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IER 607: Thales
Ta-Reflected Pu Experiment

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Outline

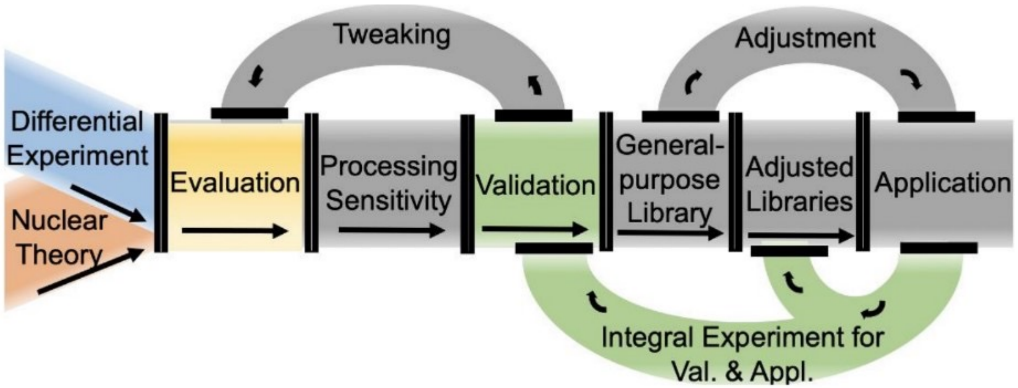
Get Excited it’s Almost Lunch!

- Introduction to Thales
- Method for Low Fidelity Optimization
- Progression to High Fidelity
- Preliminary Uncertainty
- Concluding Remarks

Motivation

Tantalum, Tantalum, and More Tantalum

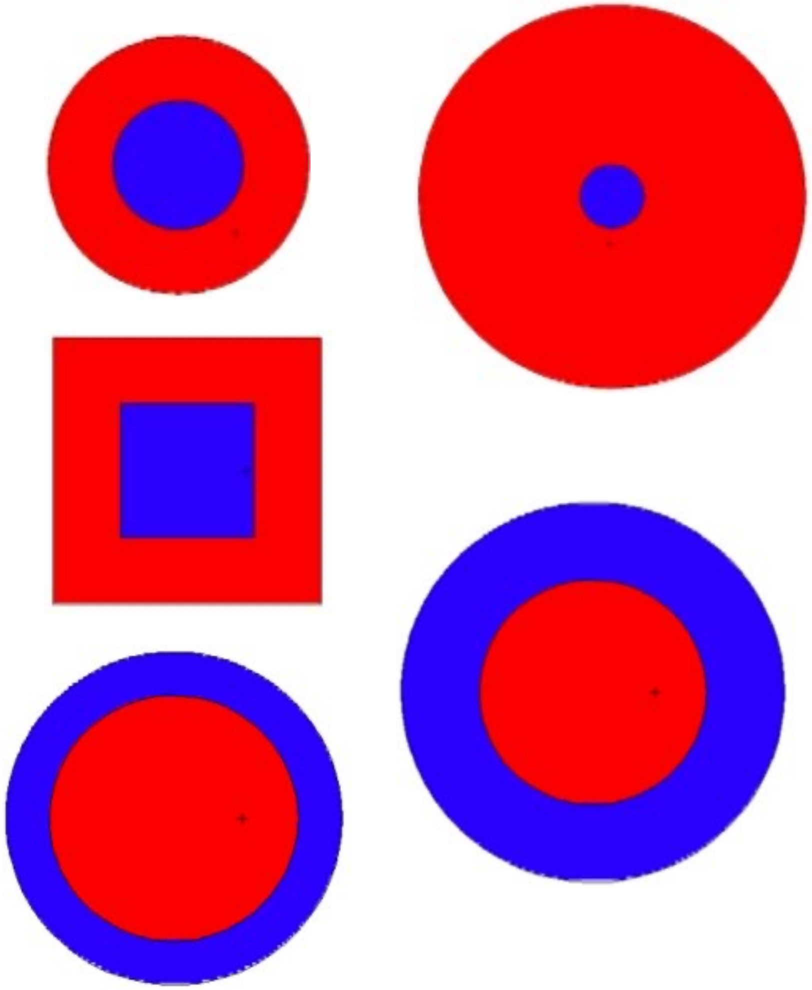
- Tantalum is a refractory metal important for Pu operations at LANL and SRS:
  - High melting point
  - Corrosion Resistant
  - Very hard, ductile, and chemically inert
- Ta has been a priority for NCSP for several years with new evaluations, measurements, and validation
- Only integral measurements that exist: PMM-03 and PMF-045



Thales

It's like EUCLID… but with Tantalum!

- Thales was conceptualized to perform uncertainty reduction on Tantalum systems
  - 40 nominal and upset criticality safety applications at LANL and SRS (A1-A40)→ Provided by NCS (R. Bulso and T. Cutler)
  - Leverage nuclear data (ND) uncertainties with nuclear data sensitivity profiles of applications
- **Combine sensitivity profiles, ND uncertainties, and Bayesian inference to design critical experiments for Ta-reflected Pu systems**



Method

- Sensitivities of the system keff to a nuclear data parameter (x) are calculated via

$$S_{k,x} = \frac{\partial k_{\text{eff}} / k_{\text{eff}}}{\partial x / x}$$

- A similarity metric, c_k, is defined via

$$c_k(A, B) = \frac{\boldsymbol{S}_A \bar{C}_{xx} \boldsymbol{S}_B^T}{\sqrt{\boldsymbol{S}_A \bar{C}_{xx} \boldsymbol{S}_A^T}\sqrt{\boldsymbol{S}_B \bar{C}_{xx} \boldsymbol{S}_B^T}}$$

  - A measure of how much nuclear-data induced uncertainty of the neutron multiplication factor is shared between two models.
  - Ranges from -1 to 1.
  - A and B can actually be any type of models.
  - Sensitivity vectors and covariance matrix can be broken down by nuclide/reaction/energy.

Terms:
x: reaction cross-section
S: vector of sensitivities
T: transpose of a vector
C_{xx}: nuclear data covariance matrix

Similarity Metric Results

All values with c_k>0.99 are shown in green.

- ck for the 40 applications.
- Values along the diagonal are 1 by definition.
- A01 has c_k>0.99 for A04 and A05.
- Application A02 has c_k<0.99 compared to other applications.
- A03 has c_k>0.99 for A06-A40.
- A maximum of three application models (A01, A02, and A03) are needed.
  - One could argue that 0.99 is too strict.
  - If so, maybe only 1 model is needed.
  - >0.99 between each pair of the 40 applications.

Application #	1	2	3
1	**1.000**	0.901	0.971
2	0.901	**1.000**	0.973
3	0.971	0.973	**1.000**
4	**0.995**	0.898	0.975
5	**0.997**	0.910	0.970
6	0.966	0.980	**0.998**
7	0.969	0.969	**0.998**
8	0.973	0.970	**0.998**
9	0.972	0.966	**0.999**
10	0.973	0.963	**0.996**
11	0.974	0.965	**0.999**
12	0.977	0.965	**0.998**
13	0.974	0.965	**0.999**
14	0.980	0.958	**0.996**
15	0.975	0.964	**0.999**
16	0.978	0.964	**0.998**
17	0.976	0.964	**0.999**
18	0.980	0.961	**0.998**
19	0.976	0.964	**0.999**
20	0.981	0.961	**0.998**
21	0.976	0.964	**0.999**
22	0.980	0.957	**0.997**
23	0.977	0.962	**0.999**
24	0.980	0.960	**0.997**
25	0.977	0.964	**0.999**
26	0.980	0.960	**0.997**
27	0.977	0.963	**0.999**
28	0.979	0.965	**0.998**
29	0.977	0.963	**0.999**
30	0.980	0.962	**0.998**
31	0.977	0.964	**0.999**
32	0.975	0.965	**0.997**
33	0.977	0.964	**0.999**
34	0.979	0.960	**0.997**
35	0.977	0.964	**0.999**
36	0.979	0.964	**0.998**
37	0.976	0.965	**0.999**
38	0.981	0.959	**0.998**
39	0.976	0.965	**1.000**
40	0.979	0.963	**0.998**

Nuclear Data Uncertainty Results

- Nuclear data uncertainties for each nuclide/reaction pair were averaged for the 40 application models.
- ^{181}Ta inelastic and elastic scattering have very large nuclear data uncertainties.
- No hydrogen reactions appear, even though some of the upset models are fairly sensitive to elastic scattering in hydrogen.
  - This reaction is well-known with low uncertainty.

Nuclide	Reaction	Avg. Unc. (pcm)
Ta181	inelastic	1891
Pu239	total nu	1254
Ta181	elastic	524
Pu239	inelastic	421
Pu239	fission	376
Pu239	elastic	275
Pu239	fission chi	242
Ta181	n,gamma	108
Pu239	n,gamma	74

*BLO covariance used

Ranked sensitivities averaged over the 40 applications.

Large nuclear data uncertainty shows clear need for additional validation experiments.

