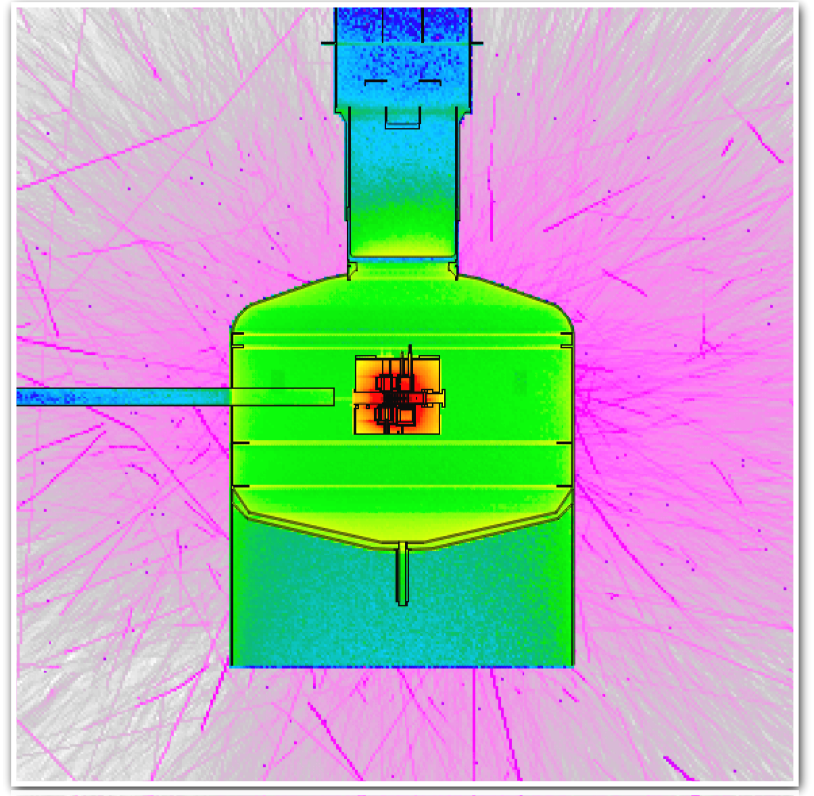
Science and Technology Facilities Council

ISIS Neutron and Muon Source

MC-driven analysis of key nuclear parameters in target design for optimised neutron yield

Insights from ISIS-TS1 and Notional Design Evaluation



Lina Quintieri, Steven Lilley

ISIS neutronics group

Abingdon, 29th October 2024

Science and Technology Facilities Council

ISIS Neutron and Muon Source

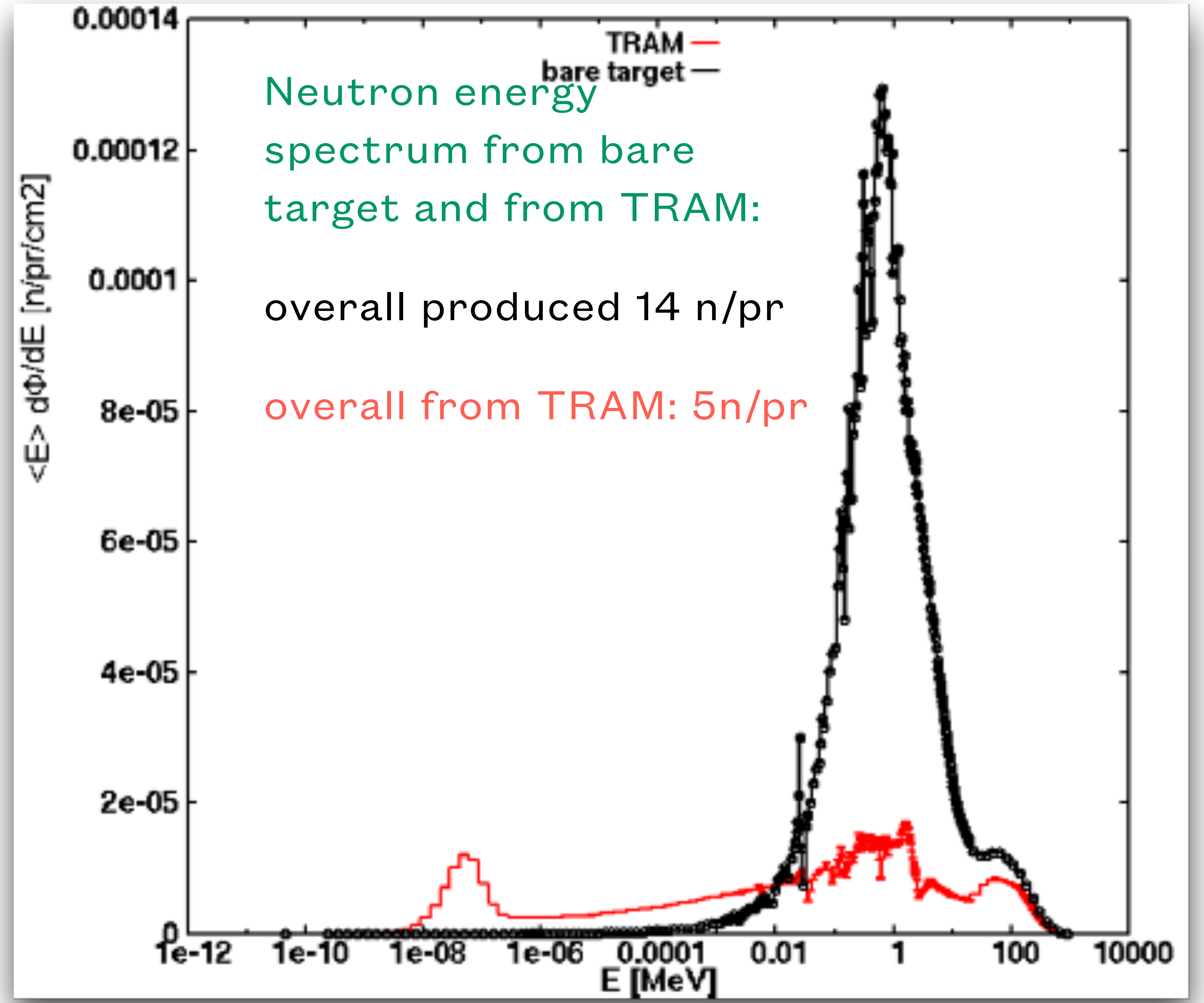
Overview

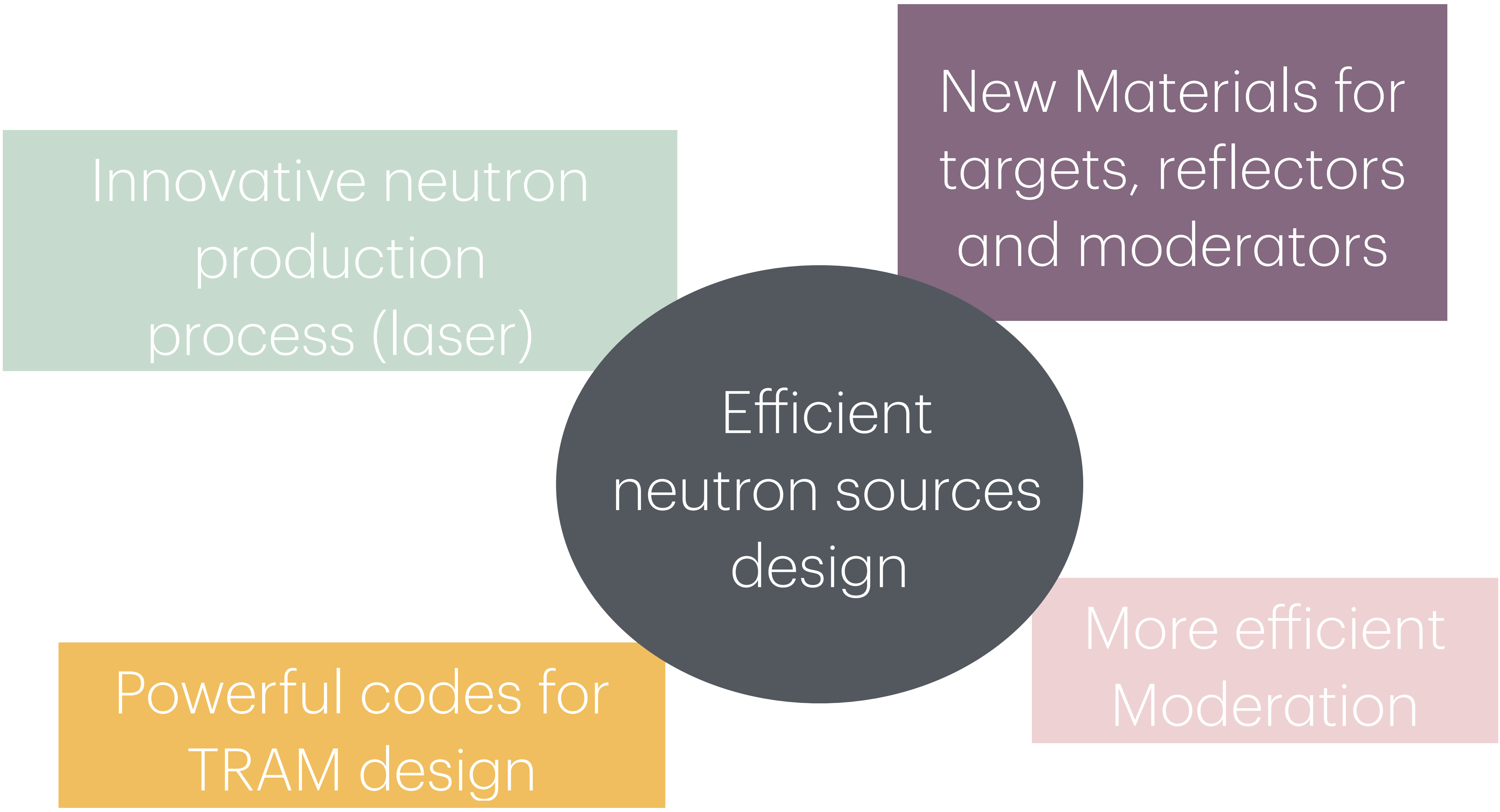
- The FLUKA models and benchmarking for ISIS-TS1
- MC analysis of the upgraded ISIS-TS1:
  - neutron yield: Optimising the target design Improving coupling between target and reflector (moderator brightness & neutron pulse shape at the instrument) (neutron leakage)
  - neutron leakage: Optimising the coupling target/reflector/moderator
  - Reducing the background: high energy neutrons, delayed neutrons, photons
  - In addition to E_dep, DH, RN, energy fluence spectrum (moderator brightness) calculation, I will show how some advanced features of MC code can help to further support in identifying an optimal spallation neutron source: lesson from ISIS-TS1

Increasing the "efficiency" of a neutron source

Scattering experiments need of intense neutron beam, low energy range and narrow pulse shape

- Make more neutrons —> powerful sources
- Reduce the neutron losses —> synergic and considerate reflector and moderator design along with the target design
- Reduce the background—> optimise the coupling of target with reflector and moderator assembly
- MC code are essential in better addressing the task !!!

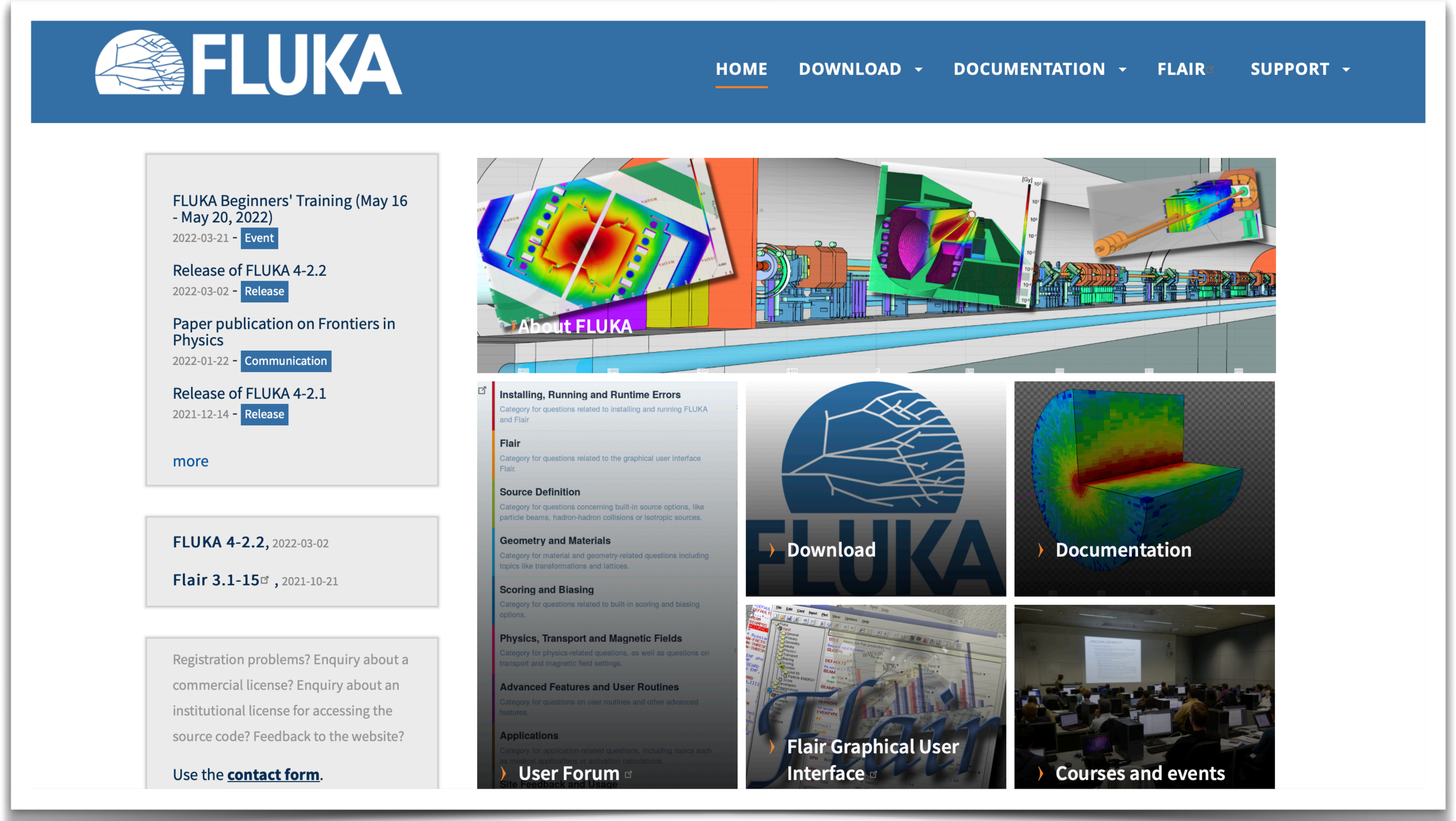




The FLUKA-CERN Updates on Neutronics

In 2019 the FLUKA collaboration split into two groups: the FLUKA-INFN and FLUKA-CERN

- Recent Important Milestones in neutronics and significant progress achieved in neutronics simulations with FLUKA-CERN
- Implementation of Point Wise XS and treatment.
- Enhanced Capabilities at low energy/temperature: Improved simulation of low-energy neutrons, particularly thermal and cold neutrons, with available scattering kernels for numerous materials at low temperatures.
- Expanded Data Library: Users now have the flexibility to select from various data libraries and file formats (e.g., ACE), enriching FLUKA's capabilities.
- All the decay products are transported and can interact in the materials (beta-+, gamma, alpha, delayed neutron)
- Uploading meshed geometry from cad files into FLUKA in progress



