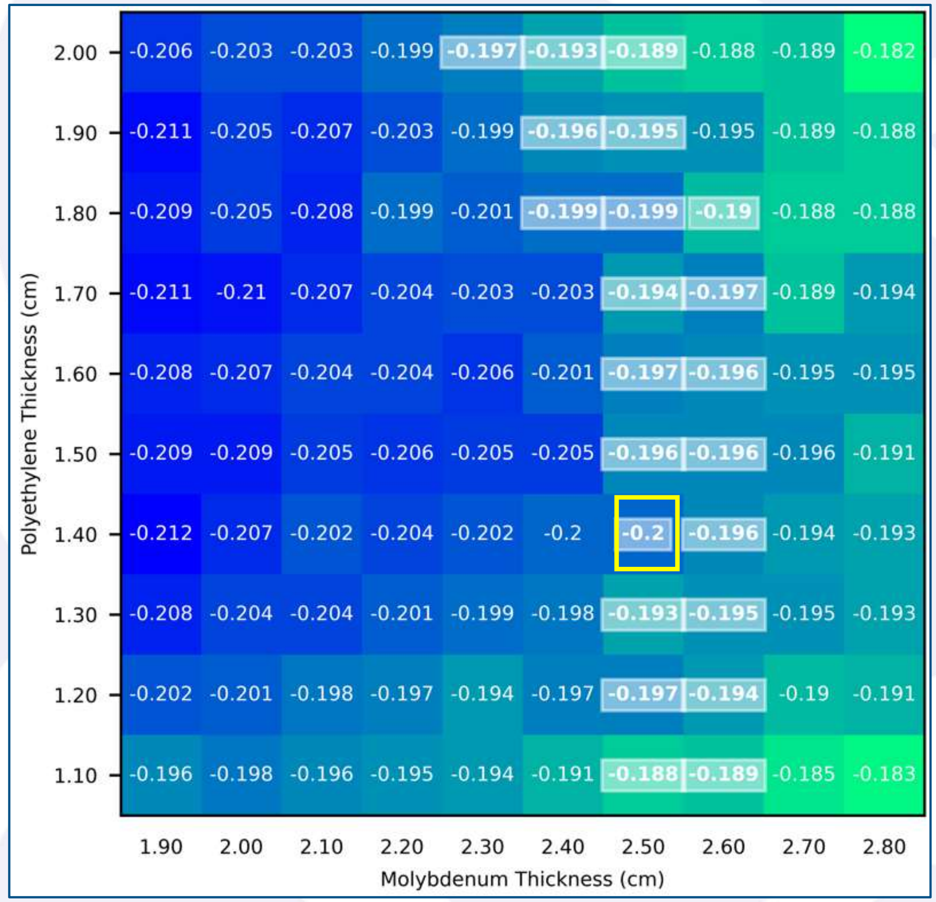
Thermal polyethylene configurations (<0.625 eV)