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Pu239	elastic	275
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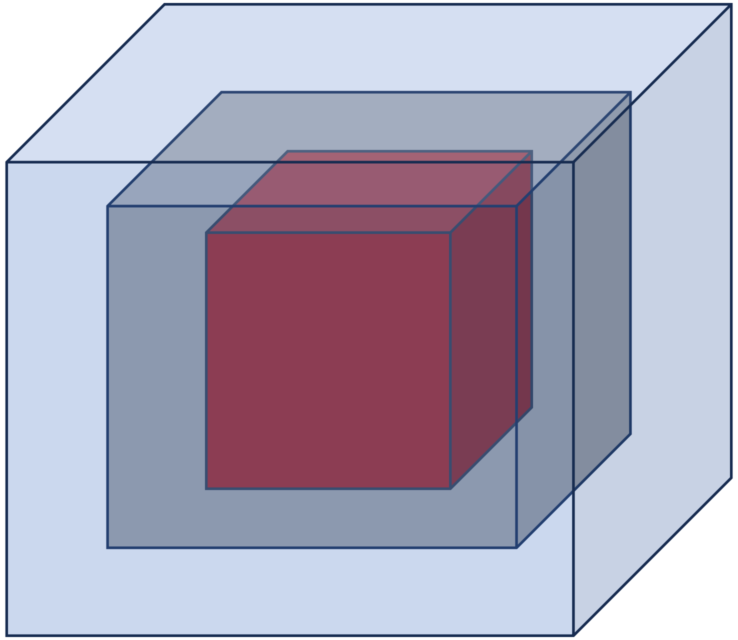
Ta181	n,gamma	108
Pu239	n,gamma	74

*BLO covariance used

No water (or poly) needed as that ND is quantified!

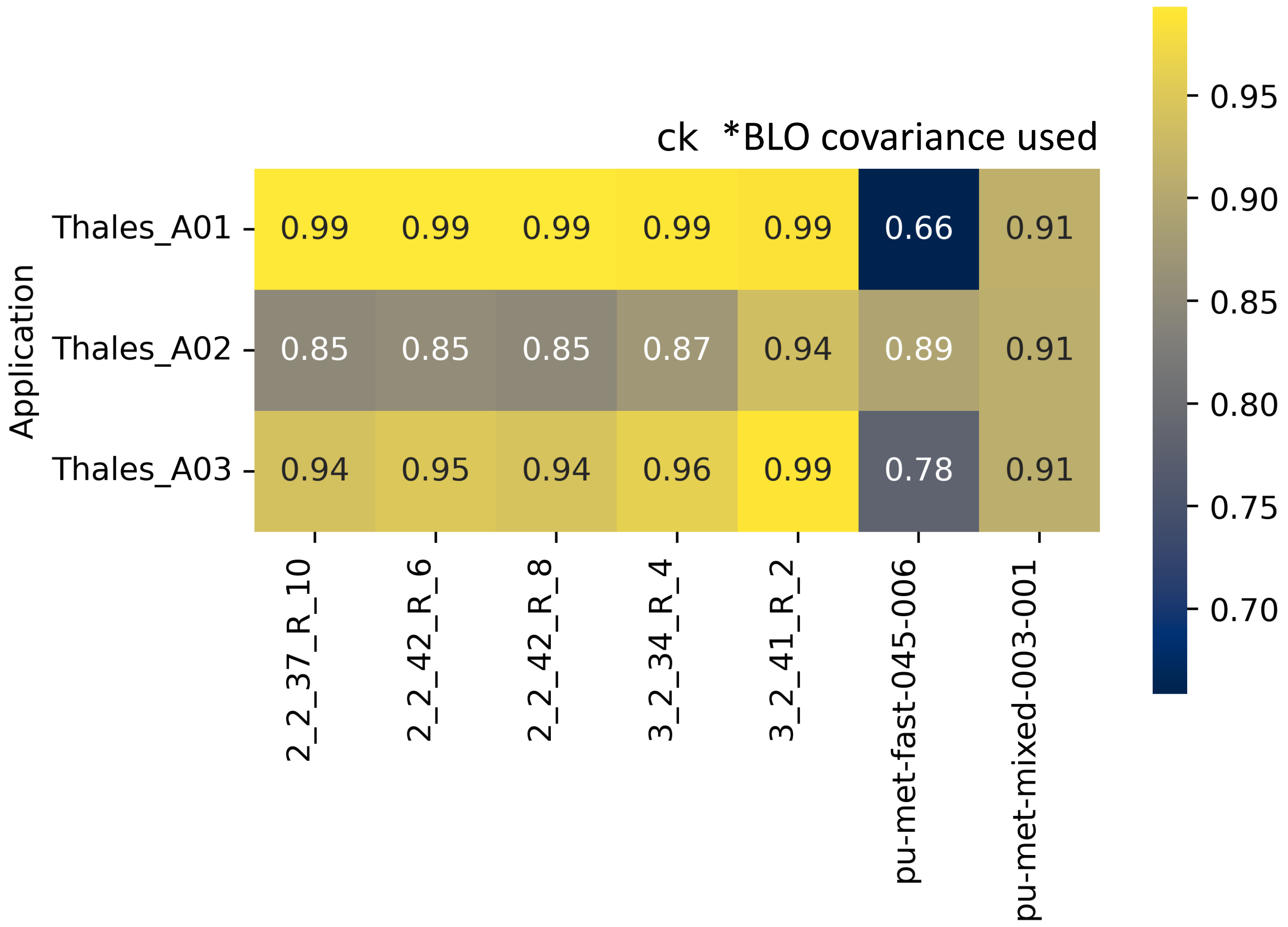
Simple Rectangular Parallelepiped (RPP) Geometry

- Early calculations showed that ZPPR plates offer the greatest flexibility in achieving criticality with multiple reflector thicknesses
- Nested RPP shells
- Pu fuel
  - ℓ, w, h between 0 to 20 cm
  - ZPPR alloy (10% Al)
  - Stainless steel cladding
- Inner Ta reflector (mold material)
  - 0 to 20 cm thick
- Outer $H_2$0 reflector (upset condition)
  - 0 to 20 cm thick



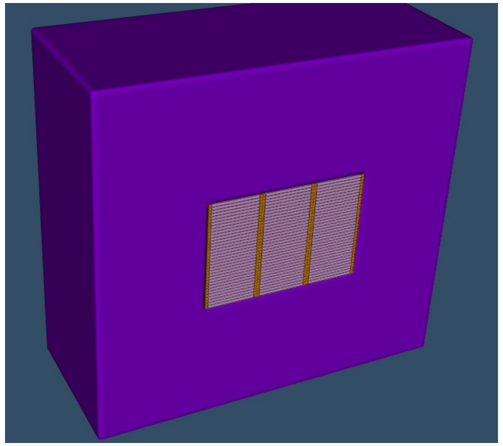
Similarity metric results

- Heatmap of the three applications shown at right.
- PU-MET-FAST-045-006: is not that useful (note that it is the most useful of all PMF045 cases).
- PU-MET-MIXED-003-001 is useful.
  - Use this case for LANL/SRS now
- It is possible to design new validation experiments with c_k>0.99 for all applications.

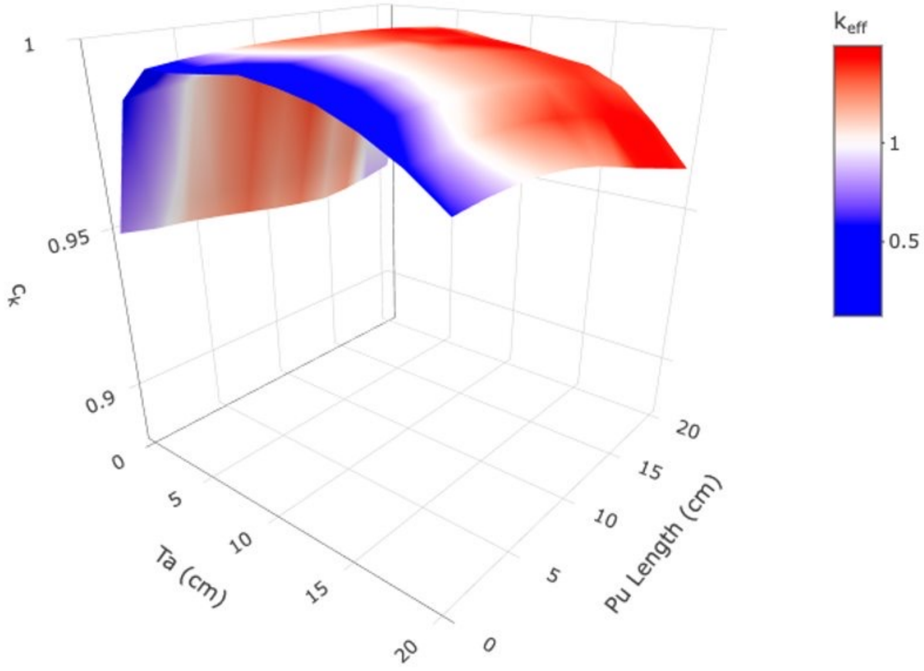


Low Fidelity Designs

- Settled on 2x3 array of ZPPR plates
  - Reminiscent of EUCLID 2x3 configuration
  - Looked at others but 6”x 6” is optimal
- Outer reflector modeled as simple RPP
- Various reflector thicknesses
- Accounted for simulations needed for CED-01 submitted in FY24