Neutron scattering in the eV range and below

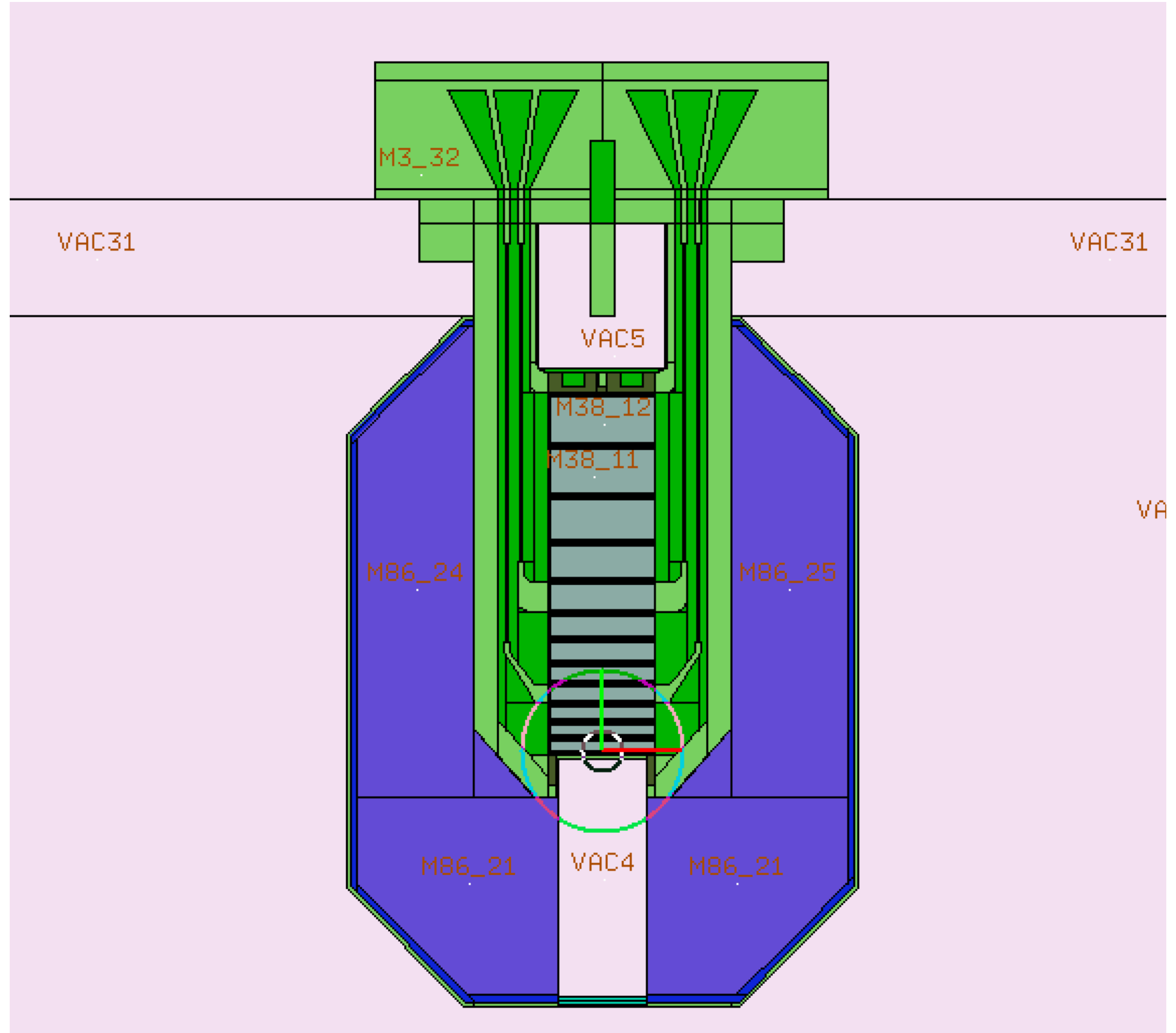
Neutrons see nuclei as bound in molecule several vibrational modes can be activate as a mechanism to lose energy.

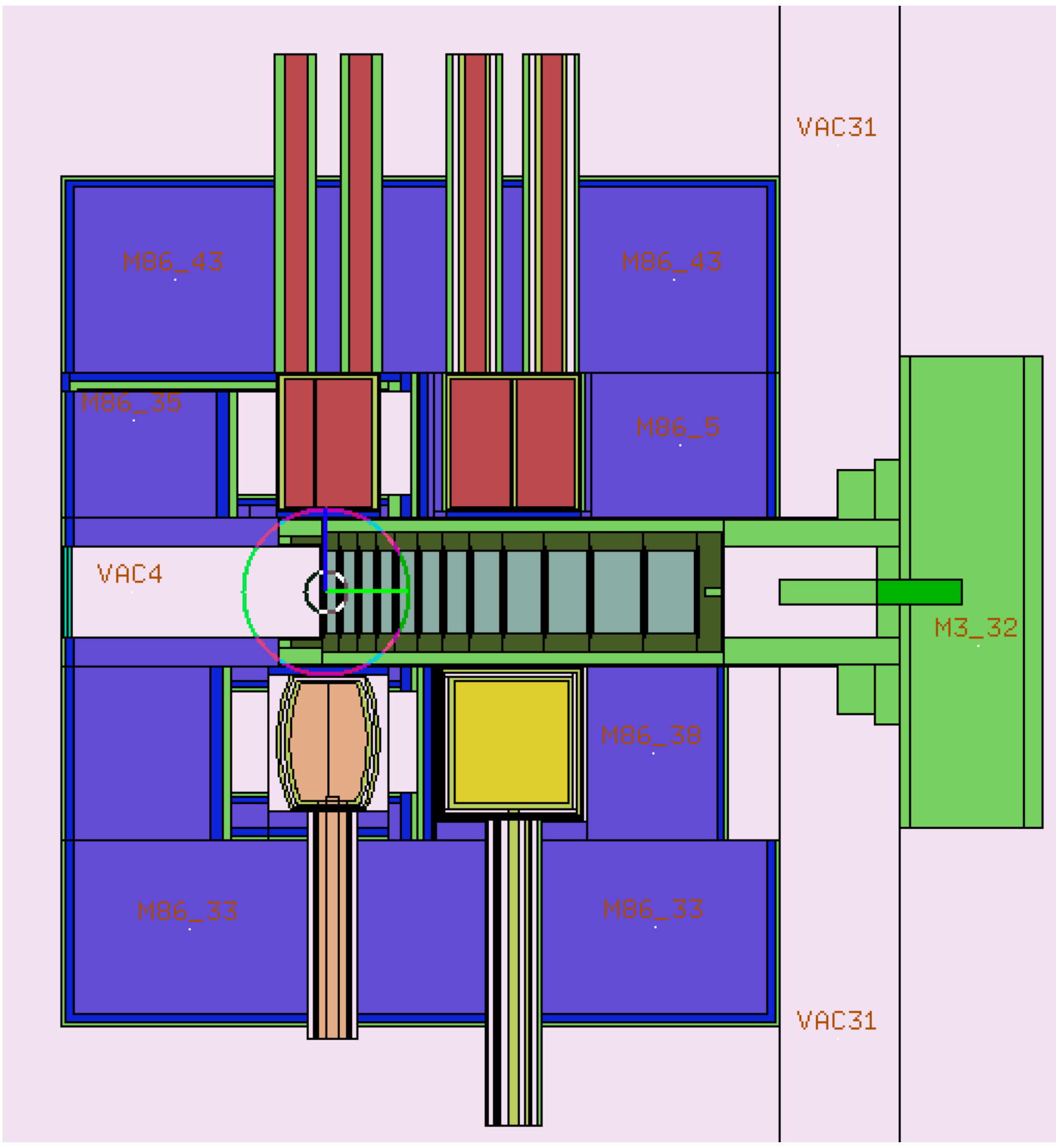
the scattering nucleus is considered at rest (KE=0)

neutron scattering elastically only changes direction

The old model of ISIS-TS1 and DH meaurement

The model of the last dismissed target has been imported via Flair from the MCNP one





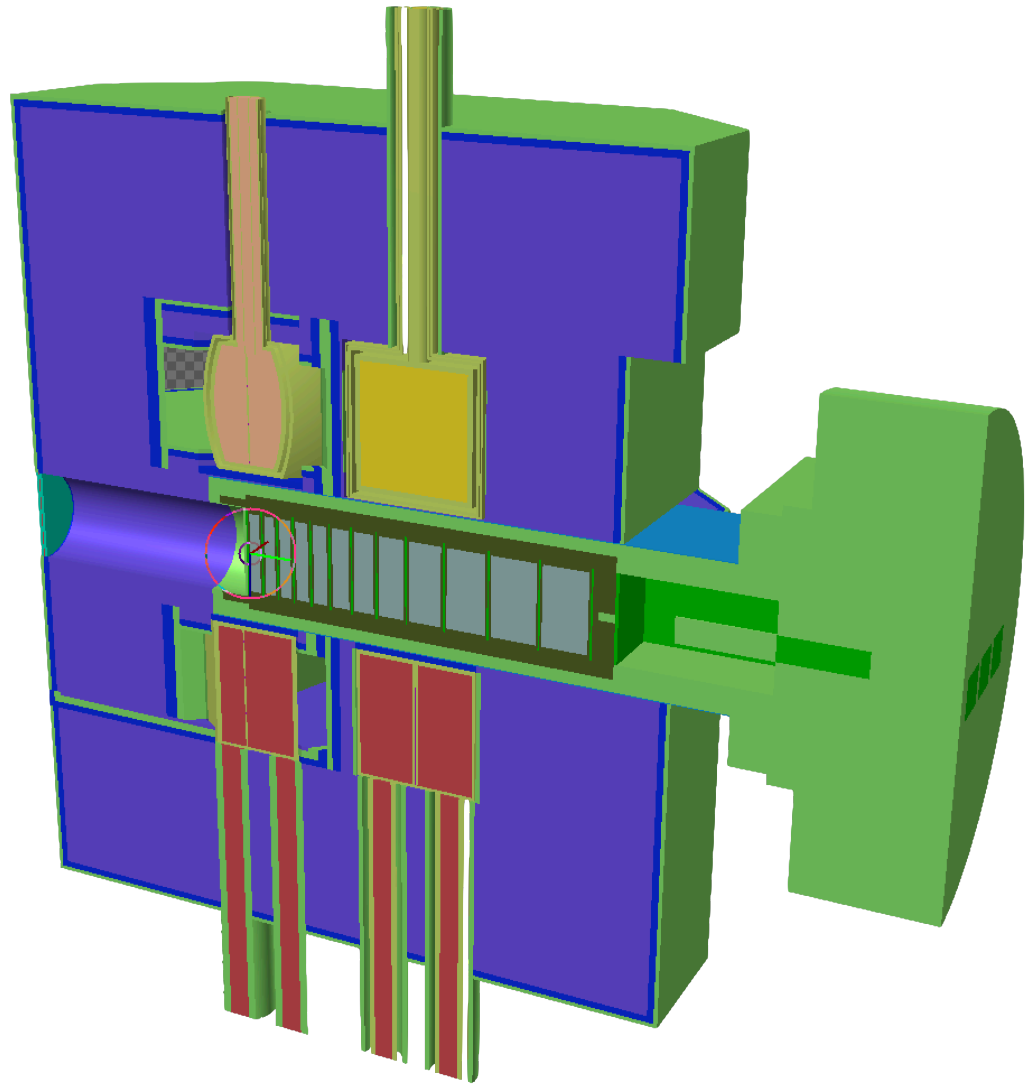


Table 4

Active cooling on and off periods during the test for heat decay measurement

Date	Cooling-off	Cooling-on
20 Dec. 2018	08:31:20	08:59:55
20 Dec. 2018	09:30:06	10:00:10
20 Dec. 2018	11:30:21	12:00:17
21 Dec. 2018	08:30:05	09:00:03
23 Dec. 2018	08:30:02	09:00:02
27 Dec. 2018	08:30:02	09:30:04
3 Jan. 2019	08:30:02	10:30:03

Thermal loads for ANSYS CFX simulations

Total Decay Heat in the target (W + Ta + SS)		
Cooling time	FLUKA [W]	MCNPX [W]
1 min	754	1274
1 hour	561	953
1 day	405	771
3 days	379	716
1 week	338	674
2 weeks	284	636

ref1 L.Quintieri et al, Journal of Neutron Research 24 (2022) 313–327-DOI 10.3233/JNR-220030

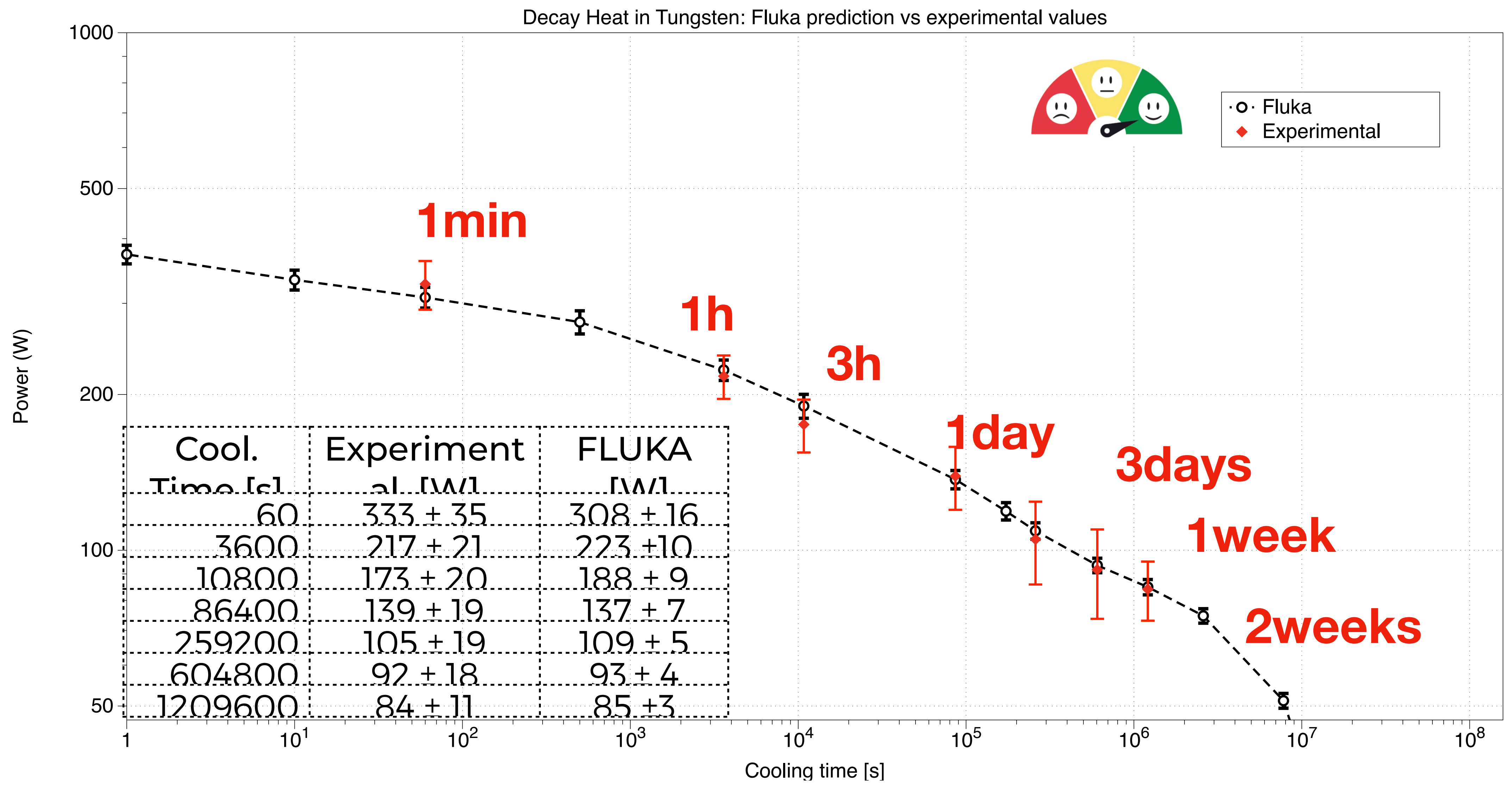
ref2 *D. Findlay* Ms. Ref. No.: NIMA-D-23-01072R1