k_{eff}



$S_{k_{eff},\sigma_{Thermal}}$



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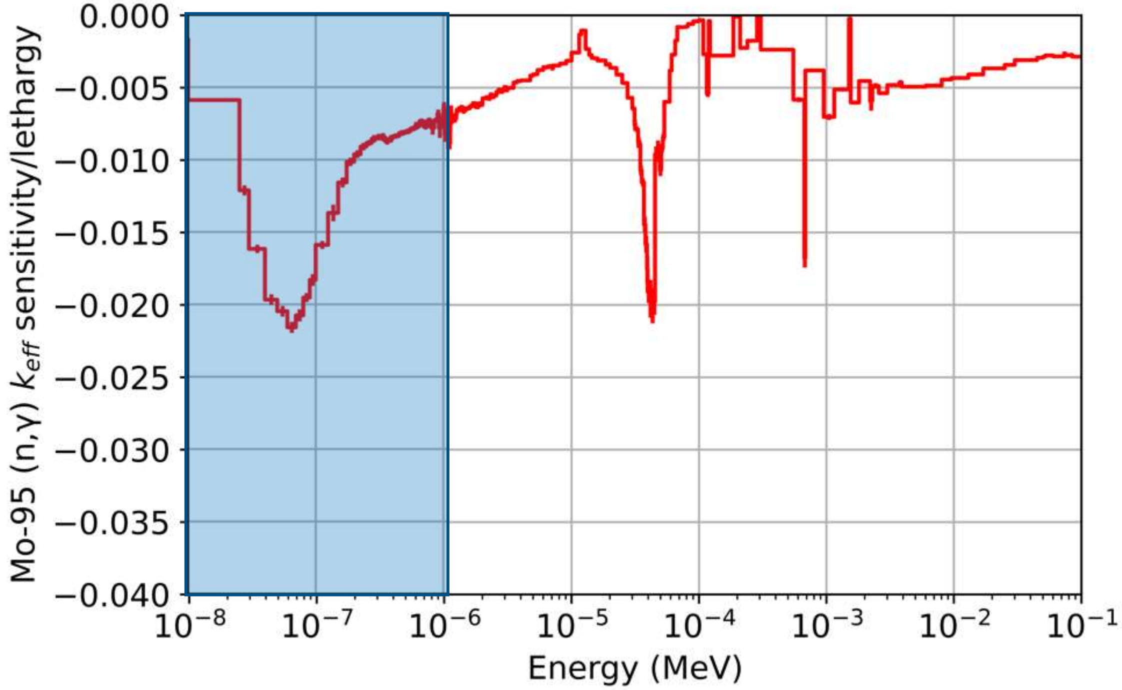
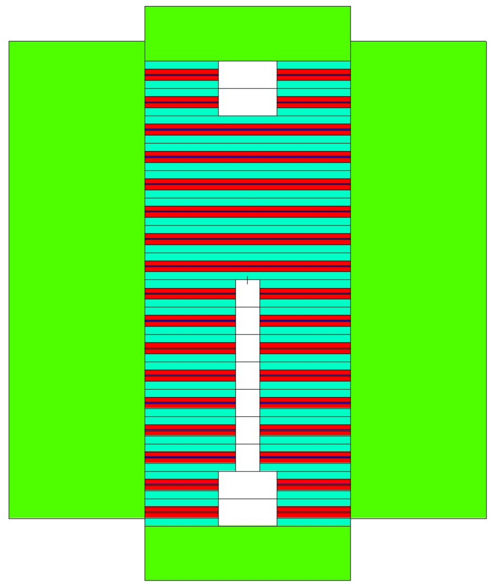
Proposed Case 4 – Thermal Case (<0.625 eV)



Moderator	Polyethylene
Formula	C_2H_4
Density [$\frac{g}{cm^3}$]	0.93
$S_{k_{eff},\sigma_{Thermal}}$	-0.2
$t_{moly}[cm]$	2.5
$t_{mod}[cm]$	1.4