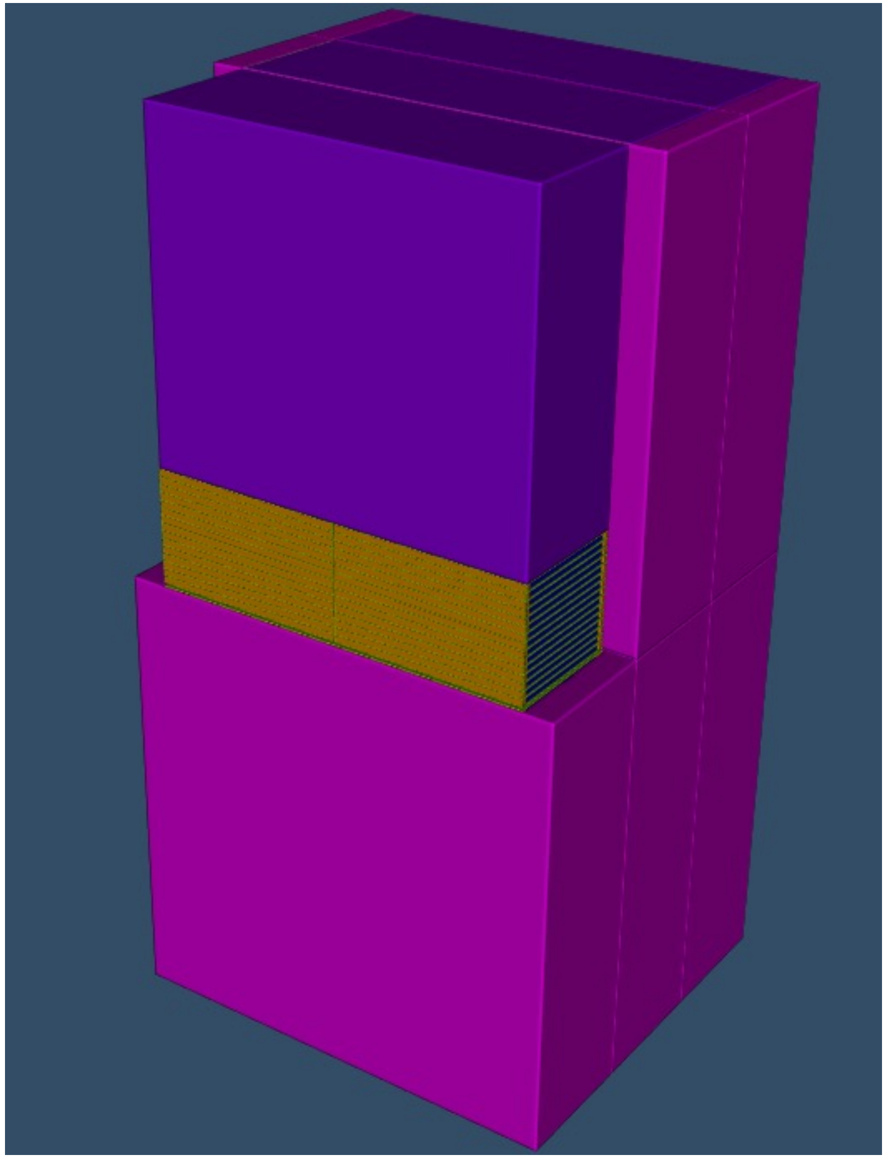
Application Ck to A-04

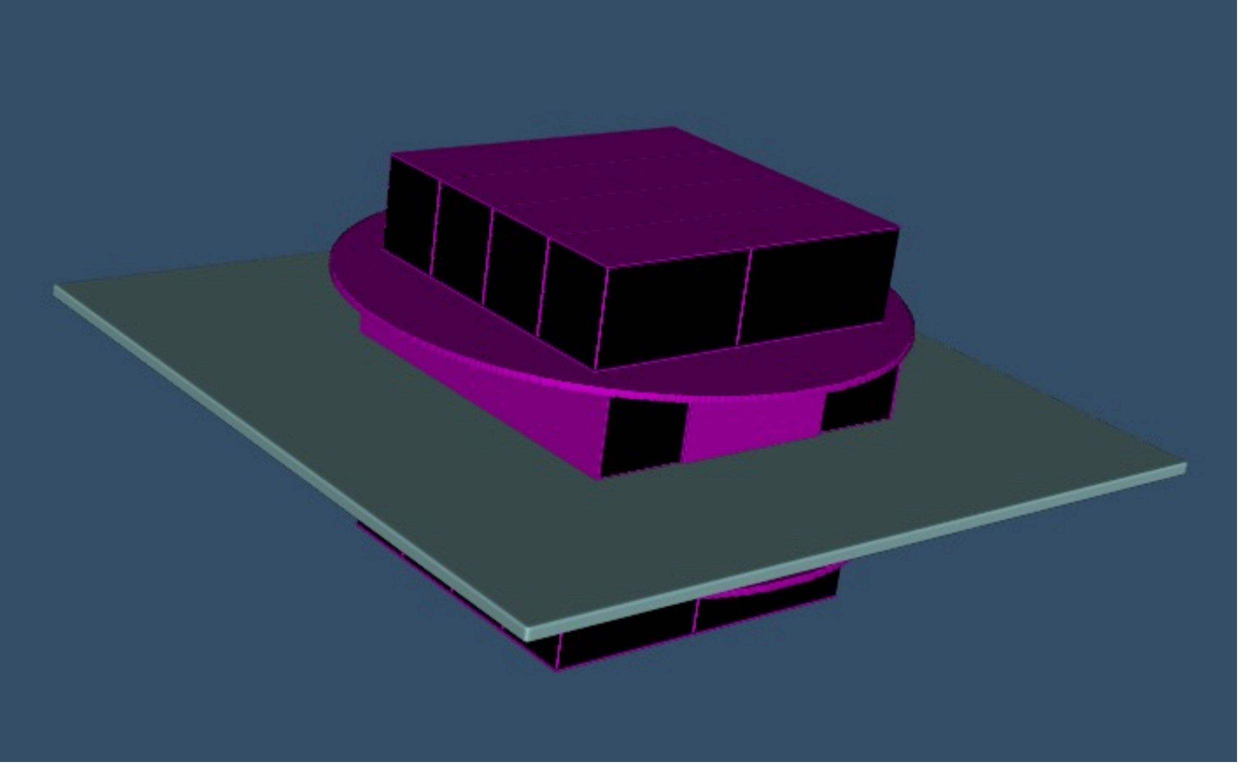


Thales Updates

High Fidelity Considerations

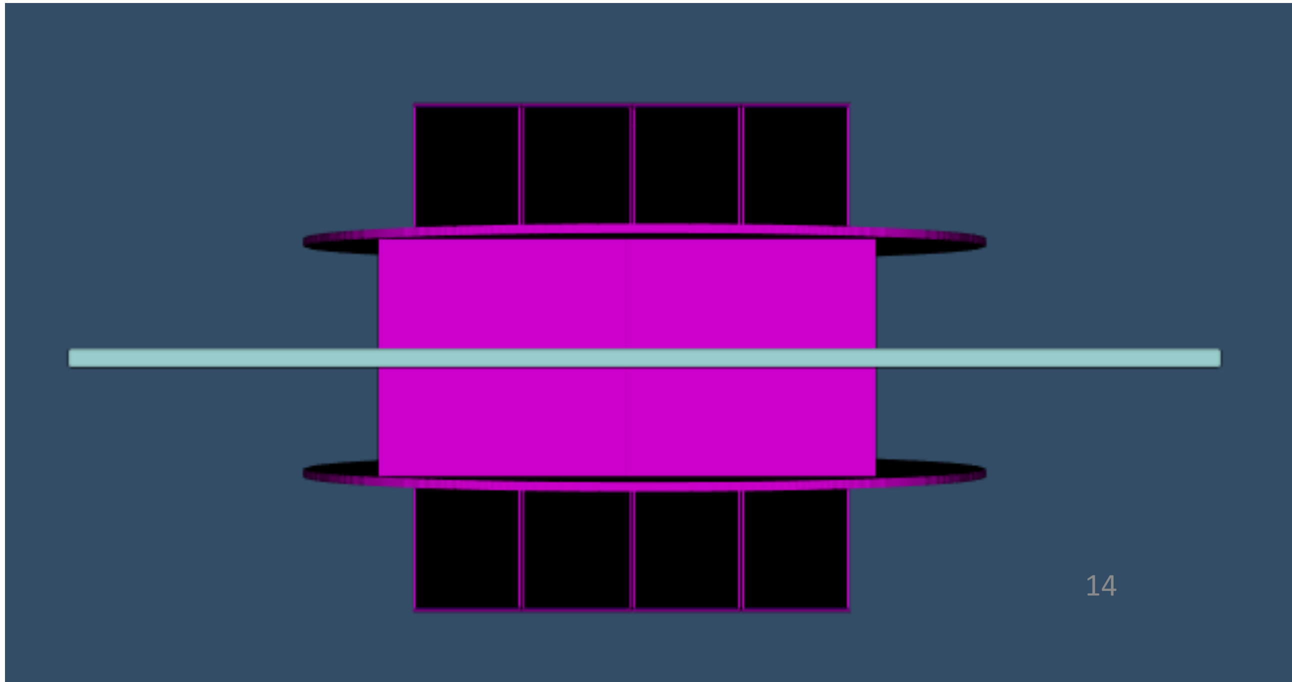
- Containerized the fuel into boxes similar to EUCLID design
- Created containers for the reflector so a square reflector could be constructed
  - Due to the containerization Ta thickness are 1.27, 2.54, 5.08, and 8.89 cm
- Performed engineering studies for materials, thickness, air tolerances, etc.