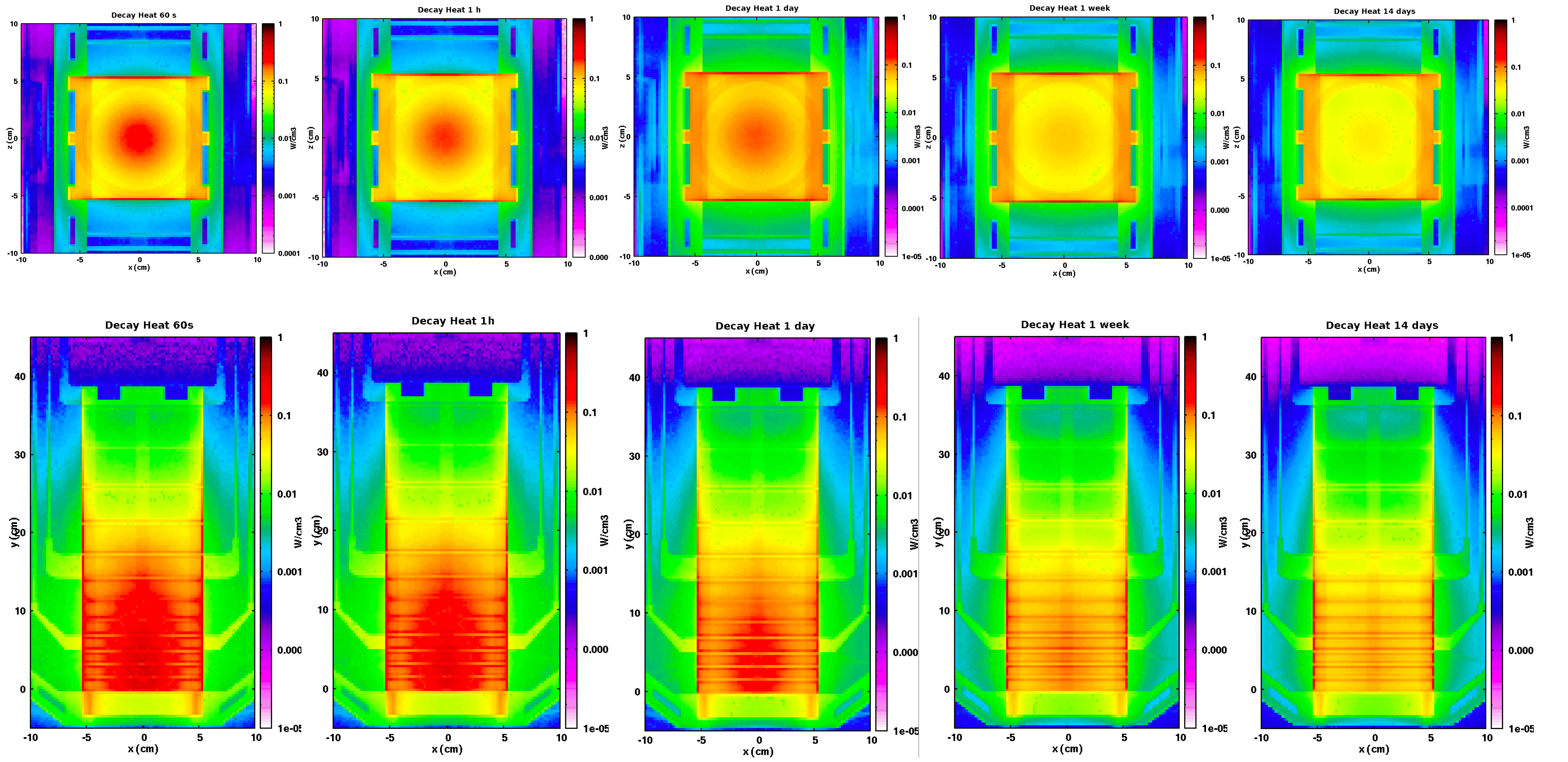
Benchmarking the Model wrt DH in W

Decay heat in tungsten at selected cooling times

Cooling time	Experimental [W]	*FLUKA** [W]	*MCNPX/CINDER90*** [W]
1 min	333 ± 35	308 ± 55	437 ± 87
1 hour	217 ± 21	223 ± 40	205 ± 57
3 hours	173 ± 20	188 ± 34	155 ± 31
1 day	139 ± 19	137 ± 25	89 ± 18
3 days	105 ± 19	109 ± 20	52 ± 10
1 week	92 ± 18	$93. \pm 17$	33 ± 7
2 weeks	84 ± 11	85 ± 15	25 ± 5

*Statistical plus systematic (as described in the text) uncertainties
**$\pm 20\%$ overall estimate uncertainties



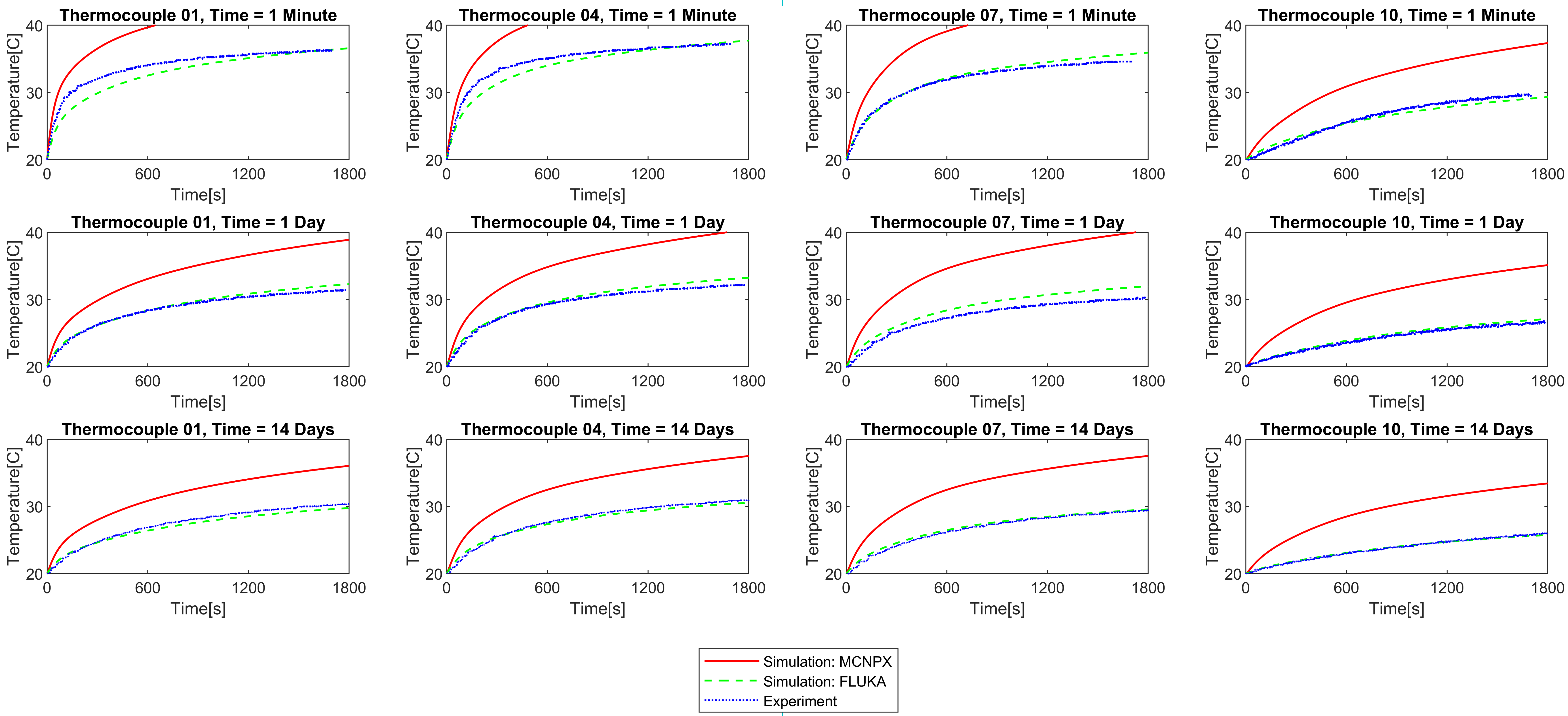


t=60 s t=1 h t= 1 day t= 7 days t= 14 days

- Thanks to two independent models, the experimental values of the decay heat deposited respectively in the inner tungsten regions and in the whole target (tungsten + tantalum cladding + stainless steel vessel) could be estimated
- The agreement between the FLUKA predictions and the experimentally derived values shows and quantifies the goodness of the FLUKA model in predicting the decay heat as relevant and indirect estimation of both the radioactive nuclei inventory produced and the correspective spatial distribution in the whole TRAM.
- Last but not least, this work attempts to highlight and propose a general empirical procedure that could be eventually applied and used to proficiently measure the decay heat at whatever cooling time in targets with similar ISIS design.

ref1 L.Quintieri et al, Journal of Neutron Research 24 (2022) 313–327-DOI 10.3233/JNR-220030

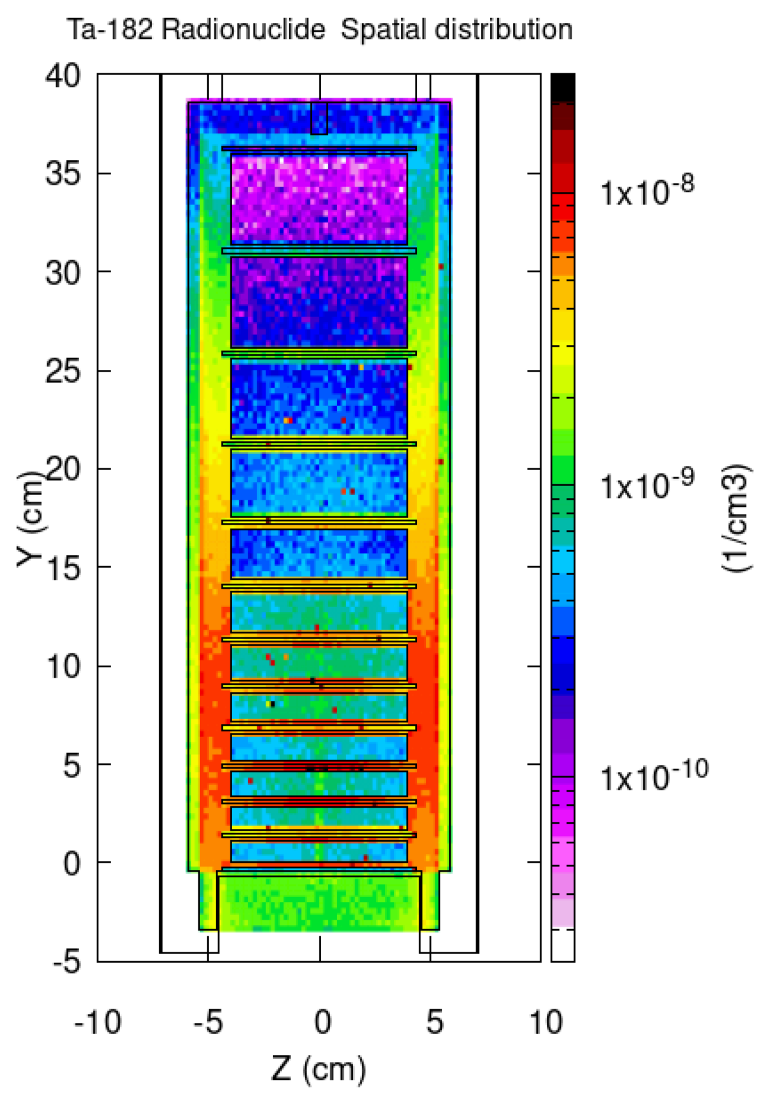
Benchmarking the Model wrt total DH

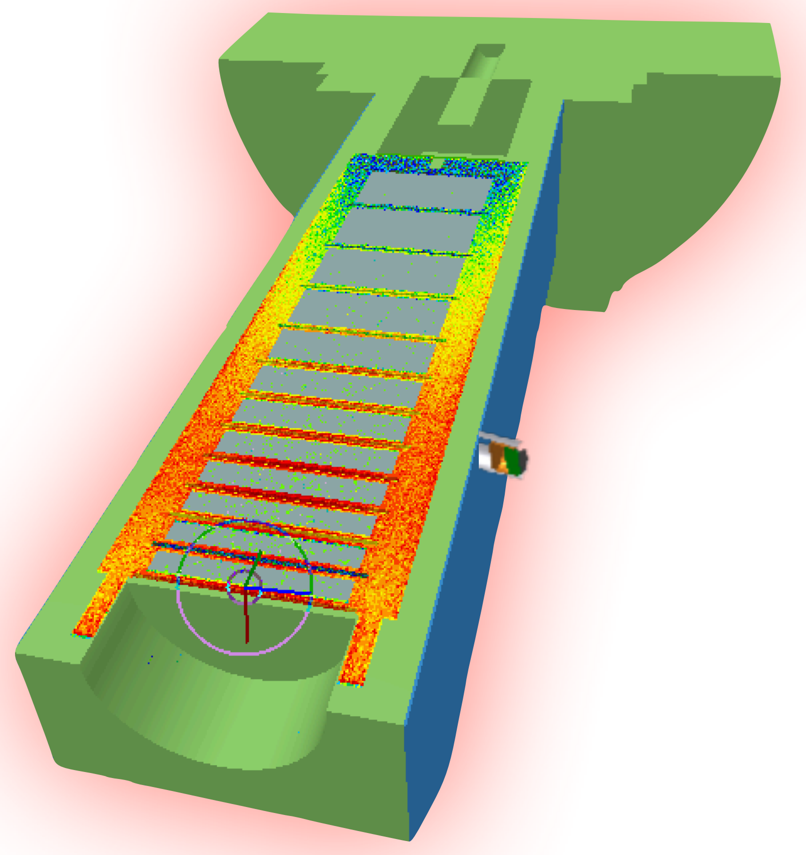


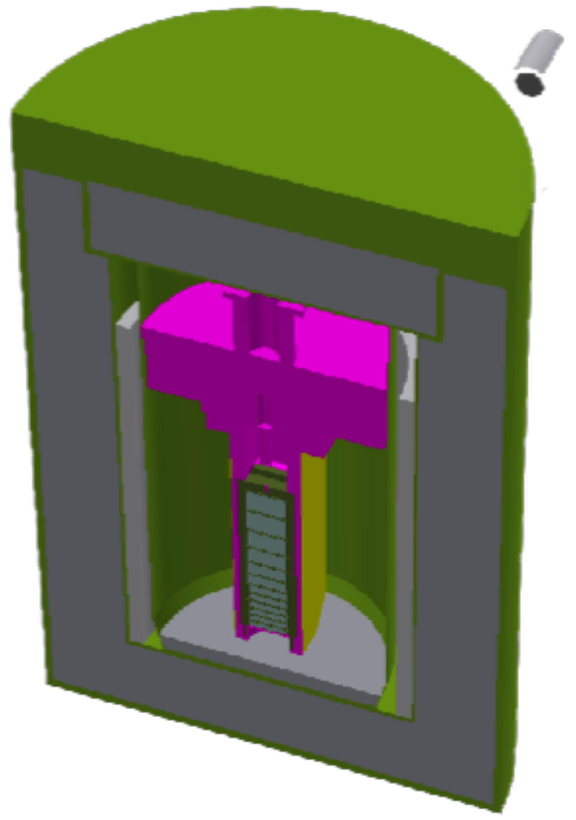
ref1 L.Quintieri et al, Journal of Neutron Research 24 (2022) 313–327-DOI 10.3233/JNR-220030