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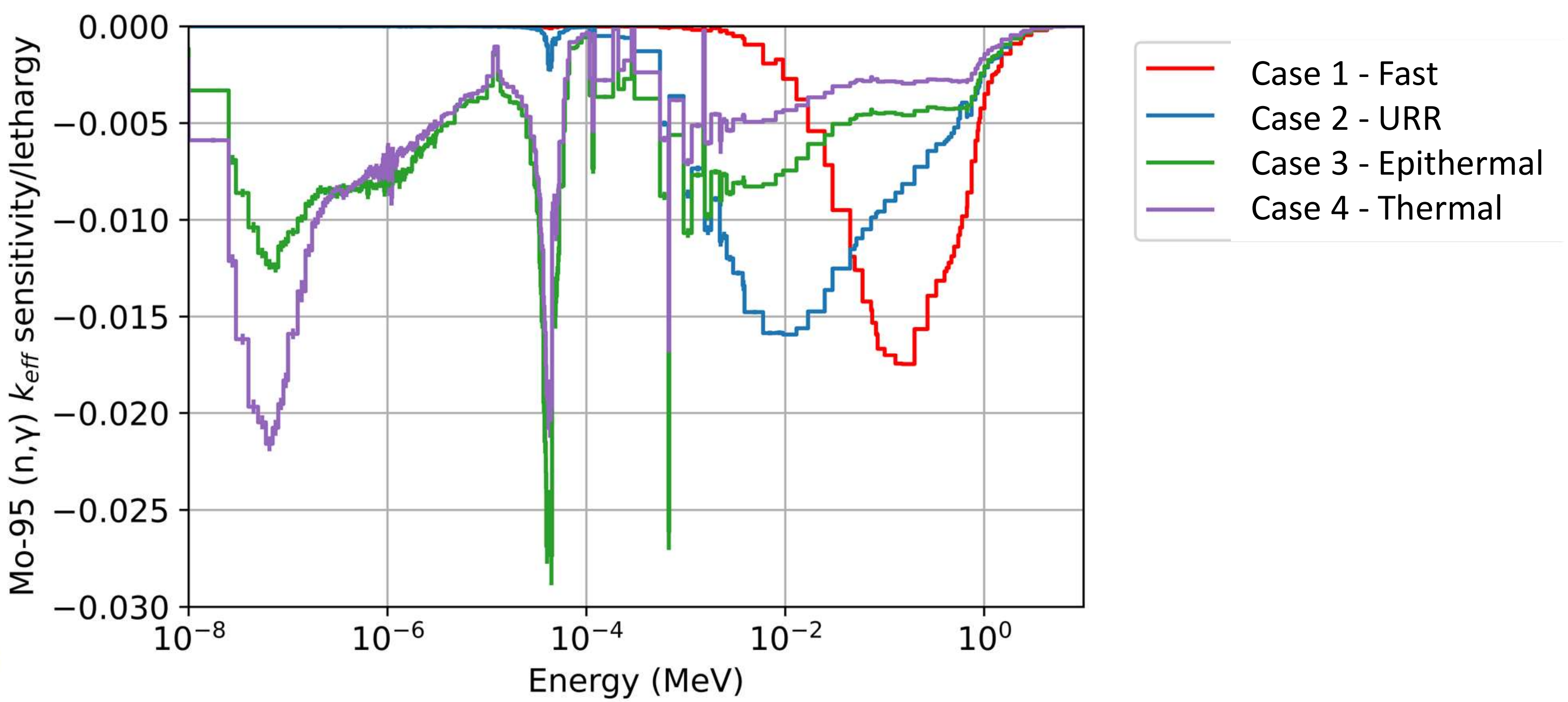
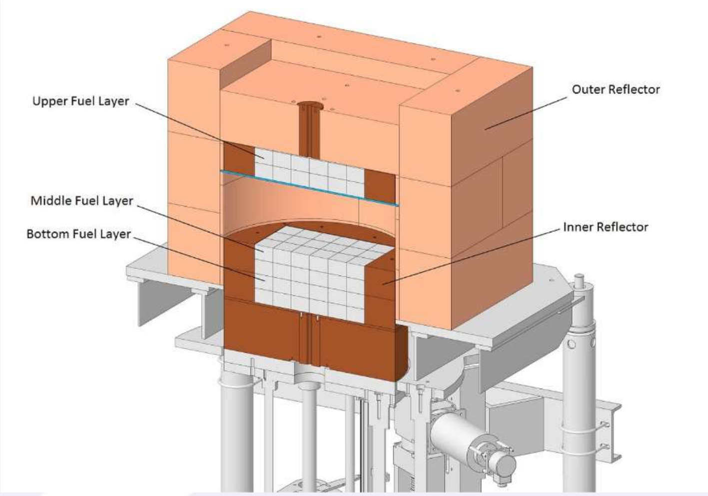
HEU Review

	Case 1 "Fast"	Case 2 "URR"	Case 3 "Epithermal'	Case 4 "Thermal"
Moderator	N/A	Beryllium or Polyethylene	Polyethylene	Polyethylene
$t_{moly}[cm]$	0.95	1.0	2.2	2.5
$t_{mod}[cm]$	N/A	0.6	0.7	1.4
Optimized Energy Range	>100 keV	2 keV – 200 keV	0.626 eV – 2 keV	< 0.625 eV
Differential Data	RPI	RPI	J-PARC	J-PARC