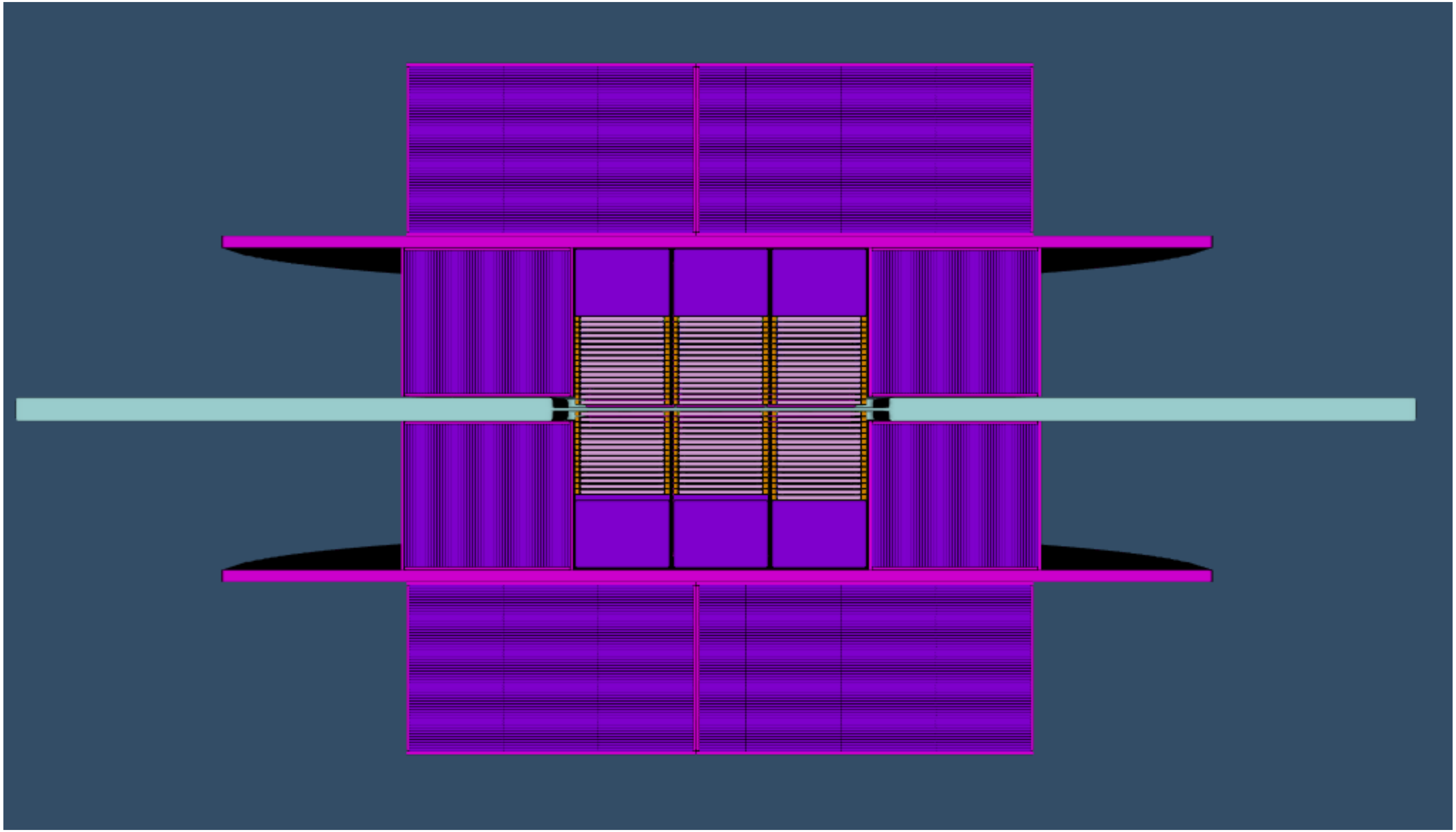


Isometric view of Thales

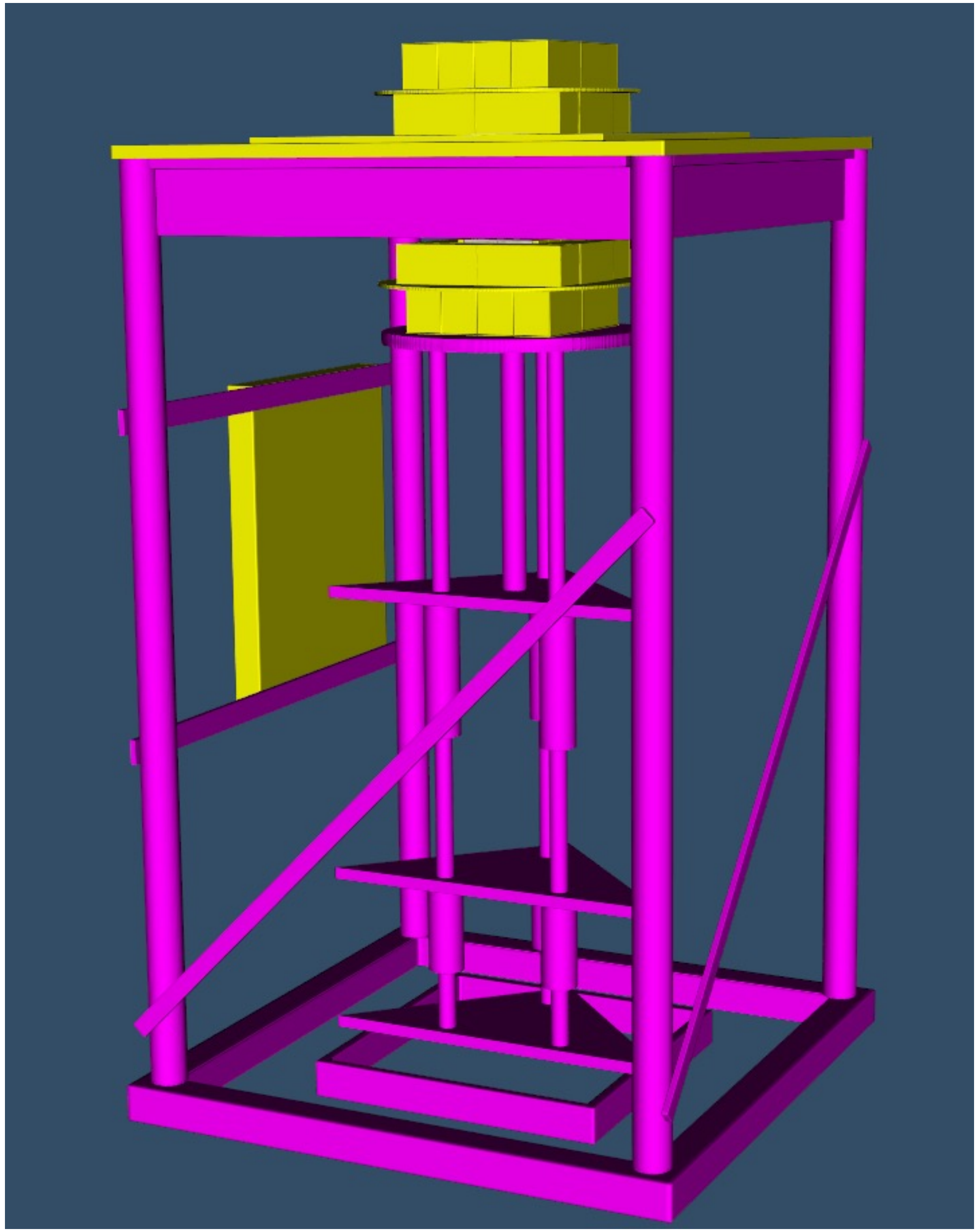
Side view of Thales



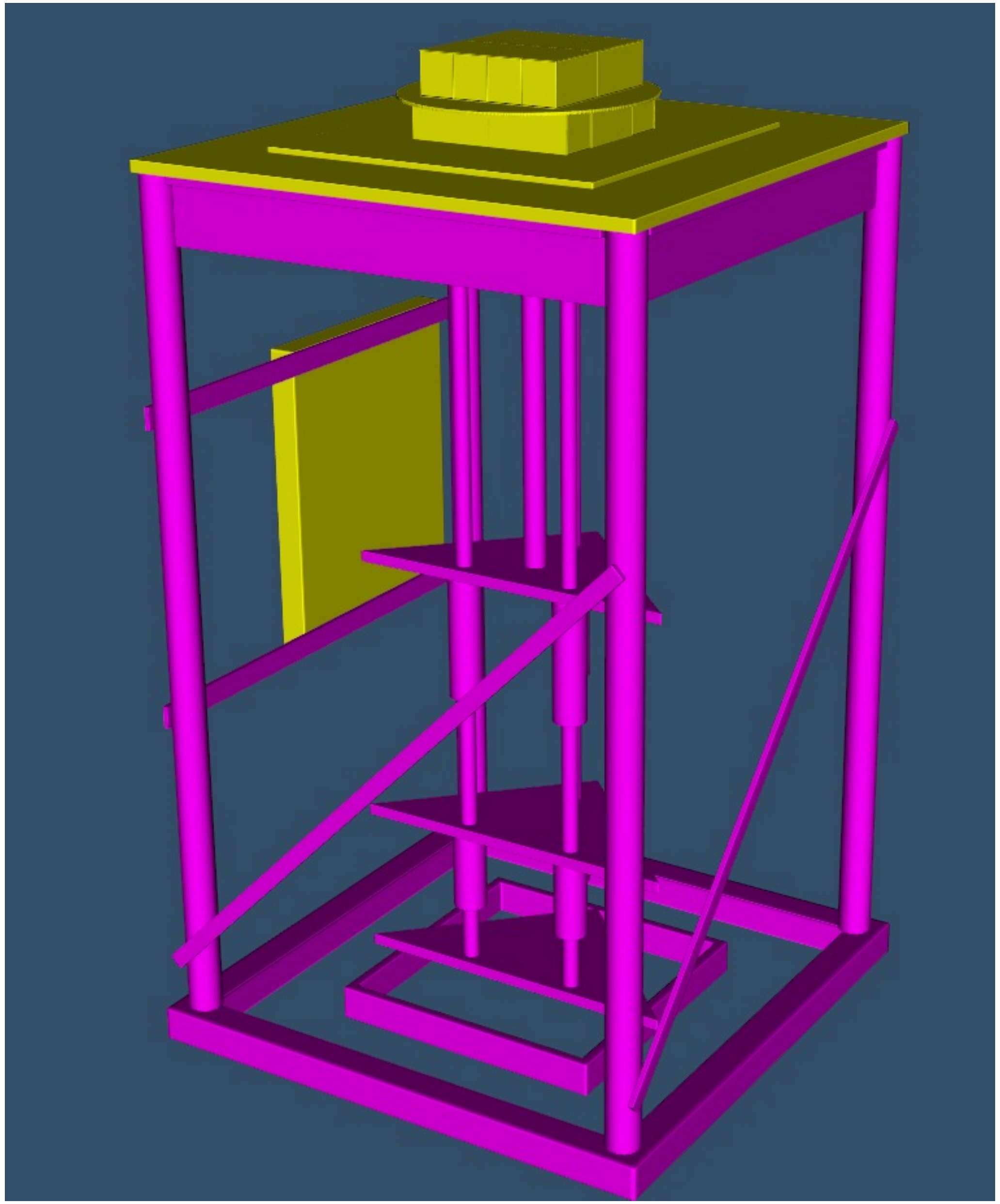
Cut away of the side view with all plates



Thales on Comet with Gap



Thales on Comet without Gap



Comparison of Thales expected unc. and PMM-03

Uncertainty Type (Perturbation)	ΔKeff
Fuel (Mass and Comp)	0.00062
Ta Plates (comp)	0.00007
Steel (comp)	0.00003
Dimensional Uncertainties	0.00150
Comet (existing/bias)	0.00200
Room (bias)	0.00020
Total Uncertainties (bias)	±162 pcm (210 pcm)

2.6.1 Table 77. Summary of Uncertainties for Case 1

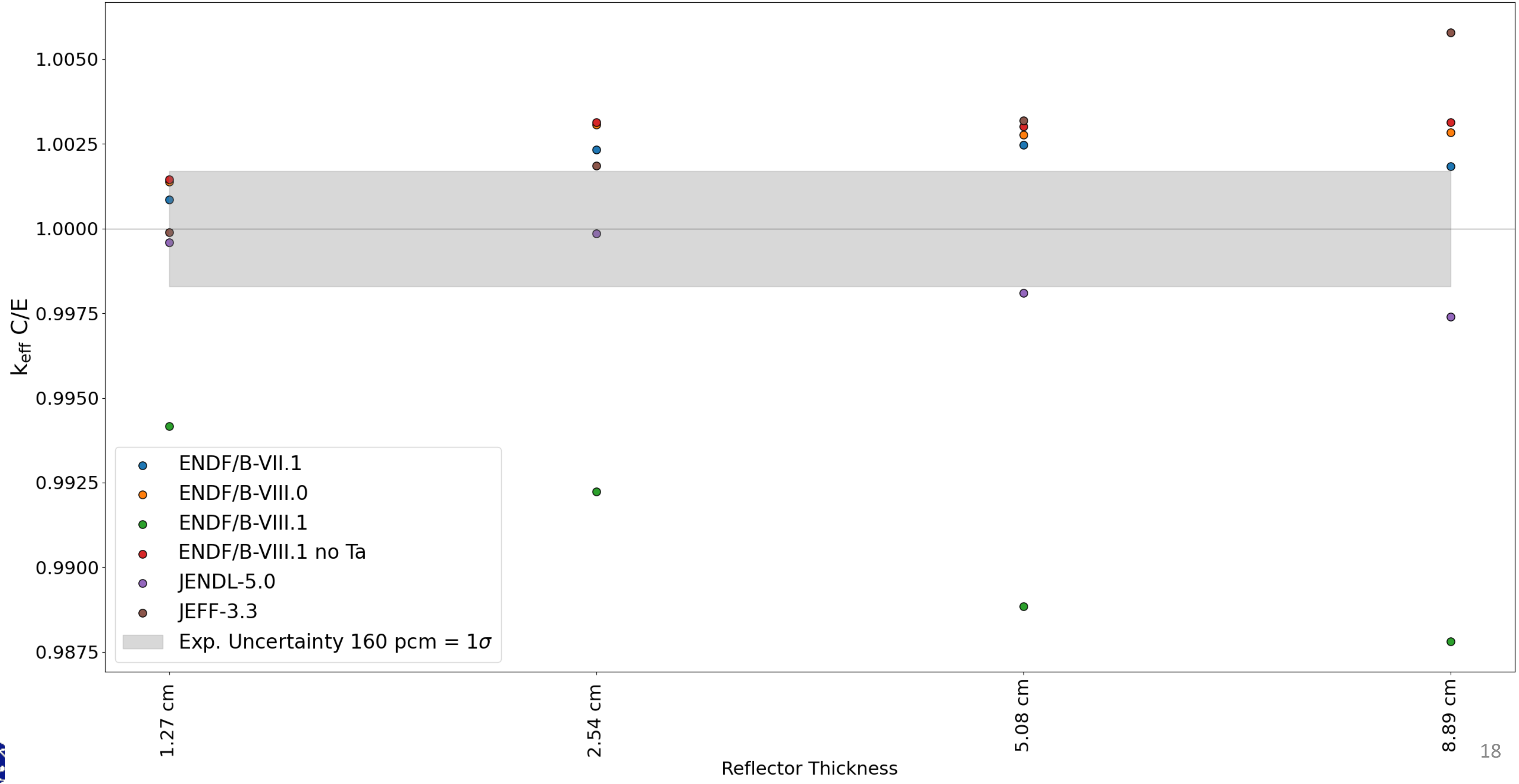
Source of Uncertainty	Parameter Value used	Parameter Variation in Calculation	Calculated Effect $\Delta k_{eff+} - \Delta k_{eff-}$	Standard Uncertainty of Parameter [A or B]	N	Standard Uncertainty in Δk_{eff}
Mass Uncertainties						