Benchmarking the FLUKA Model wrt RN inventory

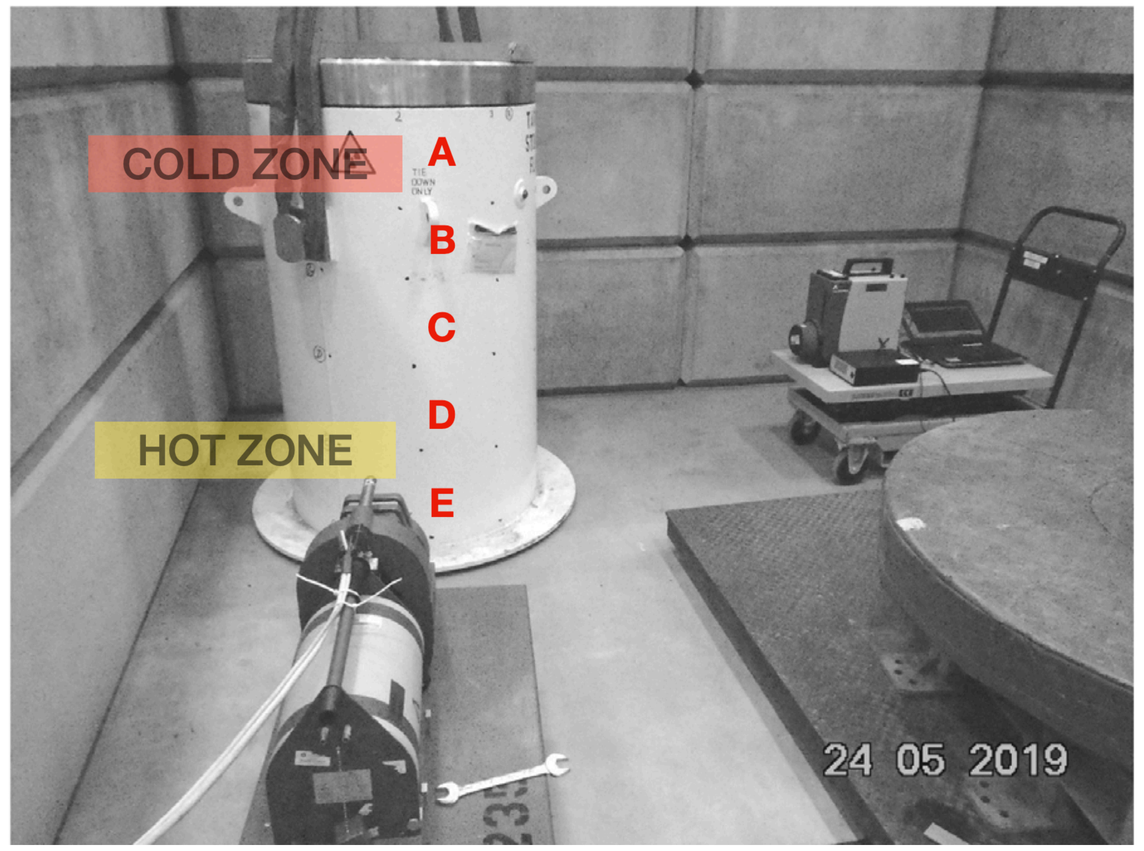
Ta-182 density spatial distribution in the target (values are per primary)







measured gammas for Ta-182	
E(keV)	Ig(%)
1121	35,17
1189	16.58
1221	27.27



$$[1]\ \ A[Bq] = \frac{CR - CRB}{f_{br} \cdot f_{eff} \cdot f_{sa} \cdot f_{shl} \cdot f_{dc}}$$

☀**RN:**

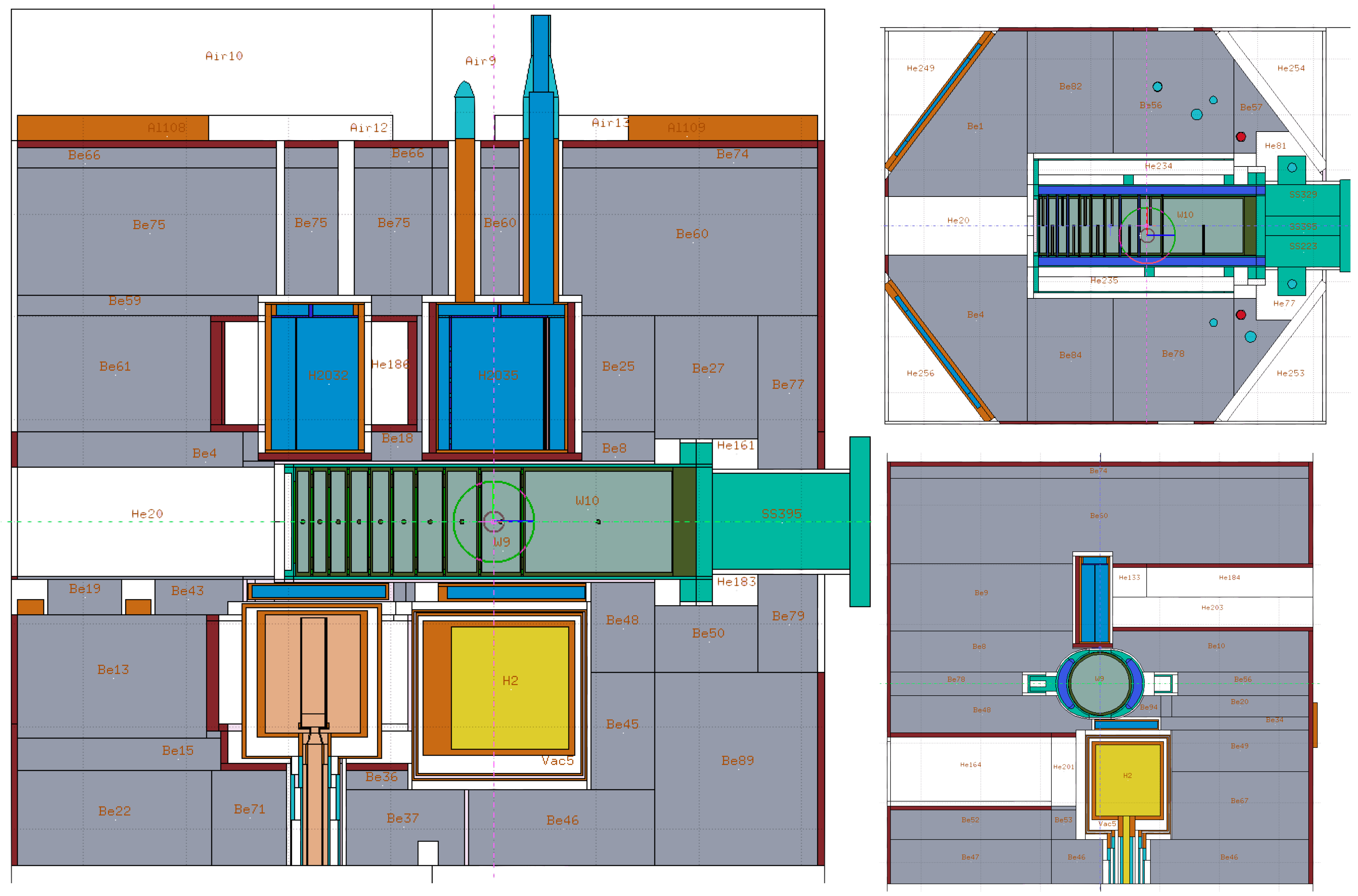
Radionuclide	Activity		Region
	FLUKA	Experimantal	
Hf-172	5.6 ±1.1 TBq	7.6±1.9T Bq	W core
Ta-182	62.6±10 GBq	82±20 GBq	Ta cladding
Co-60	5.9±1.2 TBq	5.0±1.1 TBq	SS vessel

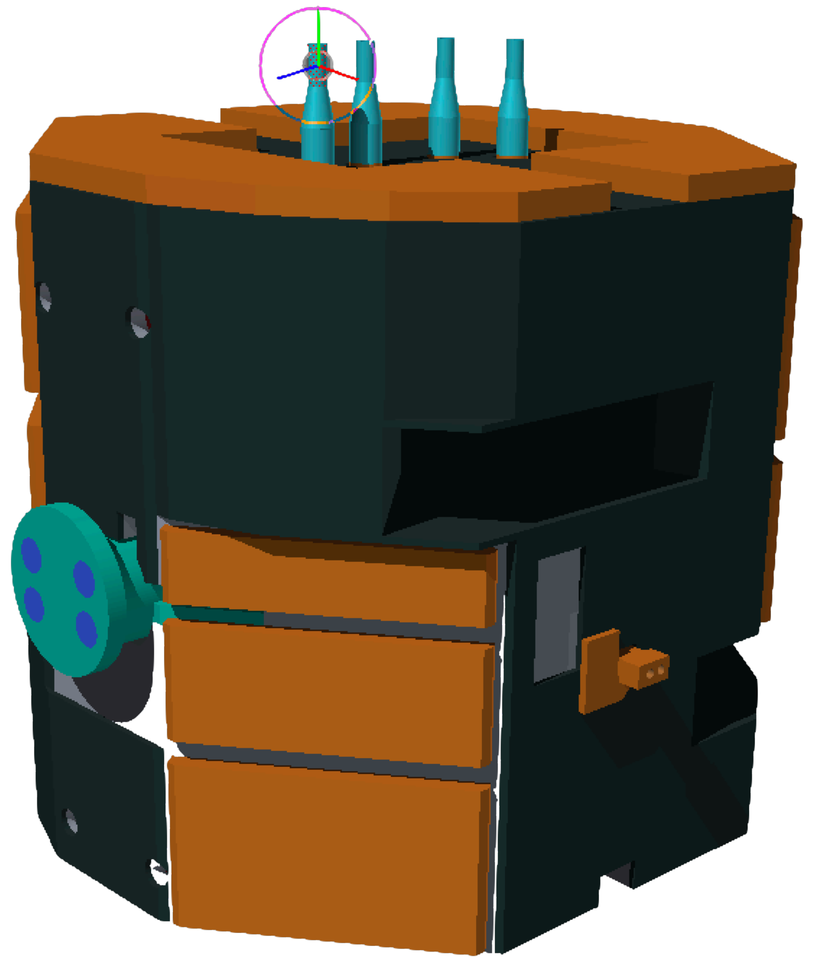
The FLUKA predictions for the activities of Hf-172 in the tungsten core, Ta-182, in the cladding, and Co-60, in the target stainless steel vessel, have been successfully validated. MC estimations agree with experimental values within the uncertainties. These results confirm FLUKA-CERN's ability to accurately reproduce both the integrated activity and the spatial distribution of the radionuclides within the targe

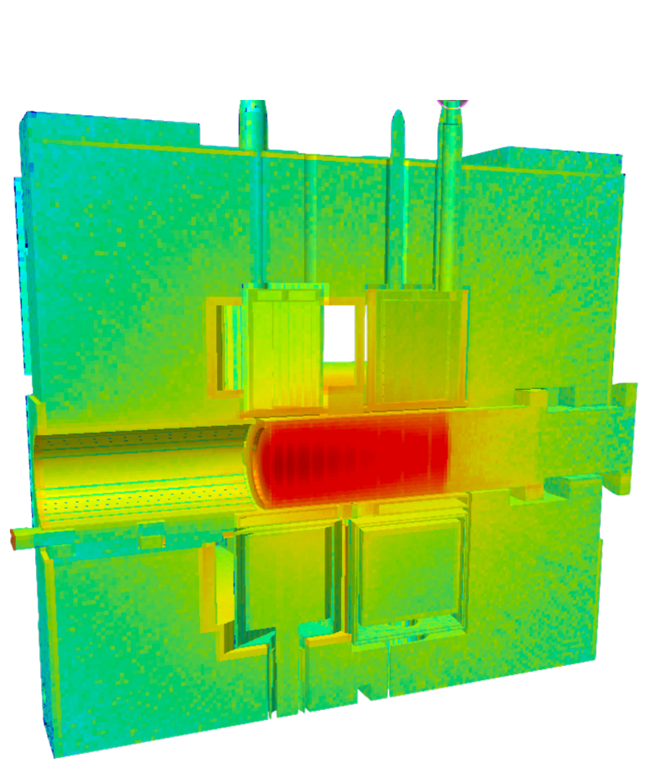
ref1 L.Quintieri et al, work presented at SATIF—16 proceeding in progress

The upgraded FLUKA model of ISIS-TS1

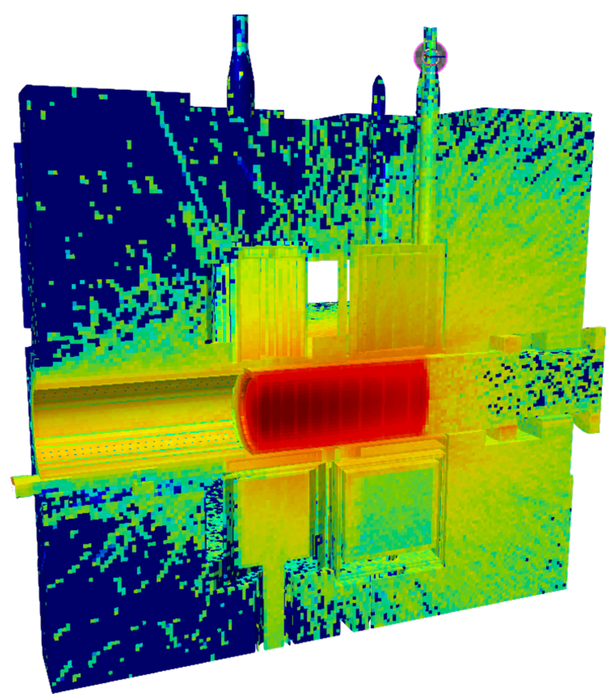
The model of the new TRAM has been implemented by scratch based on the CAD designs