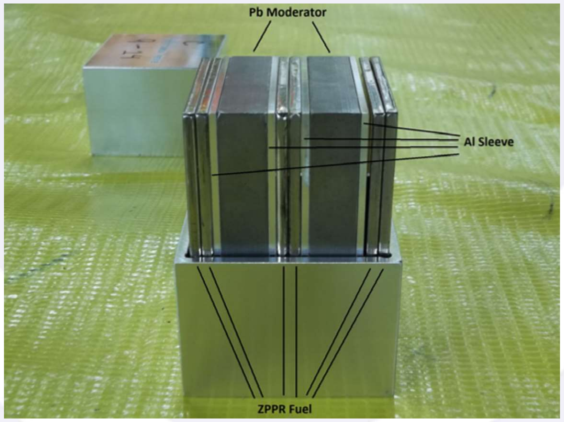


Present Work - Plutonium

- Same goals as HEU configurations, maximize ^{95}Mo(n,γ) sensitivity in :
  - Fast, >100 keV
  - URR, 2 keV – 200 keV
  - Epithermal, 0.625 eV – 2 keV
  - Thermal, <0.625 eV
- Using the ^{239}Pu ZPPR plates as fuel



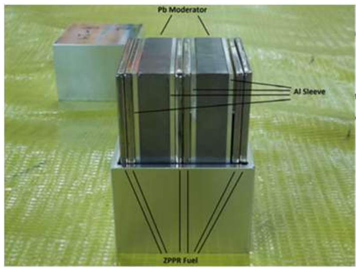
Jupiter Pu/Pb experiment on COMET

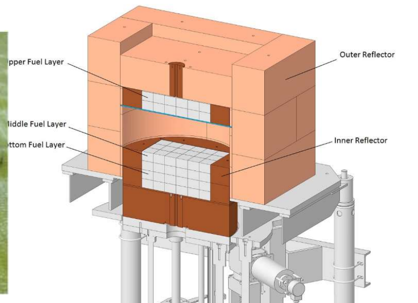


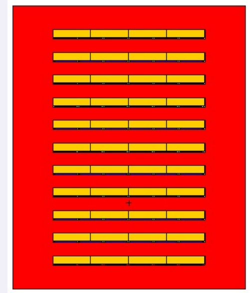
Fuel unit

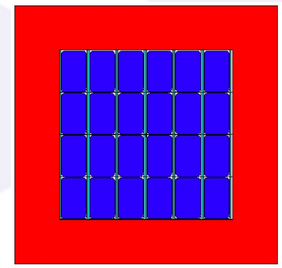
Present Work - Plutonium Configurations

Fast (x1) Intermediate (x2) Thermal (x1)









Case 1
- "Fast Case"
- Similar to Jupiter
- Maximize ^{95}Mo(n,γ) sensitivity in fast range (>100 keV)

Case 2
- "URR Case"
- Similar to Jupiter
- Maximize ^{95}Mo(n,γ) sensitivity in URR (2 keV – 200 keV)

Case 3
- "Epithermal Case"
- Moderated and reflected
- Maximize ^{95}Mo(n,γ) sensitivity in epithermal range (0.625 eV – 2 keV)

Case 4
- "Thermal Case"
- Polyethylene moderated and reflected
- Maximize ^{95}Mo(n,γ) sensitivity in thermal range (<0.625 eV)