Plutonium Core Mass	105.384 g	±0.01 g	0.00022	0.01g [B]	1	0.00011
Plutonium Mass Distribution	48 Heavy/Light Plates	n/a	0.00046	n/a [B]	1	0.00046
Stainless Steel Cladding Mass	24.767 g	±0.01 g	0.00003	0.01 g [B]	1	0.00001
Tantalum Plate Mass	101.95 g	±1.1547 g	0.00026	1.1547 g [B]	648	0.00001
Polyethylene Mass:						
• 3/16 in Tray Frame Density	0.964 g/cm³	±0.002 g/cm³	0.00019	1.321E-03 g/cm³ [A]	1	0.00006
• 1/16 in Sheet (Tray Moderator) Density	0.961 g/cm³	±0.002 g/cm³	0.00012	1.321E-03 g/cm³ [A]	1	0.00005
• 15/16 in Sheet (Lower Reflector) Density	0.972 g/ cm³	±0.002 g/cm³	0.00025	1.202E-03 g/cm³ [A]	1	0.00007
• 15/16 in Sheet, 1/16 in Sheet (Upper Reflector) Density	0.972 g/ cm³, 0.961 g/ cm³	±0.002 g/cm³	-0.00003	1.202E-03, 1.321E-03 g/cm³ [A]	1	0.00001
Heat Dispersal Plate Mass	Examined in Conjunction with Heat Dispersal Plate Dimensional Uncertainty					