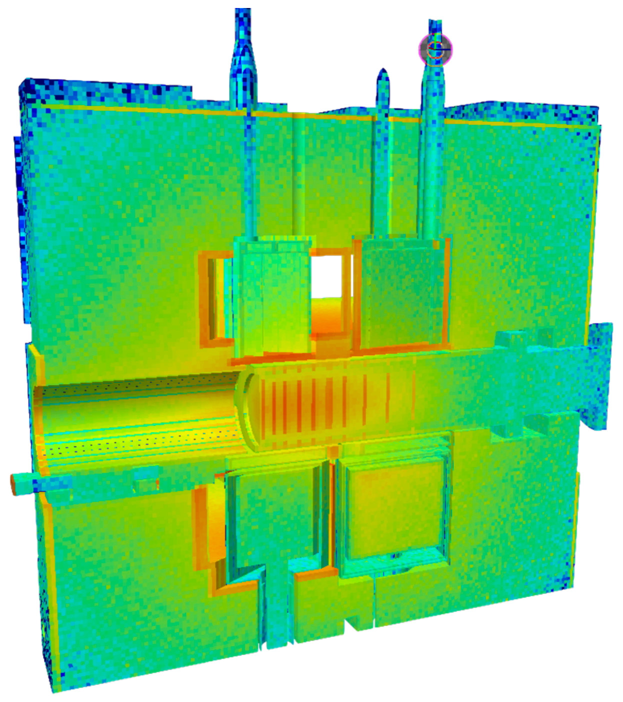




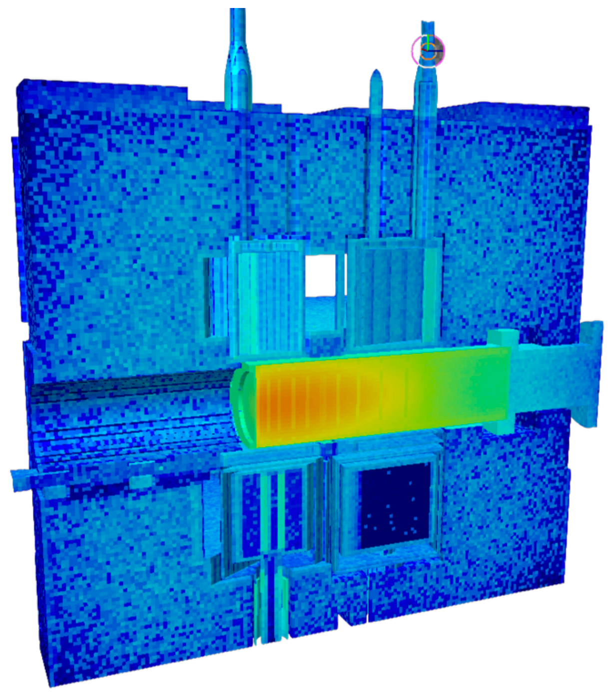
Total E_dep



Proton E_dep

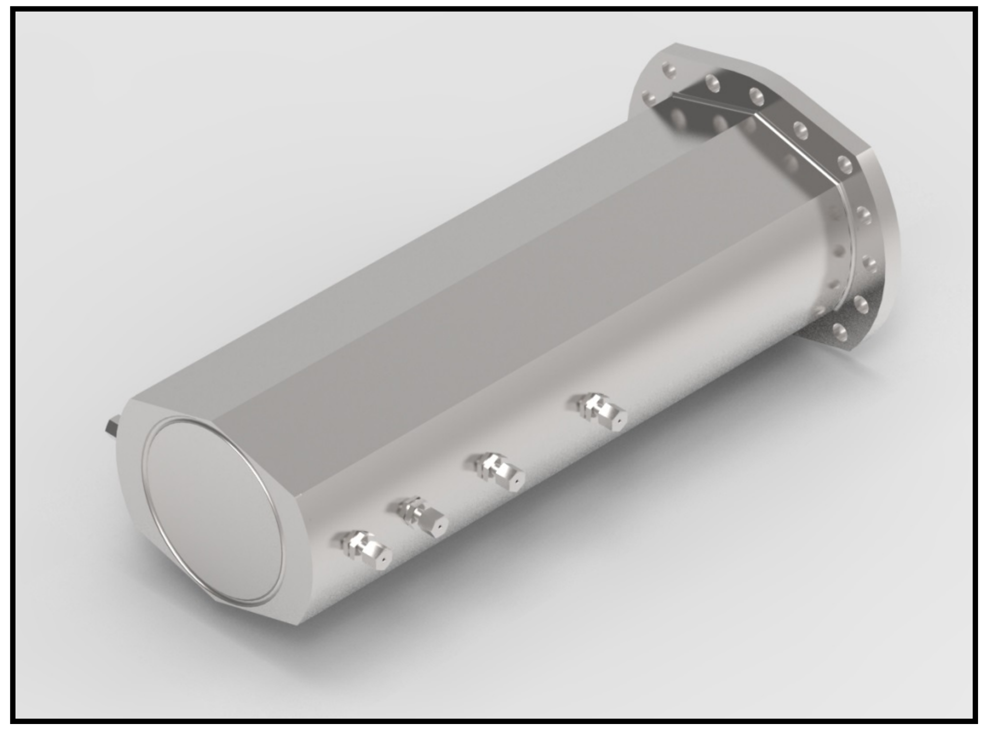


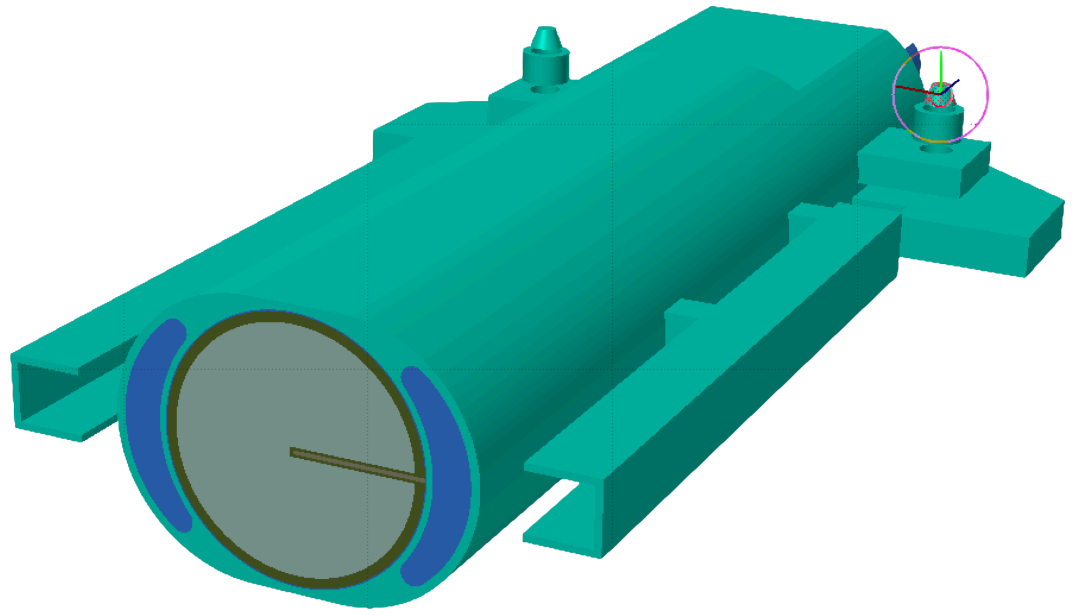
Neutron E_dep

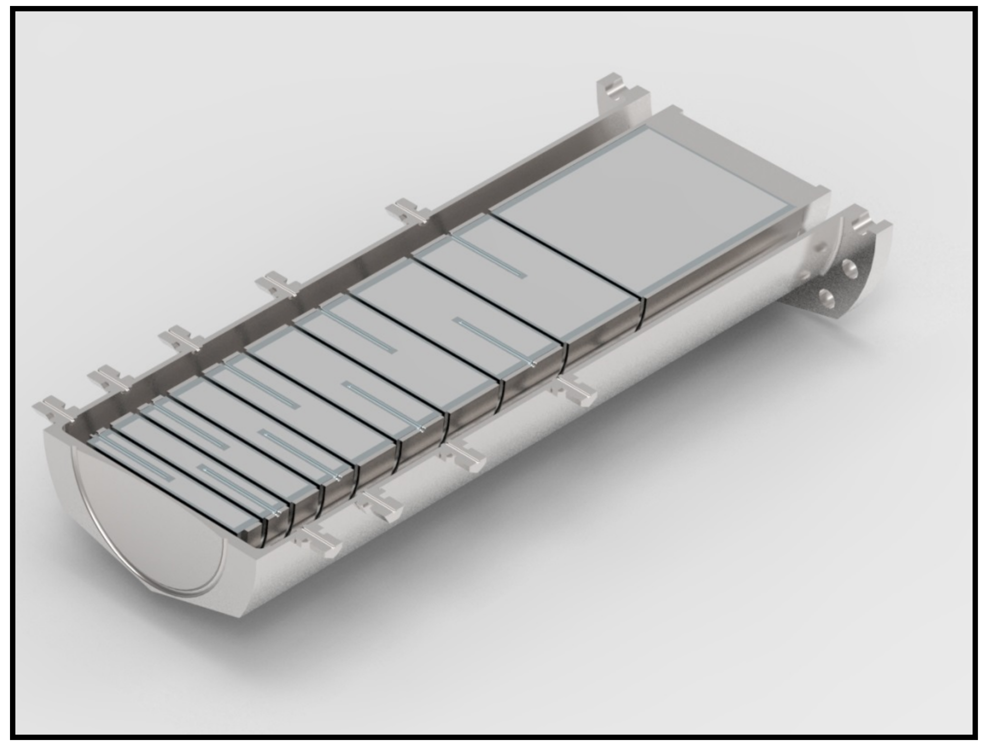


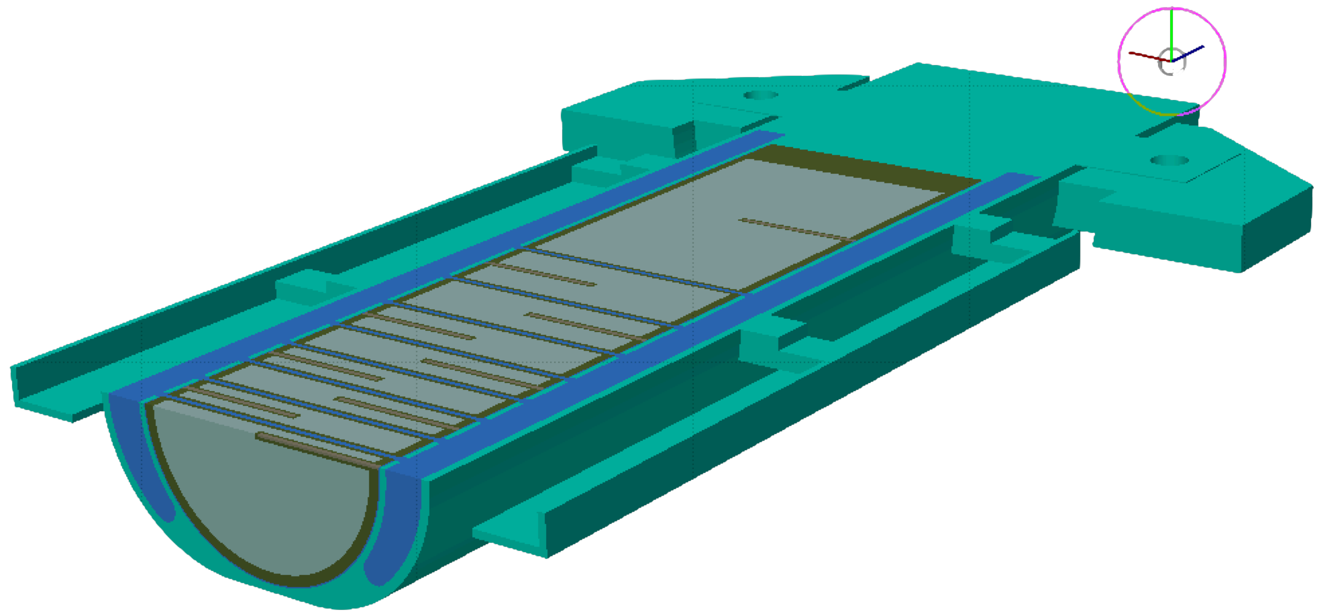
Gamma E_dep

Geometric accuracy of the model









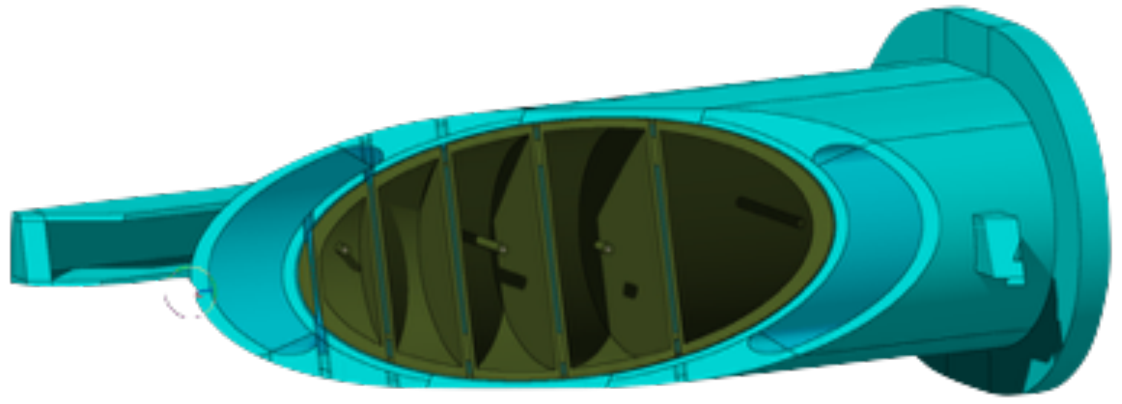
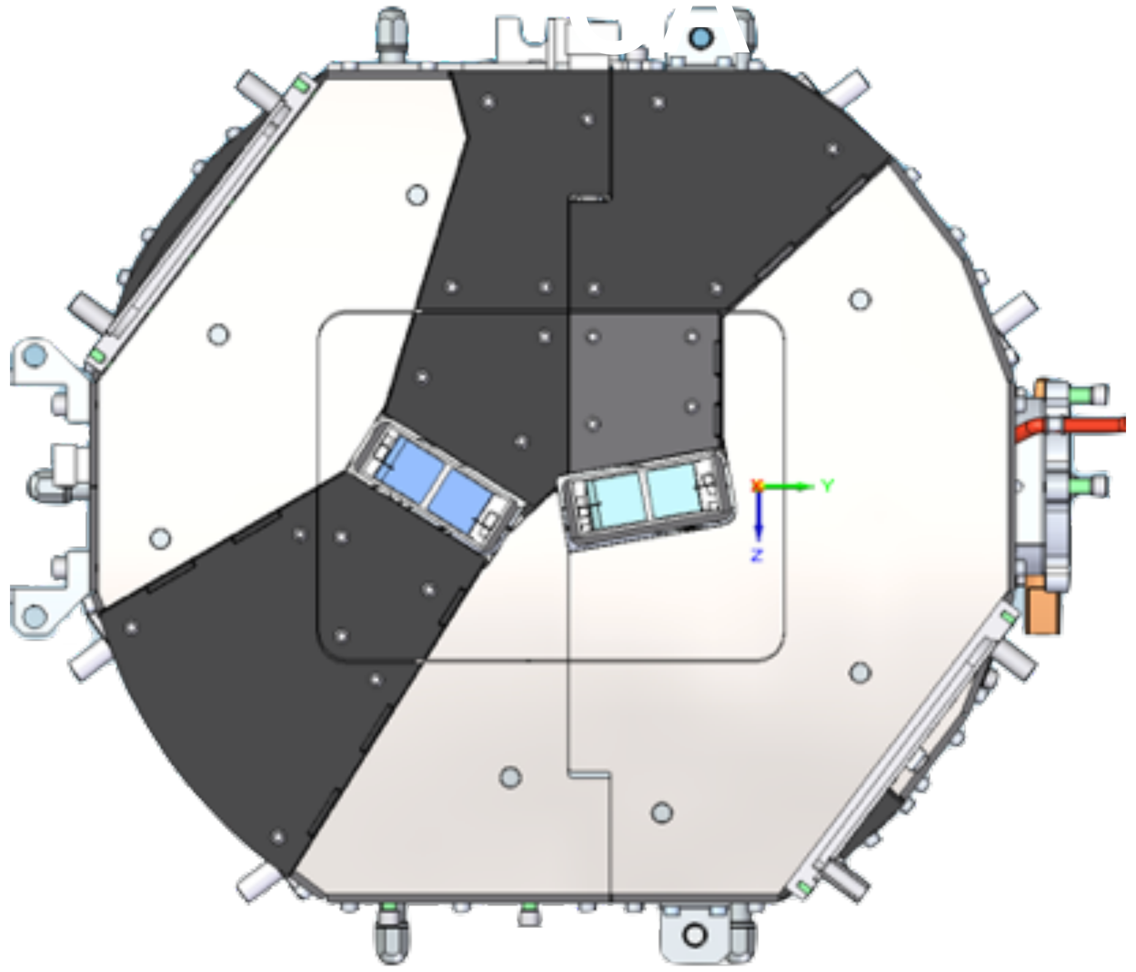