Energy

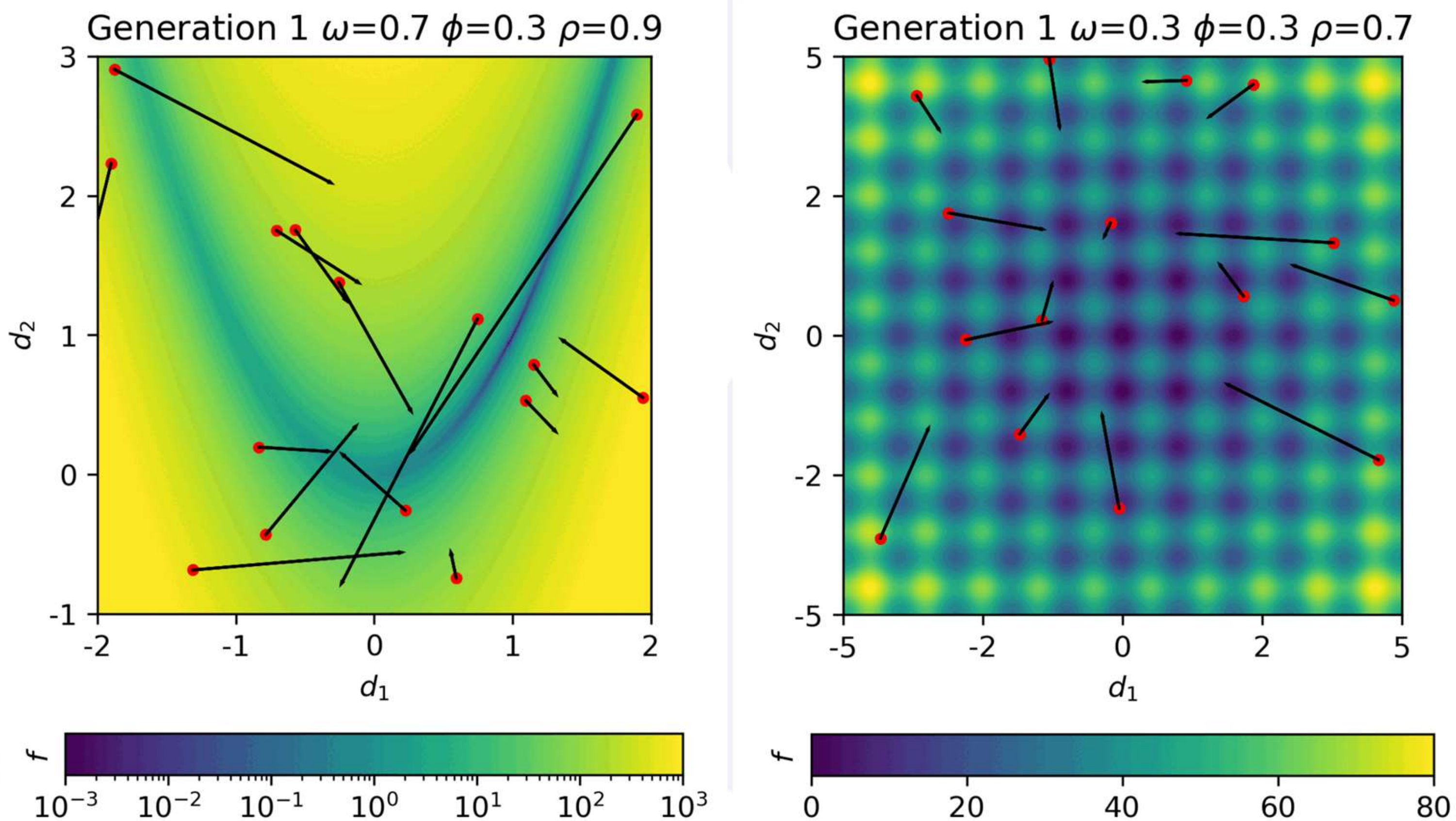
Particle Swarm Optimization (PSO)

- PSO algorithms are used to locate global maxima or minima of functions without using its gradient
- A PSO-MCNP coupled algorithm was developed to aid in the design of critical experiments
- This new method is being used to design the Plutonium cases of this IER