Table 100. Expected Benchmark Model k_{eff} for Detailed Cases

Case	Experimental $k_{eff} \pm 1\sigma$	Simplification Bias $k_{eff} \pm 1\sigma$	Benchmark Model k_{eff}
1	1.00043 ± 0.00195	-0.00090 ± 0.00008	0.99953 ± 0.00195
2	1.00021 ± 0.00154	-0.00083 ± 0.00008	0.99938 ± 0.00154
3	1.00021 ± 0.00154	-0.00013 ± 0.00008	1.00008 ± 0.00154
4	1.00037 ± 0.00142	+0.00041 ± 0.00008	1.00078 ± 0.00142
5	1.00031 ± 0.00121	-0.00160 ± 0.00008	0.99871 ± 0.00121

Critical Configurations with Different Libraries

New Ta makes a big ol' difference



Conclusions

- There is limited validation data for fast applications with Pu-reflected Ta.
  - The recent PU-MET-MIXED-003 evaluation is useful for Ta validation.
  - Especially the fastest case, PU-MET-MIXED-003-001.
- 40 different application models were created/provided.
  - Pu operations at LANL and SRS under normal and upset conditions.
  - A maximum of three application models are needed to represent all 40 models.
- High fidelity neutron and CAD models developed and CED-02 is underway!
- Expected uncertainties are below 200 pcm, more than enough to validate the new Tantalum evaluation

Acknowledgments

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- We'd like to thank LANL and SRS Nuclear Criticality Safety

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Backup Slides

Summary of Keff and Sensitivities
Condense all the inputs into a single table

Configs	Original w/ RPP Reflector Keff	Original w/ RPP Reflector Sens	Euclid w/ RPP Reflector Keff	Euclid w/ RPP Reflector Sens	New Least Keff (Al box)	New Least Sens (Al box)	New Most Keff (Ta box)	New Most Sens (Ta box)
32 Layers 8.90 cm reflector	1.090946	0.114 (El) 0.095 (Inel)	1.066311	0.105 (El) 0.086 (Inel)	1.010248	0.0979 (El) 0.0834 (Inel)	1.014625	0.105 (El) 0.0876 (Inel)
36 Layers 5.08 cm reflector	1.072730	0.105 (El) 0.097 (Inel)	1.052834	0.097 (El) 0.088 (Inel)	1.046267	0.0906 (El) 0.0804 (Inel)	1.050325	0.093(El) 0.085 (Inel)
44 Layers 2.54 cm reflector	1.04377	0.0743 (El) 0.0767(Inel)	1.05829	0.0710 (El) 0.0684 (Inel)	1.043921	0.0701 (El) 0.0676 (Inel)	1.052596	0.078 (El) 0.076 (Inel)
55 Layers 1.27 cm reflector	1.006921	0.060 (El) 0.062 (Inel)	0.999840	0.057 (El) 0.058 (Inel)	1.029687	0.0432 (El) 0.0467 (Inel)	1.039995	0.055 (El) 0.057 (Inel)

Critical Configuration Search

Subcritical, Critical, and Keff+0.01

Configuration	Subcritical	Num. Layers	Critical	Num. Layers	Super Critical	Num. Layers
1.27 cm	0.994181	42.33	1.001374	43.5	1.010648	45.33
2.54 cm	0.996163	37	1.003063	37.83	1.011729	39
5.08 cm	0.992325	33.33	1.002767	33.33	1.012935	34.33
8.89 cm	0.990959	30.33	1.002844	31.33	1.014299	32.33

Container and Membrane Studies

1.27 cm reflector

Membrane	Al_Al_Al	Ta_Al_Al	Ta_Ta_Al	Ta_Ta_Ta
Tantalum	1.006328	1.006973	1.010984	1.014969
Aluminum	1.001379	1.002013	1.006364	1.010482
Stainless Steel	1.005966	1.006612	1.010673	1.014749

Membrane	All Al El.	All Al Inel	Ta/Al/Al El.	Ta/Al/Al Inel.	Ta/Ta/Al El.	Ta/Ta/Al Inel.	All Ta El.	All Ta Inel.
Tantalum	5.6310E-02	5.8643E-02	5.6853E-02	5.9195E-02	6.1445E-02	6.2849E-02	6.6031E-02	6.7141E-02
Aluminum	4.9612E-02	5.2788E-02	5.0946E-02	5.3669E-02	5.5180E-02	5.7726E-02	5.9950E-02	6.1987E-02
Stainless Steel	5.0343E-02	5.2525E-02	5.1055E-02	5.3349E-02	5.5714E-02	5.7318E-02	6.0075E-02	6.1393E-02

Container and Membrane Studies

2.54 cm reflector

Membrane	Al_Al_Al	Ta_Al_Al	Ta_Ta_Al	Ta_Ta_Ta
Tantalum	1.008418	1.008896	1.012431	1.015588
Aluminum	1.003083	1.003592	1.007502	1.010857
Stainless Steel	1.007904	1.008493	1.012029	1.015320

Membrane	All Al El.	All Al Inel	Ta/Al/Al El.	Ta/Al/Al Inel.	Ta/Ta/Al El.	Ta/Ta/Al Inel.	All Ta El.	All Ta Inel.
Tantalum	8.0542E-02	7.8323E-02	8.0708E-02	7.8696E-02	8.5445E-02	8.1872E-02	8.8834E-02	8.4306E-02
Aluminum	7.2766E-02	7.2526E-02	7.3810E-02	7.2867E-02	7.8440E-02	7.6337E-02	8.1866E-02	7.9355E-02
Stainless Steel	7.3796E-02	7.2059E-02	7.4234E-02	7.2593E-02	7.7984E-02	7.5862E-02	8.1777E-02	7.9062E-02

Container and Membrane Studies

5.08 cm reflector

Membrane	Al_Al_Al	Ta_Al_Al	Ta_Ta_Al	Ta_Ta_Ta
Tantalum	1.007688	1.008018	1.010630	1.012912
Aluminum	1.002767	1.003125	1.006189	1.008679
Stainless Steel	1.007729	1.008072	1.010838	1.013188

Membrane	All Al El.	All Al Inel	Ta/Al/Al El.	Ta/Al/Al Inel.	Ta/Ta/Al El.	Ta/Ta/Al Inel.	All Ta El.	All Ta Inel.
Tantalum	9.9498E-02	8.9037E-02	9.8958E-02	8.9345E-02	1.0281E-01	9.0848E-02	1.0709E-01	9.3203E-02
Aluminum	9.2311E-02	8.4172E-02	9.2174E-02	8.3887E-02	9.5897E-02	8.6301E-02	9.9155E-02	8.8800E-02
Stainless Steel	9.2965E-02	8.3579E-02	9.3232E-02	8.4045E-02	9.6370E-02	8.5943E-02	9.8953E-02	8.8123E-02

Container and Membrane Studies

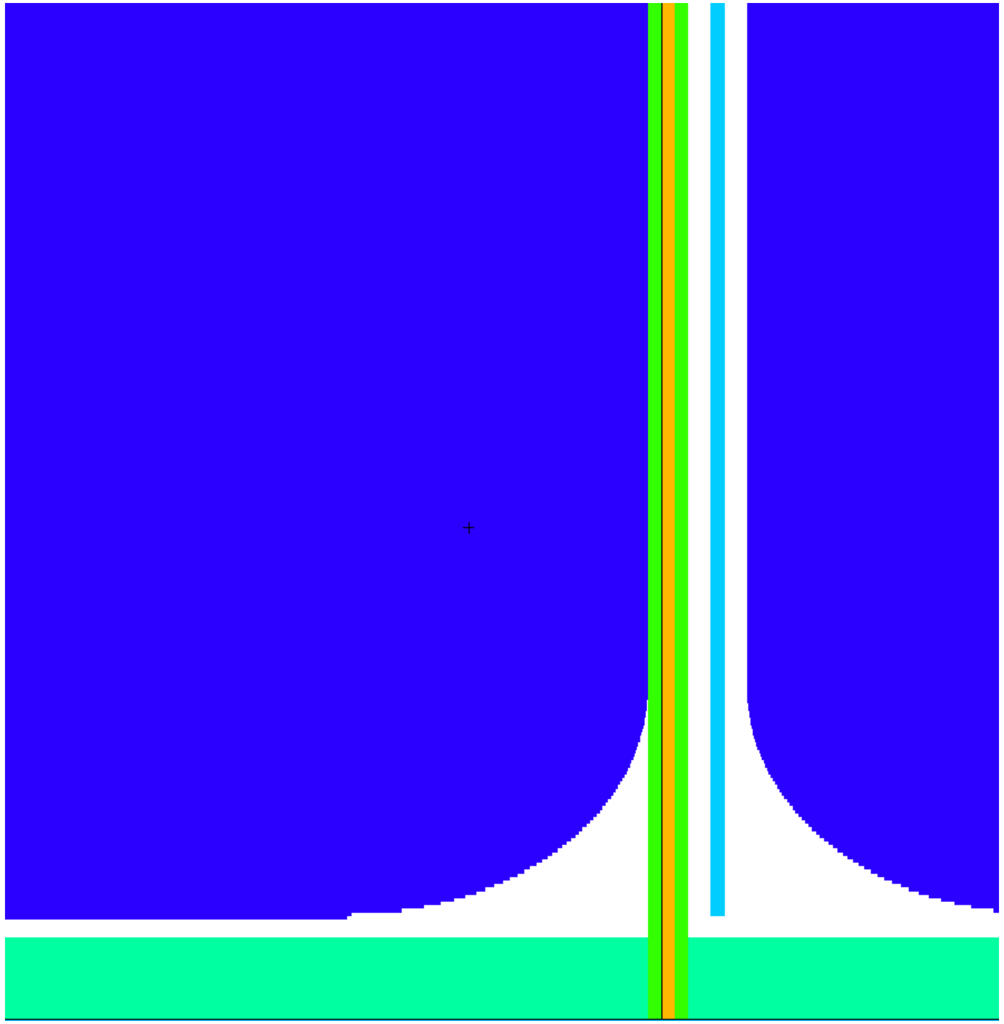
8.89 cm reflector

Membrane	Al_Al_Al	Ta_Al_Al	Ta_Ta_Al	Ta_Ta_Ta
Tantalum	1.006411	1.006579	1.008141	1.009971
Aluminum	1.002812	1.003006	1.005156	1.007080
Stainless Steel	1.007527	1.007674	1.009513	1.011310