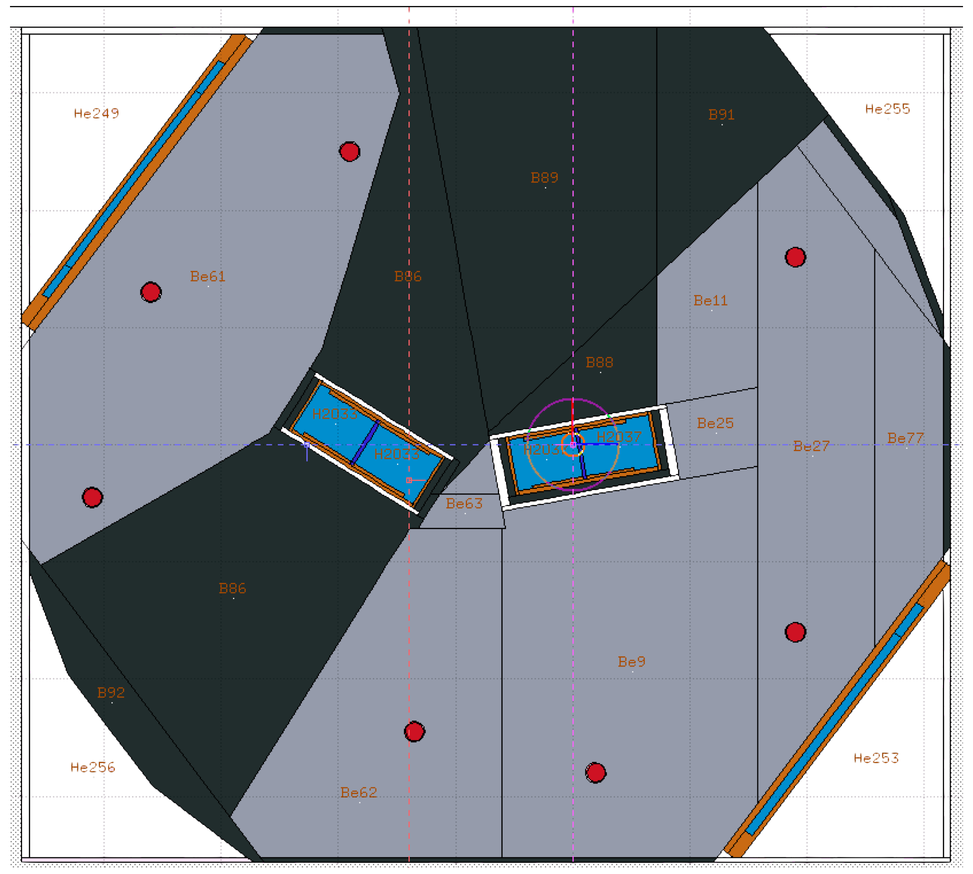
Table 3: Thickness of each tungsten plate

plate	cm
1	1.1
2	1.2
3	1.4
4	1.6
5	1.6
6	1.9
7	2.3
8	2.9
9	3.7
10	14.3



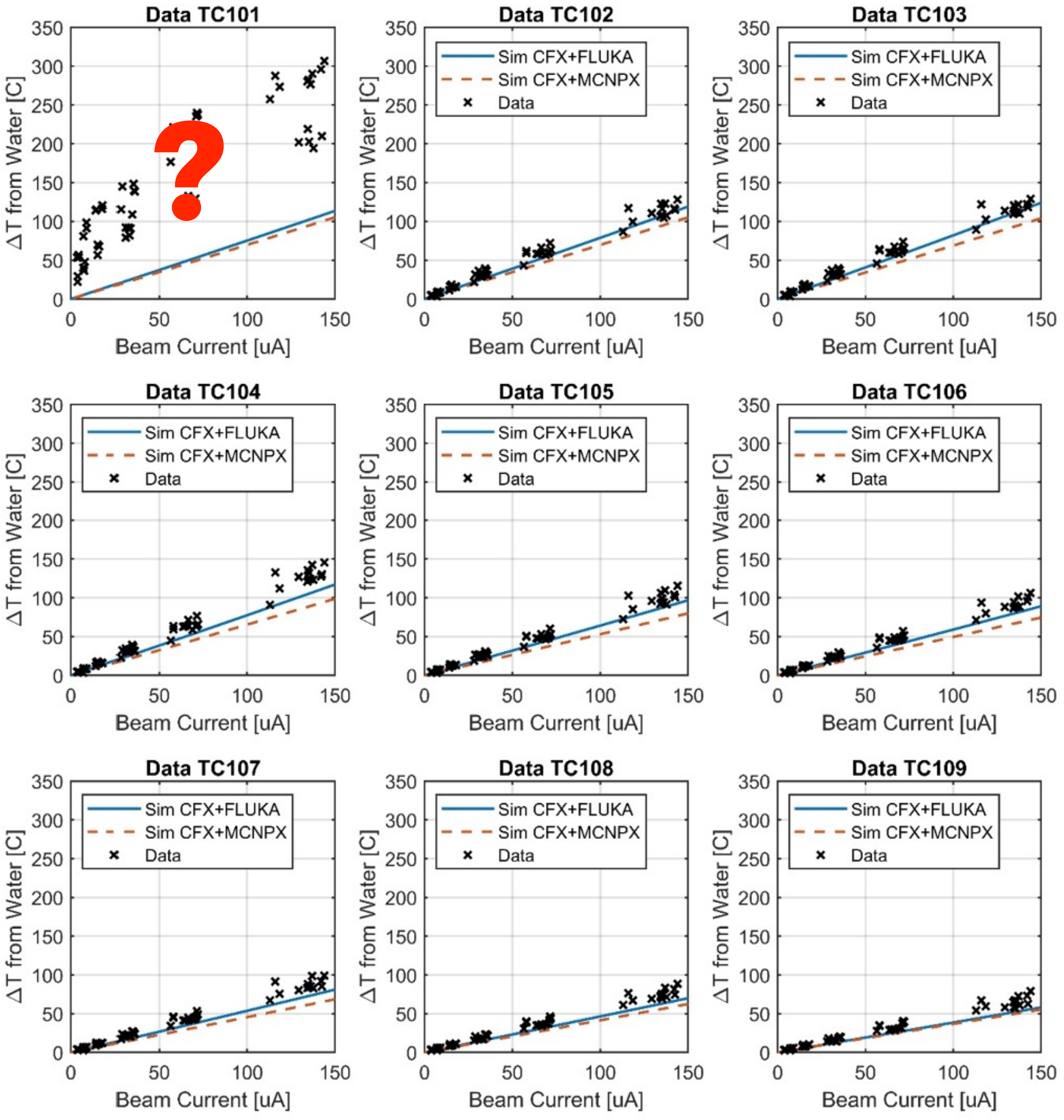
Very accurate model of the whole TRAM: between CAD and FLUKA model, the maximum difference in the volumes for each components is always less than 3%

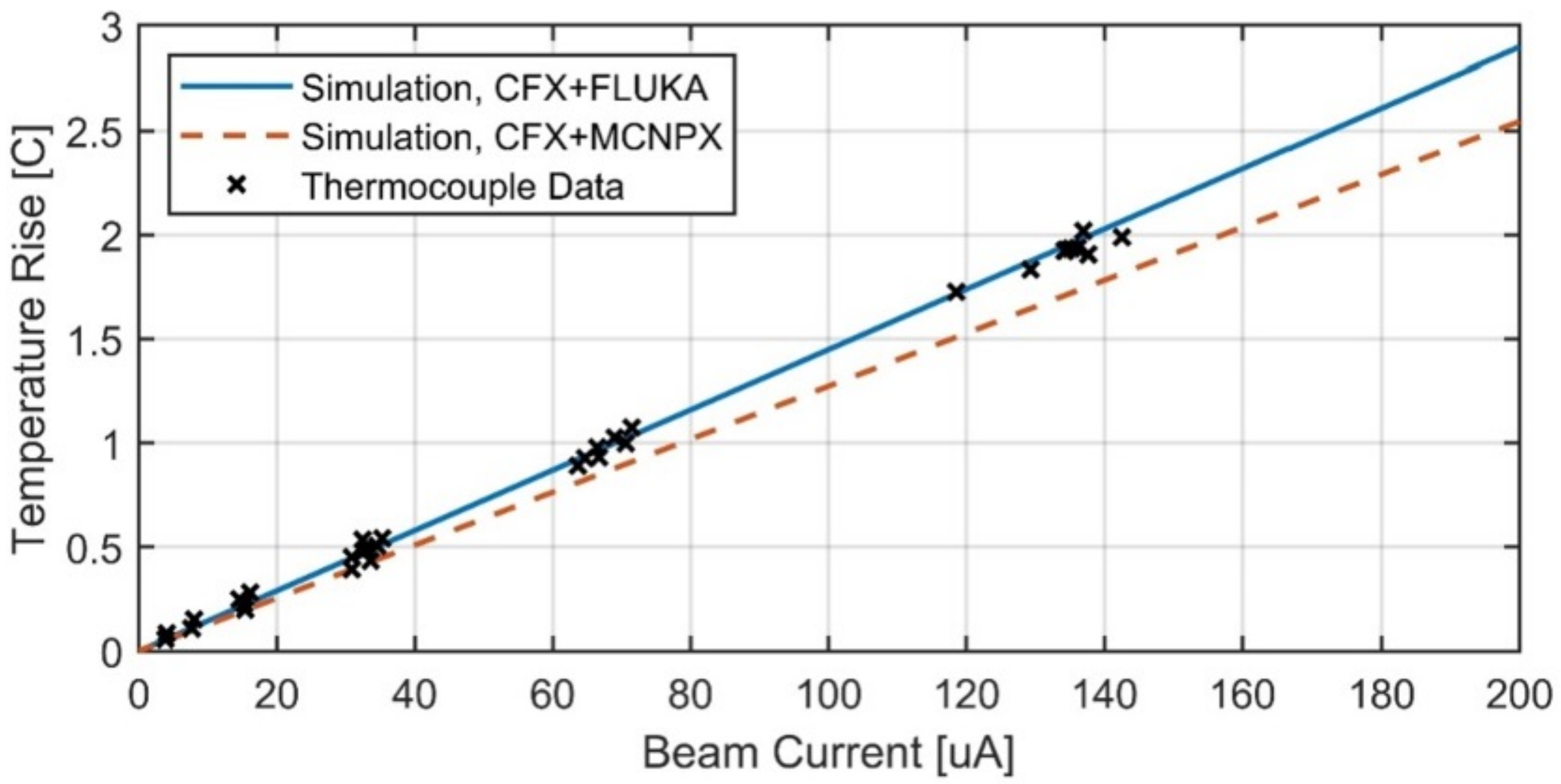
Ta cladded thermocouples are introduced in the Fluka model as well



The target core is made of 10 tungsten plates, each of 4.9 cm radius, cladded with tantalum (cladding thickness is 0.2 cm).

Benchmarking the Model wrt Energy deposition





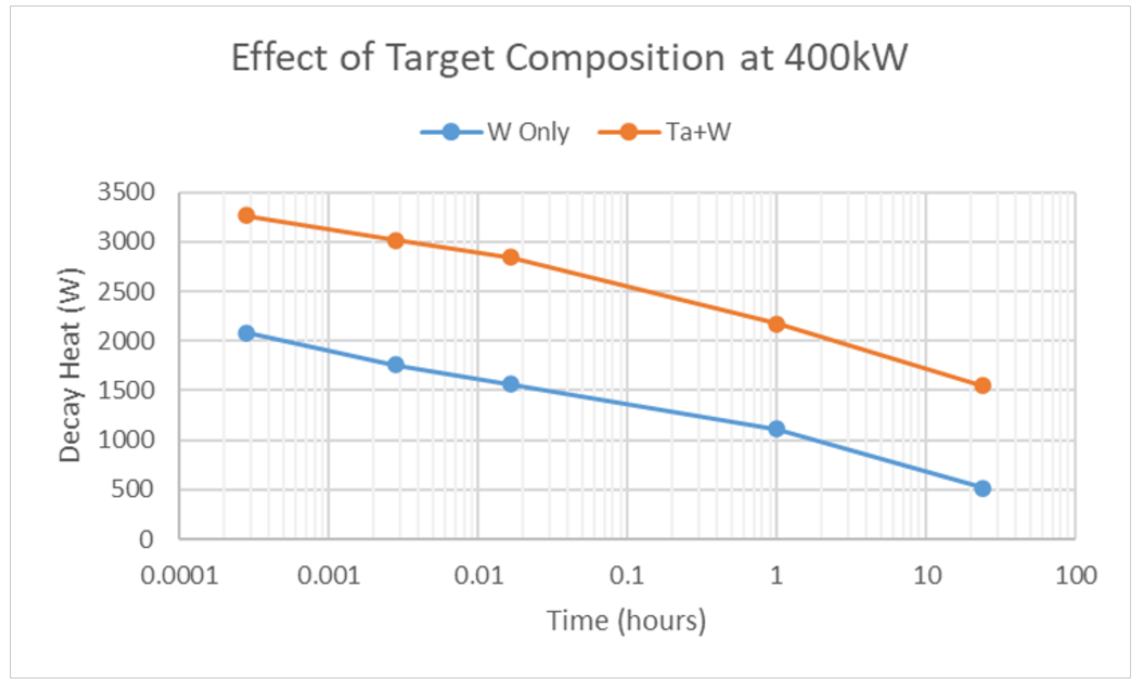
For further details —> talk of Dan Wilcox today

Thermal performance of the recently installed TS-1 Project target was measured and compared to predictions from FEA simulations. Steady state and transient thermal simulation results agree well with measured temperatures on 9 out of 10 target plates. The thermal performance of the target appears to be in line with expectations, with the exception of the front target plate, the temperature of which was elevated compared to predictions.