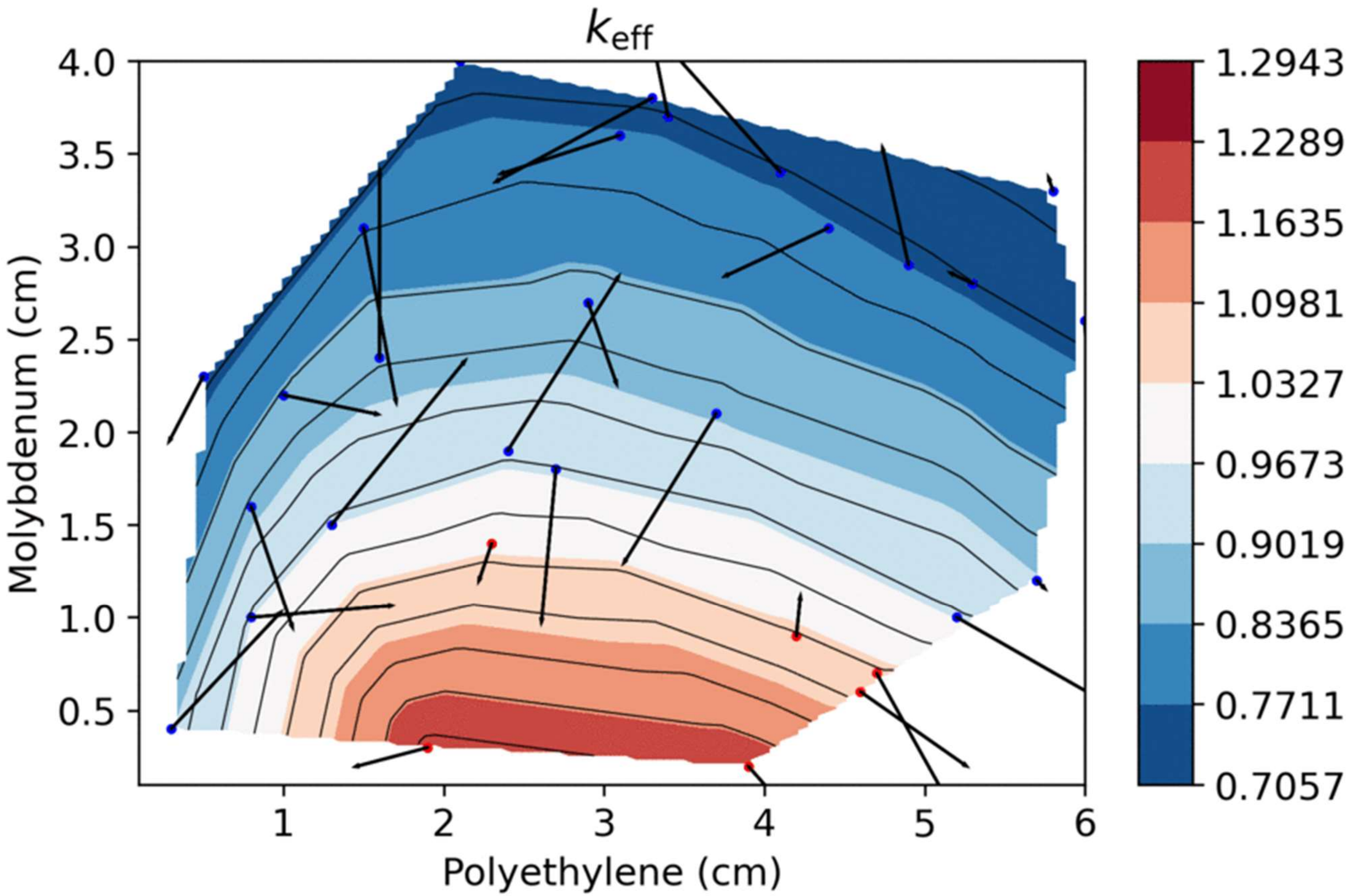
Analytical PSO Examples

For each dimension d of particle i

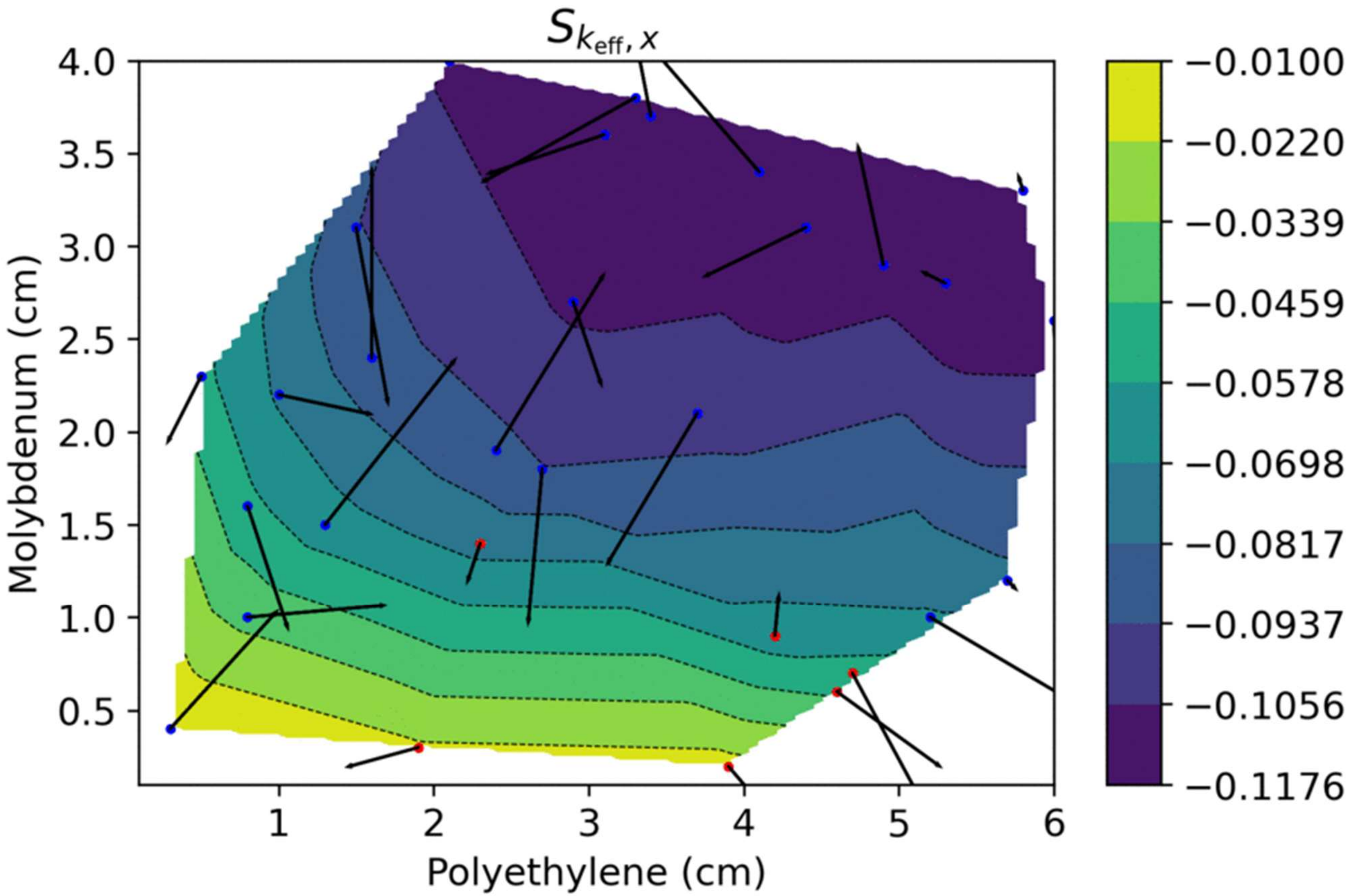
$$\boldsymbol{v}_{i,d} \leftarrow \underbrace{\omega \boldsymbol{v}_{i,d}}_{\text{Previous velocity}} + \underbrace{\varphi_p r_p (\boldsymbol{p}_{i,d} - \boldsymbol{x}_{i,d})}_{\text{Particle best}} + \underbrace{\varphi_g r_g (\boldsymbol{g}_d - \boldsymbol{x}_{i,d})}_{\text{Swarm best}}$$