Membrane	All Al El.	All Al Inel	Ta/Al/Al El.	Ta/Al/Al Inel.	Ta/Ta/Al El.	Ta/Ta/Al Inel.	All Ta El.	All Ta Inel.
Tantalum	1.0405E-01	8.6767E-02	1.0461E-01	8.7032E-02	1.0712E-01	8.8320E-02	1.0797E-01	8.9965E-02
Aluminum	9.8182E-02	8.3318E-02	9.7297E-02	8.3564E-02	1.0073E-01	8.4271E-02	1.0329E-01	8.6503E-02
Stainless	9.8859E-02	8.2621E-02	9.7326E-02	8.2045E-02	1.0064E-01	8.4224E-02	1.0285E-01	8.5838E-02

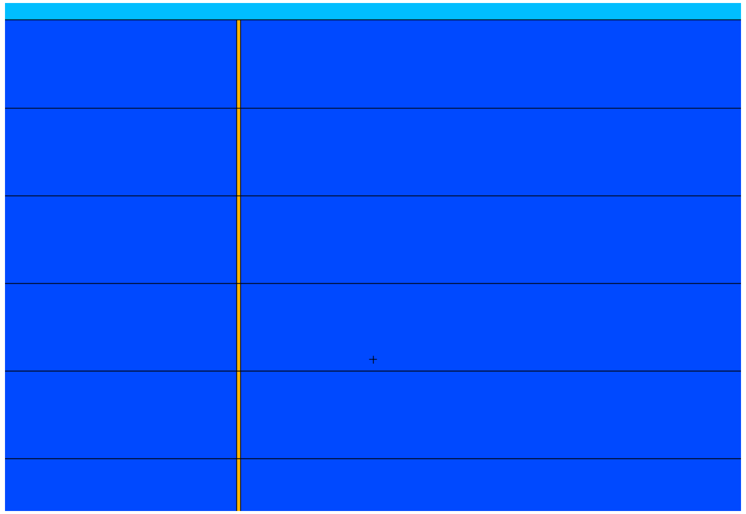
Uncertainty Analysis – ZPPR Air Gaps (0.03 cm)

Configuration	Baseline	Air Gap	ΔKeff
1.27 cm	1.001374	1.000207	-110 ± 2 pcm
2.54 cm	1.003063	1.002011	-105 ± 2 pcm
5.08 cm	1.002767	1.001821	-95 ± 2 pcm
8.89 cm	1.002844	1.001882	-96 ± 2 pcm



Uncertainty Analysis – Ta Plate Gaps

Only added air gaps between plate rows (gravity is in effect) (x=0.018cm, y = 0.0125cm)



Configuration	Baseline	Air Gaps	Diff
1.27 cm	1.001374	1.001087	-28 ±2 pcm
2.54 cm	1.003063	1.002620	-38 ±2 pcm
5.08 cm	1.002767	1.002265	-49 ±2 pcm
8.89 cm	1.002844	1.002305	-52 ±2 pcm

2.2.4 Tantalum Plate Dimensions

Original drawings or historical dimensional measurements for the ZPPR program's tantalum plates were not found. As mentioned in Section 1.2.2, twenty five tantalum plates were chosen at random by LLNL and measured with electronic calipers with a precision of 0.001 in. The results of these measurements are shown in Table 58.

Table 58. Measurement Results for 25 Randomly-Chosen Tantalum Plates

Measured Parameter	Mean (in)	Standard Deviation (in)	Mean (cm)	Standard Deviation (cm)
Plate Length	2.993	0.0010	7.60222	0.00254
Plate Width	1.995	0.0009	5.0673	0.00229
Plate Height	0.062	0.0007	0.15748	0.01778

The uncertainty in the tantalum plate dimensions was taken to be the standard deviation of the recent measurements with the addition of the measurement uncertainty of $0.0025/\sqrt{3}$ cm. The uncertainty in tantalum dimensions was assessed by varying the tantalum plate length and width by ± 0.005 cm, while adjusting the density to maintain the same tantalum mass, scaling the resulting calculations by the total uncertainty, and dividing by the $\sqrt{N}$ (total number of tantalum plates) to determine the effect on k_{eff}.

Uncertainty Analysis – Fuel

Configuration	Mass (0.01g/105g)	Impurities Isotopics
1.27 cm	7.3 pcm	67 pcm
2.54 cm	7.2 pcm	64 pcm
5.08 cm	7.1 pcm	62 pcm
8.89 cm	7.0 pcm	61 pcm

Uncertainty Analysis - Steel Cladding Impurities

Following PMM-03

- 1% uncertainties for Cr, Ni, Mn
- 0.1% for Fe
- 10% for everything else

Configuration	Clad Unc ΔKeff
1.27 cm	3.62 pcm
2.54 cm	3.16 pcm
5.08 cm	2.58 pcm
8.89 cm	2.42 pcm

Table 62. 304-L Stainless Steel Cladding Composition for the PANN Plates

Component of 304-L SS	Mass per plate (g)	Mass Fraction per plate (%)	Assumed 1σ Uncertainty (g)	Typical 304-L Mass Fraction Range (%)
Fe	16.26	65.657	--	--
Cr	4.57	18.453	0.0457	18.00-20.00
Ni	2.22	8.964	0.022	8.00-12.00
Mn	0.42	1.696	0.042	≤ 2.00
Si	0.118	0.476	0.0118	≤ 1.00
Mo	0.079	0.319	0.0079	--
Cu	0.069	0.279	0.0069	--
C	0.016	0.065	0.0016	≤ 0.08
P	0.006	0.024	0.0006	≤ 0.045
S	0.005	0.020	0.0005	≤ 0.030
Steel Spring (estimated)	0.258	1.042	--	--
Unknown	0.744	3.004	--	
Totals	24.765	100	--	--

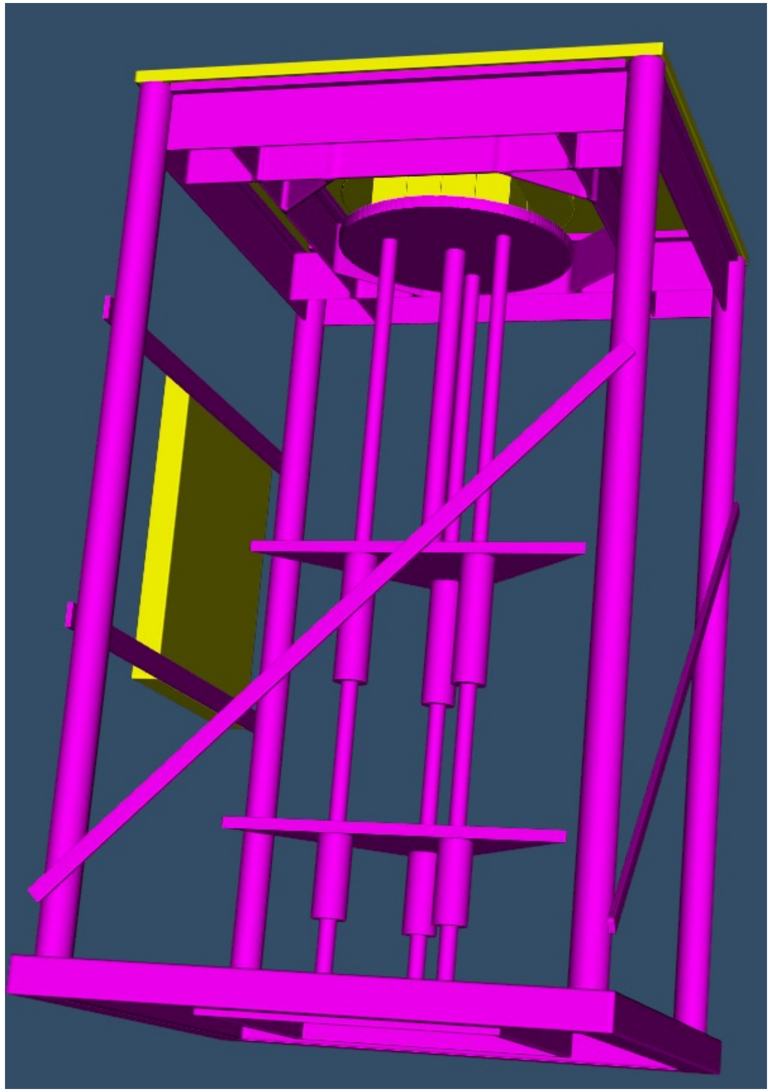
Uncertainty Analysis – Ta Impurities

Configuration	Baseline	Max Impurities	ΔKeff
1.27 cm	1.001374	1.001480	11 ± 2 pcm
2.54 cm	1.003063	1.003185	12 ± 2 pcm
5.08 cm	1.002767	1.002828	5 ± 2 pcm
8.89 cm	1.002844	1.002750	-9 ± 2 pcm