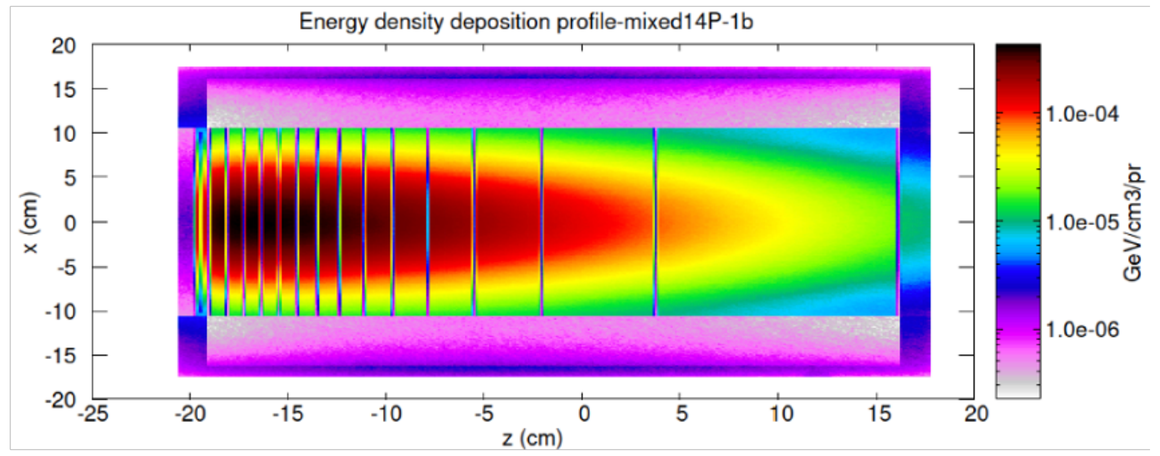
ref1 **Dan Wilcox** Journal of Neutron Research 26 (2024) 47–58 47 DOI 10.3233/JNR-24

New target dpa predictions: comparison between codes

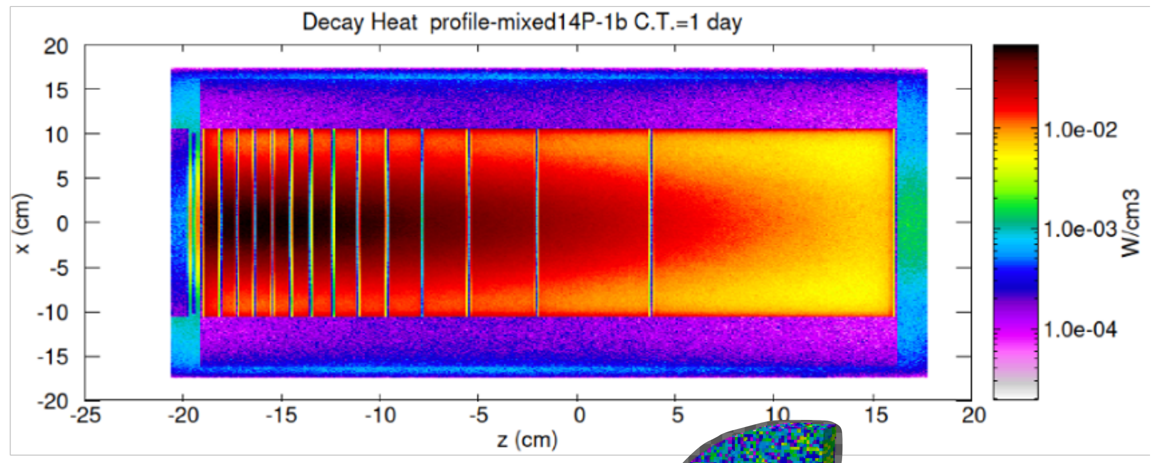
- FLUKA can perform within the same model:
- 1)Prompt Energy deposition calculations
- 2)RN inventory and DH calculations
- 3)DPA estimations

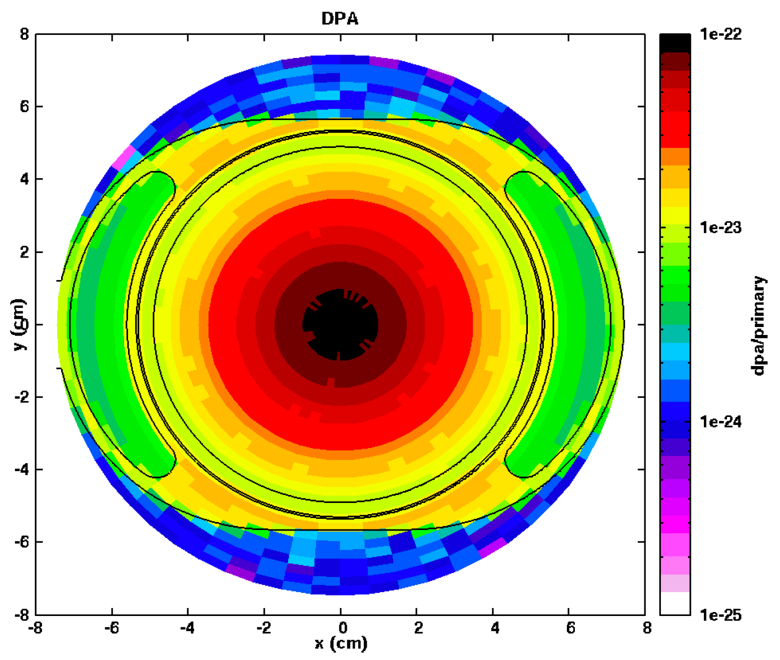


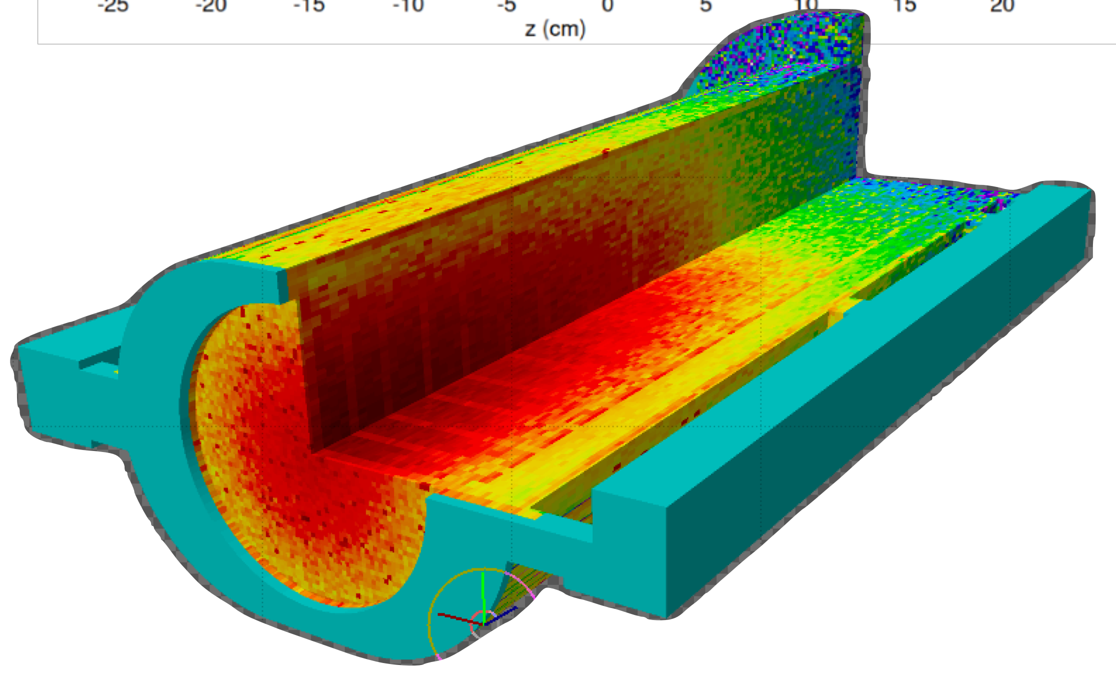
Ta+W Direct beam:



Ta+W Decay heat:







Case	Peak dose per Amp-hour (DPA/Ah)
TS1 (FLUKA-ISIS)	8.6
TS1 (MCNPX-IFN)	8.5
SNS (MCNP)	9.9

Details of dpa calulations:

- NRT-dpa as dpa-sco by "usrbin"
- charged particle transport has been set to 1.0 keV
- Values for the DAMAGE ENERGY THRESHOLD assumed for the materials in the models(based on NJOY suggested values):
- Tungsten: 90 eV
- Tantalum: 90 eV
- IRON: 40 eV
- Nickel: 40eV

All Monte Carlo simulations used DPA-NRT, with the possible exception of the SNS studies which did not report any particular DPA standard

Neutron yield: target design optimisation

MC parameters for optimisation: proton range, nuclear collision mean free path, absorption XS of relevant materials

The Role of the Target in Spallation Sources

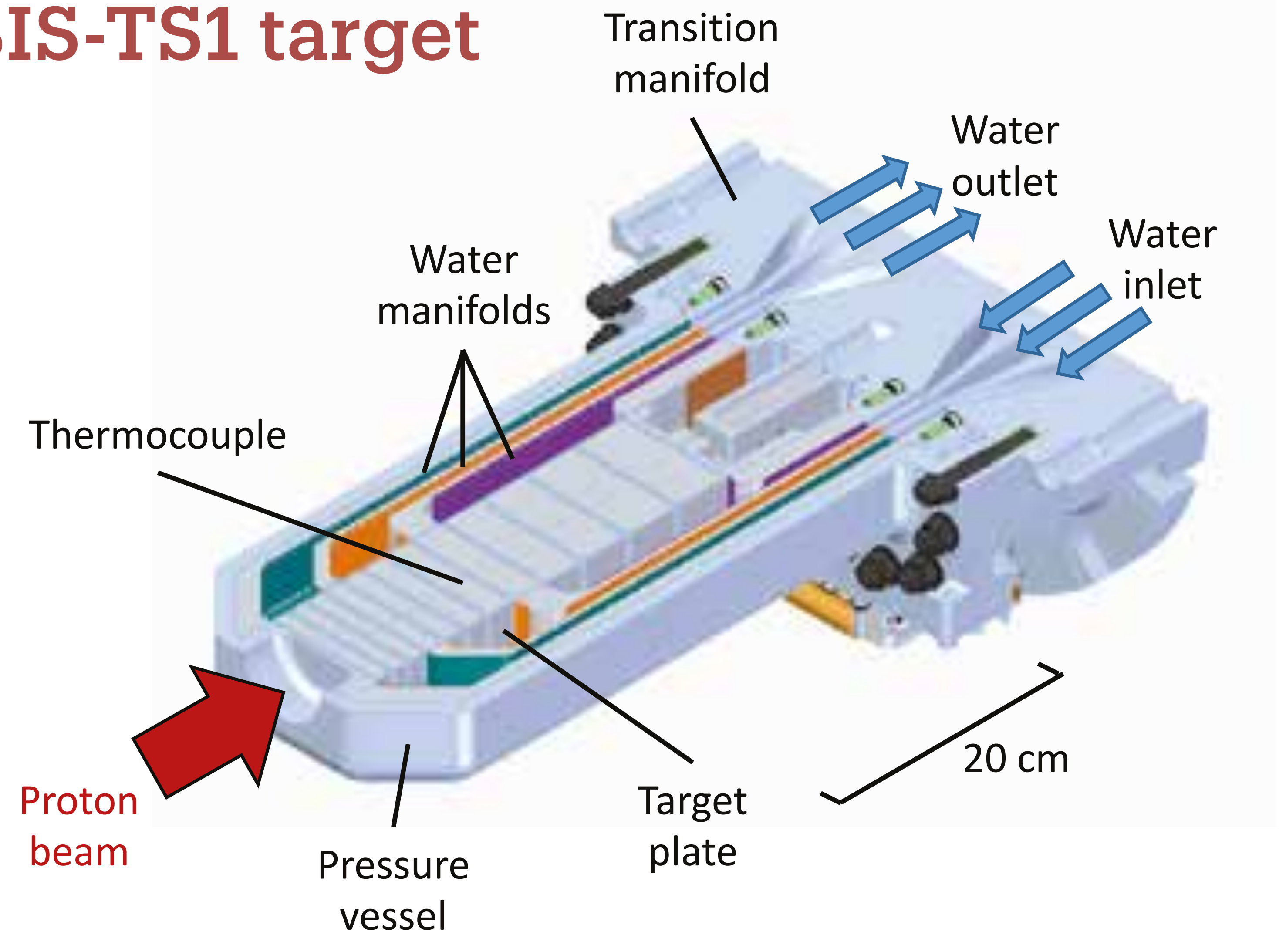
- The essential function of the targets in spallation sources is to convert the high-energy proton beam into as many neutrons as possible, whilst occupying as small a volume as possible.
- Minimising the volume within which protons are converted to neutrons results in the highest neutron fluxes.

nucl. parameters

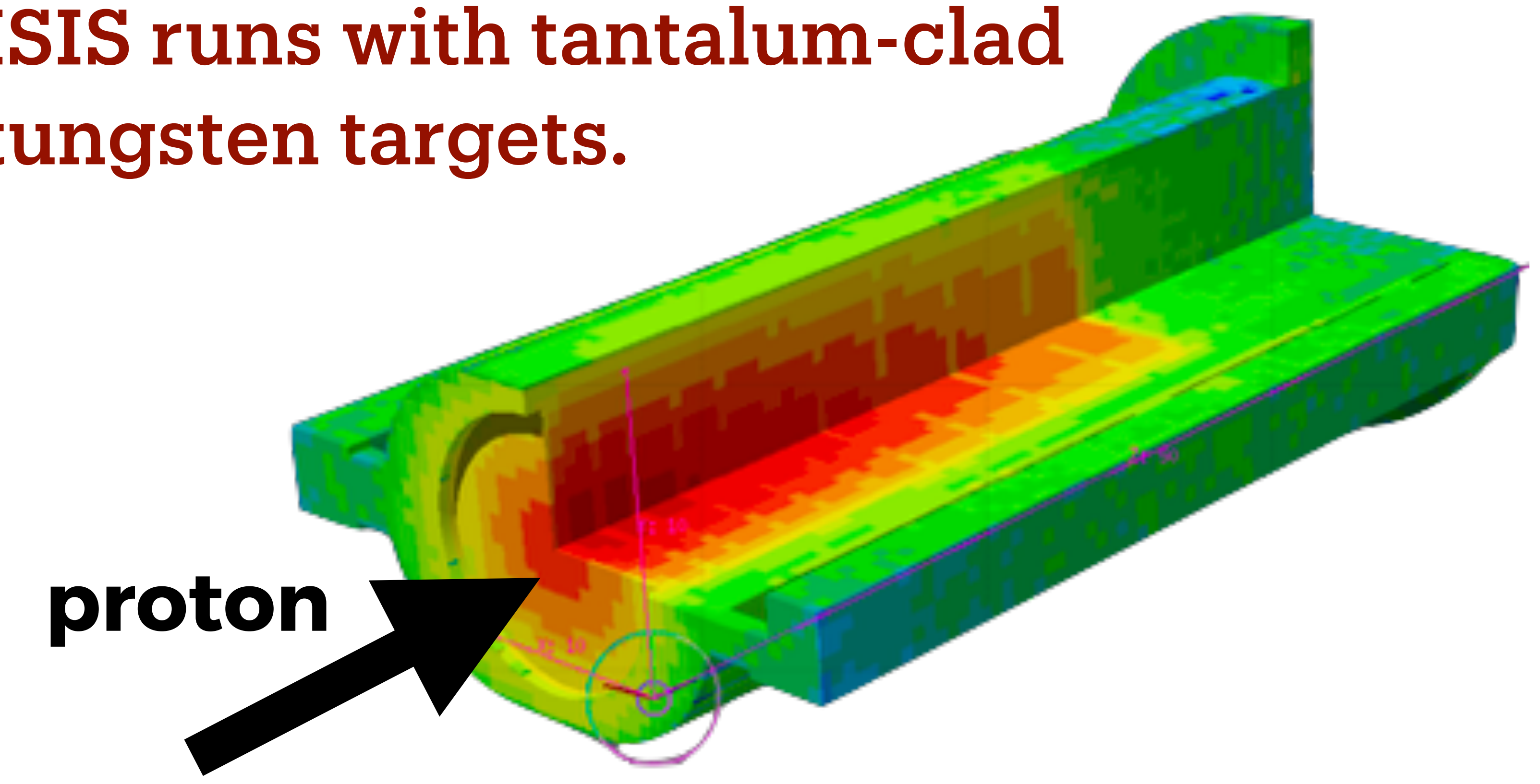
- Within the target, most of the power in the proton beam appears as heat, which has to be carried away by cooling
- In addition to the maximise neutron yield, the choice of target material is determined by a number of considerations, such as thermal conductivity, melting point, machinability, chemical reactivity, induced radioactivity, availability and cost.

engin. parameters

Schematic diagram of (the old) ISIS-TS1 target



ISIS runs with tantalum-clad tungsten targets.