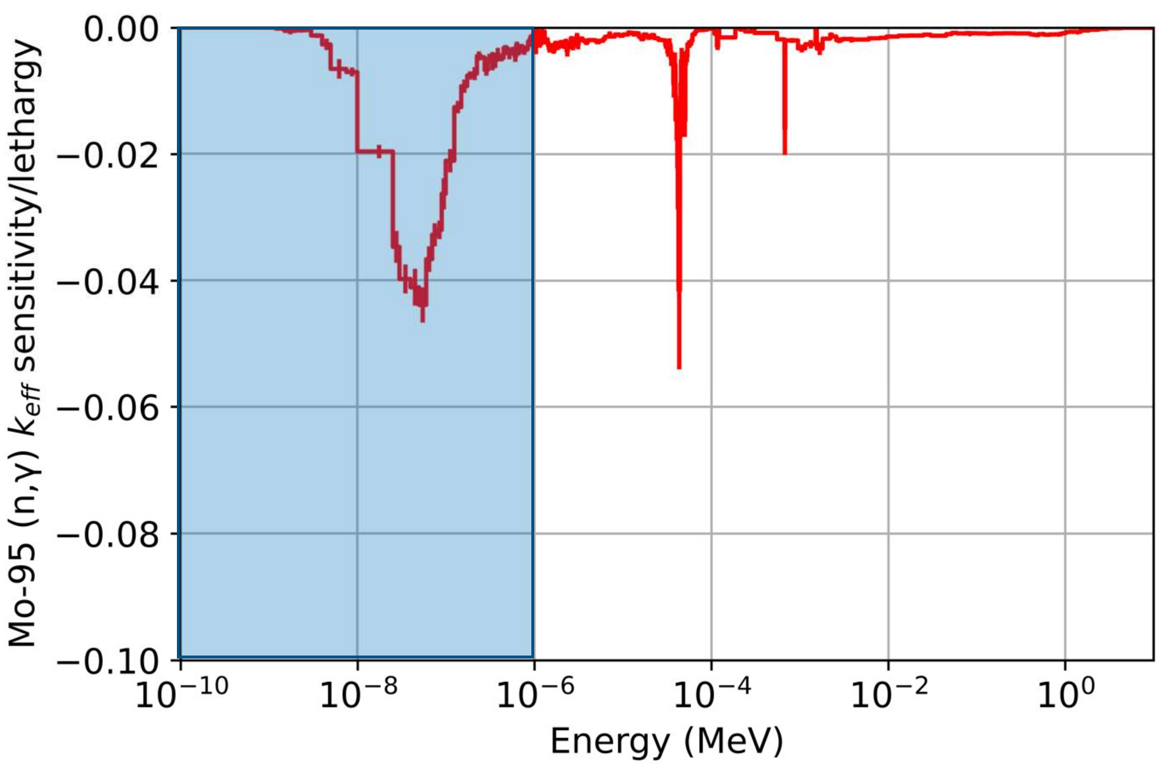
Thermal Plutonium Case (<0.625 eV)



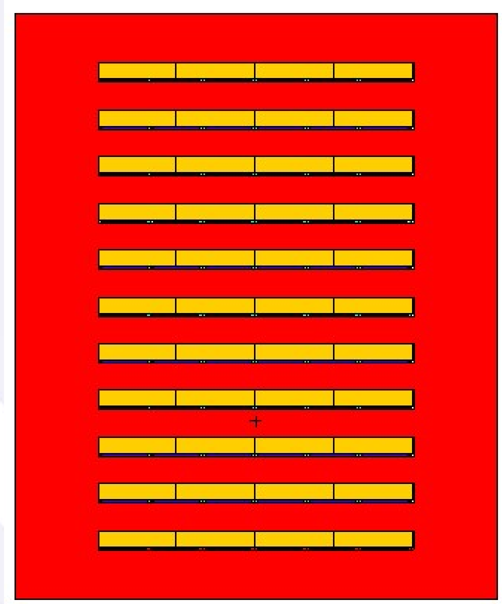
Thermal Plutonium Case (<0.625 eV)



Thermal Plutonium Case (<0.625 eV)



Moderator	Polyethylene
Formula	C_2H_4
Density $[\frac{g}{cm^3}]$	0.93
$S_{k_{eff},\sigma_{Thermal}}$	-0.0907
$t_{moly}[cm]$	1.7
$t_{mod}[cm]$	2.6



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Future Work

- Complete Plutonium for epithermal, URR, and fast configurations using PSO algorithm
- Investigate different moderators for epithermal and URR configurations
- Finalize CED-1 report

Acknowledgments

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NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

NCERC NATIONAL CRITICALITY EXPERIMENTS RESEARCH CENTER

Questions?