Element	Typical max. value [µg/g]	Guaranteed max. value [µg/g]
Fe	17	50
Mo	10	50
Nb	10	100
Ni	5	50
Si	10	50
Ti	1	10
W	20	50
C	11	50
H	2	15
N	5	50
O	81	150
Cd	5	10
Hg	-	1
Pb	5	10

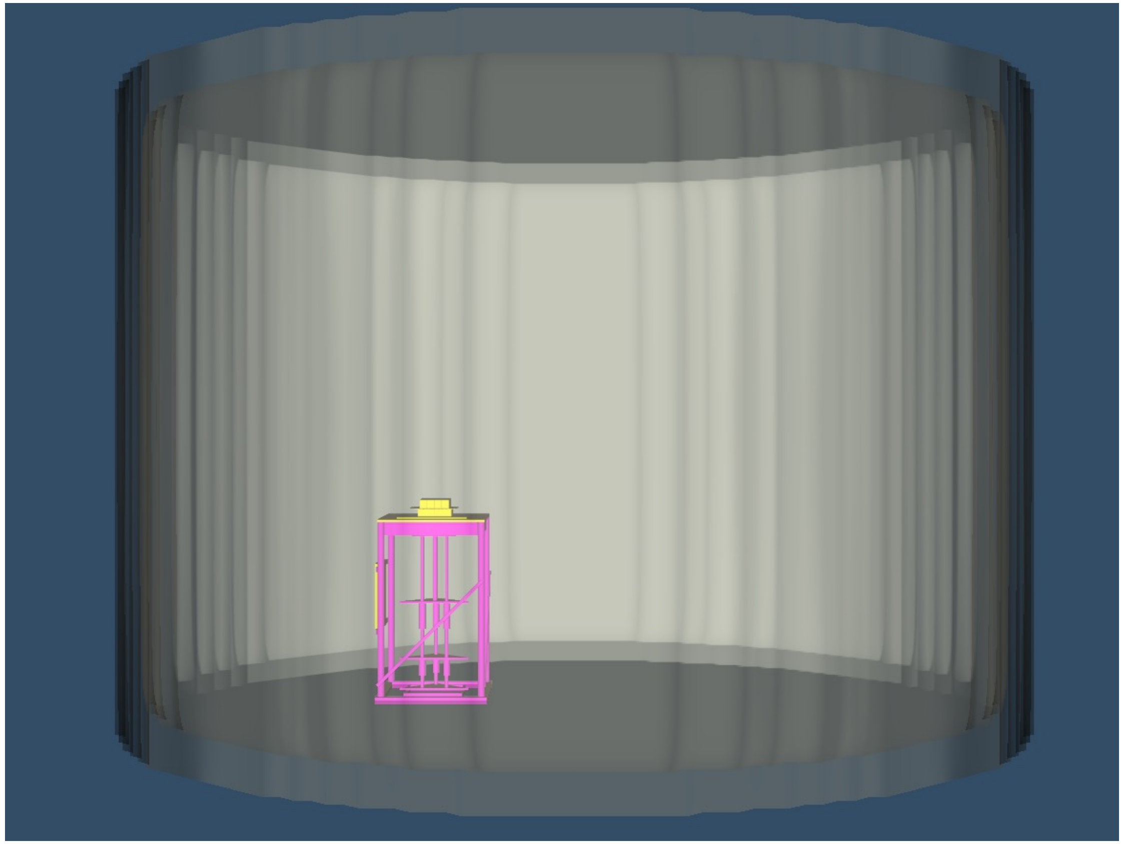
The presence of Cr (VI) and organic impurities can be excluded definitely because of the production process (multiple heat treatment at temperatures above 1000 °C in H2-atmosphere)

Uncertainty Analysis – Comet Platform

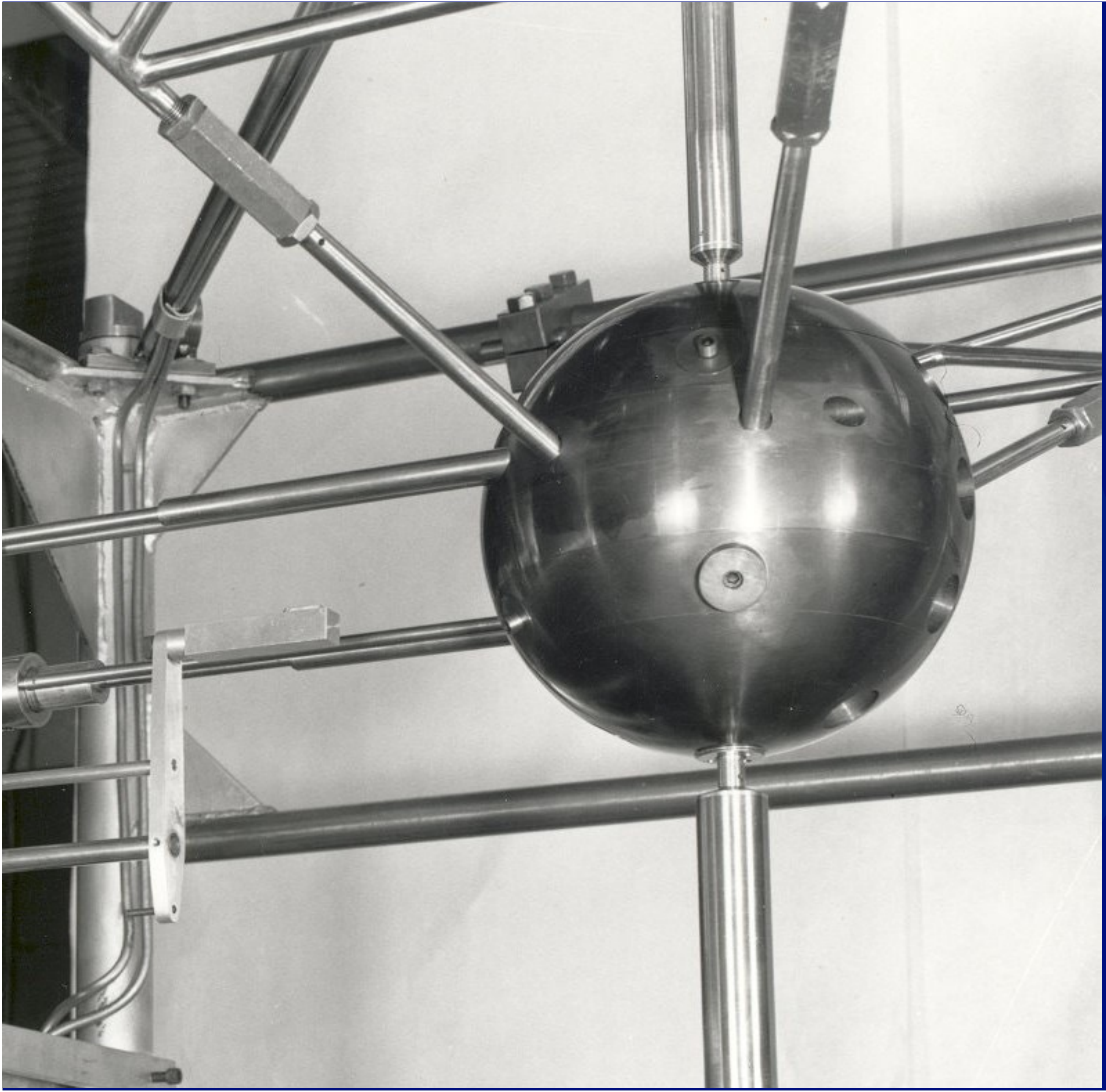


Configuration	Baseline	Comet Included	ΔKeff
1.27 cm	1.001374	1.005684	430 ± 2 pcm
2.54 cm	1.003063	1.006347	328 ± 2 pcm
5.08 cm	1.002767	1.004754	199 ± 2 pcm
8.89 cm	1.002844	1.003828	198 ± 2 pcm

Uncertainty Analysis – Room Return



Configuration	Baseline	Room Included	ΔKeff
1.27 cm	1.001355	1.001749	39 ± 2 pcm
2.54 cm	1.003025	1.003316	29 ± 2 pcm
5.08 cm	1.002756	1.002878	13 ± 2 pcm
8.89 cm	1.002828	1.002904	8 ± 2 pcm



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