Results of MC Simulation of Energy deposited profile in the new target

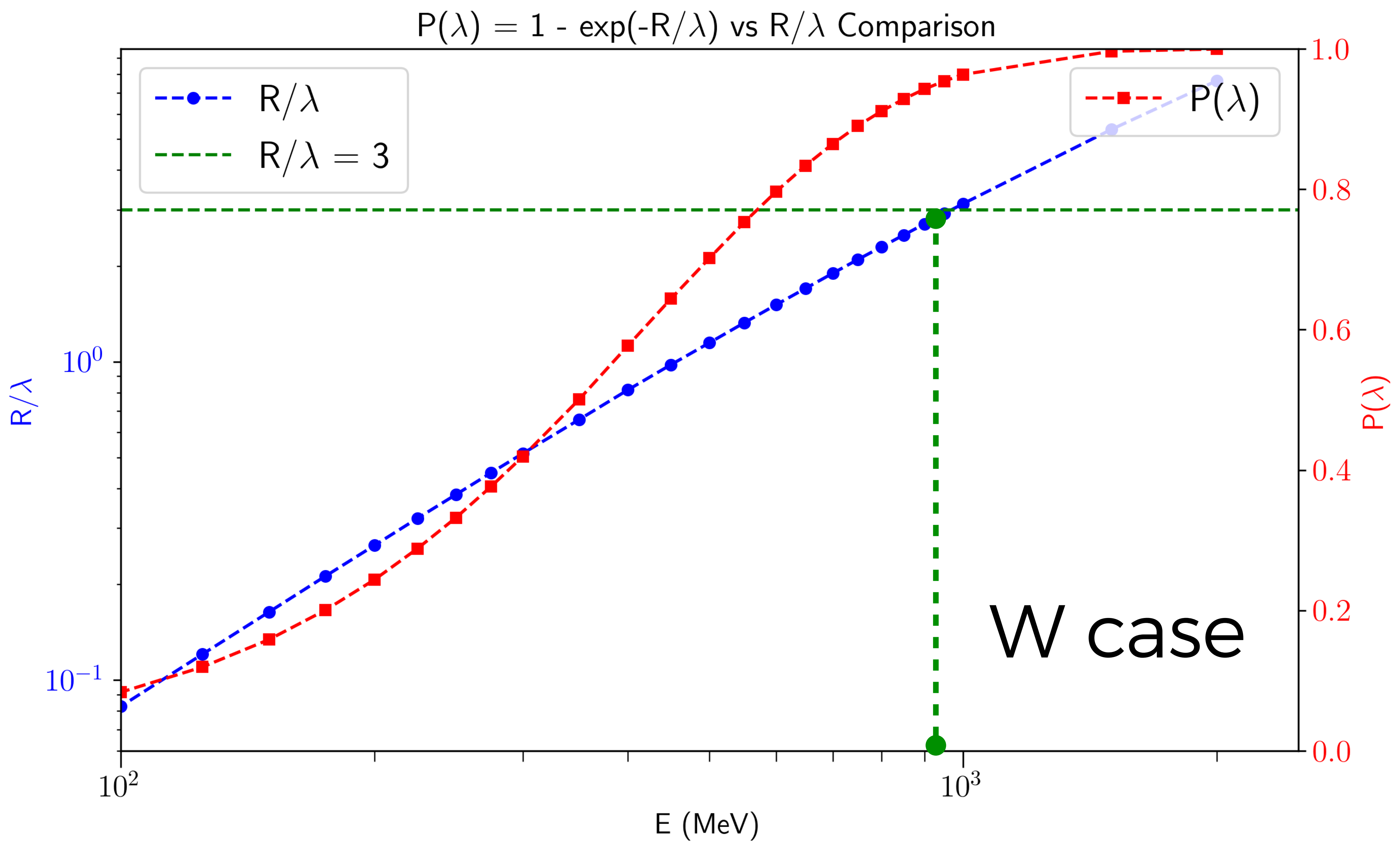
Target thickness: Range vs inelastic Length

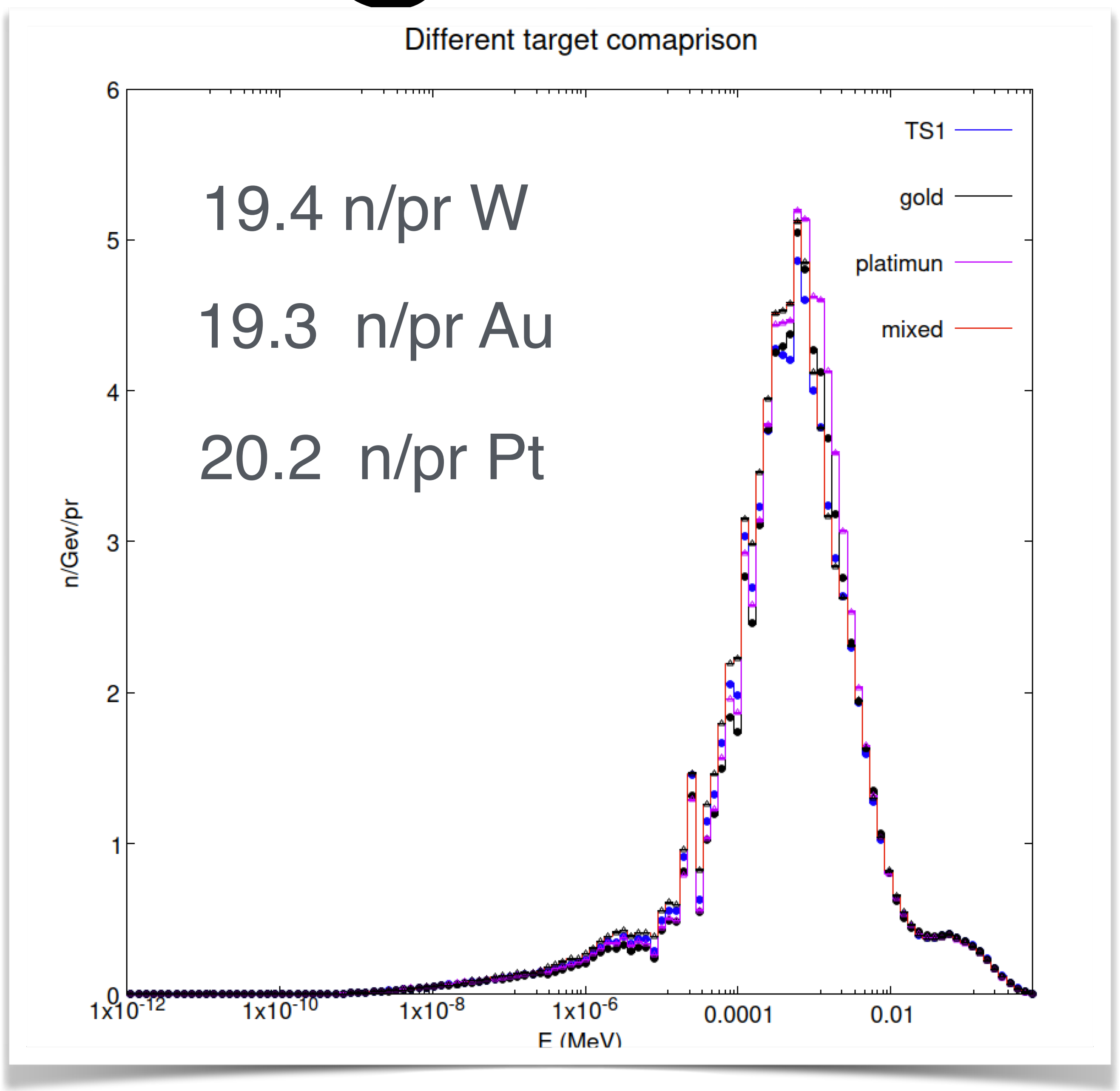
Target thickness—>fully absorption of the primary protons. Confine the hadronic shower and beam power, minimising the energy released around

This means a depth comparable to the range of the proton at a given E

- For neutron production to occur, nuclear collisions must take place before the incident particle reaches the end of its range.
- To obtain a reasonably high NUCLEAR COLLISION PROBABILITY Pn (~ 0.95) the particle energy must satisfy the condition

$$R(E_p) > 3\lambda$$





λ inelastic length (cm)				
E	W	Au	Pt	Ta
800 MeV	9.5	9.7	8.7	10.9

$$\lambda[g/cm^{-2}] \rightarrow$$ nuclear collision mean free path

λ is almost constant above 200 MeV

ISIS TS1: W optimised thickness

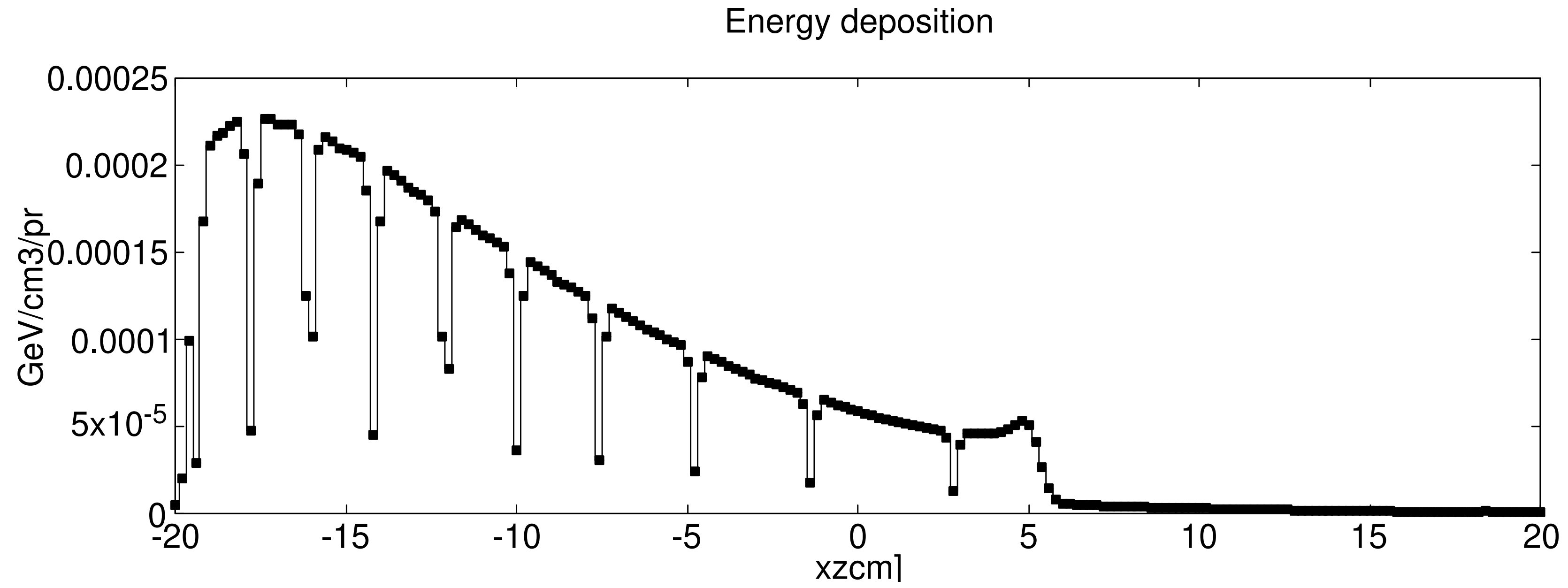
Table 4: Neutron balance* per primary proton

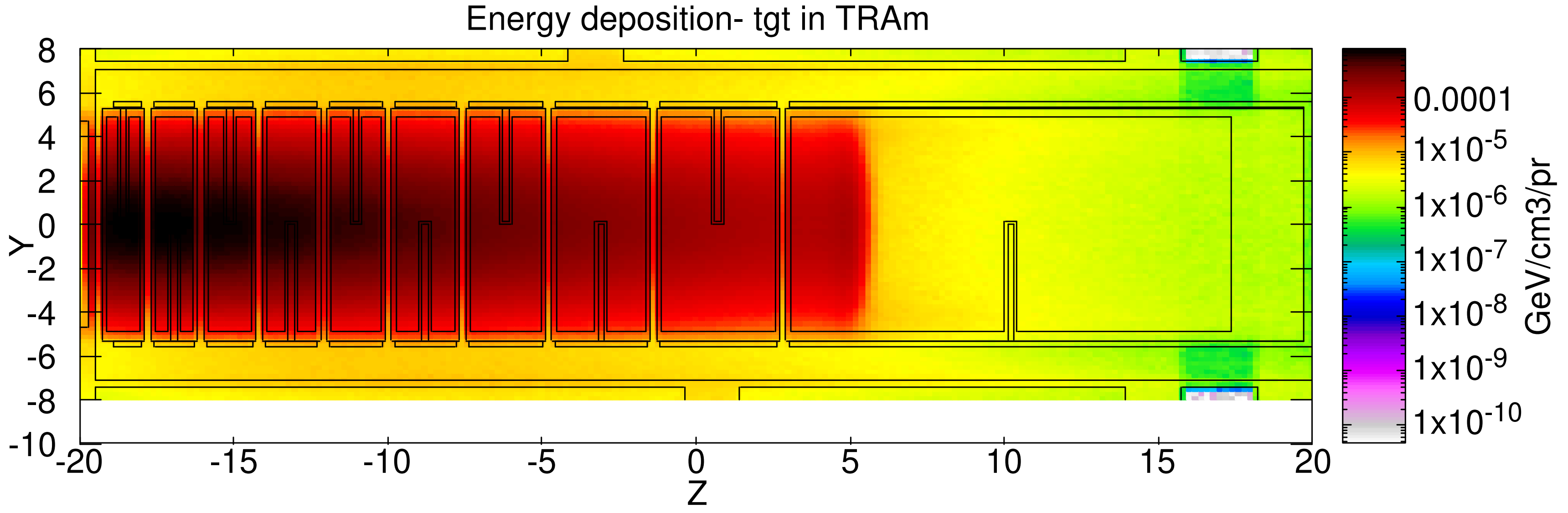
800 MeV proton		Bare Target [n/p]	TRAM [n/p]
Target	W	11.88±0.4%	11.14±0.5%
	Ta	2.07±0.9%	0.81±2.9%
	SS	0.19±1.5%	-0.28 ±1.7%
	Ni (thermocouples)	0.003±13.7%	0.003±18.9%
	MixWater**	0.029±3.1%	0.023±4.8%
Reflector	Be	-	1.43±0.6%
Poisons and liners	Boral	-	-7.07±0.2%
	Gd	-	-0.28±0.9%
Cold Moderators	Liquid CH4	-	-0.02±3.3%
	Liquid H2	-	-0.002±7.9%
Water moderators	Water	-	-0.09±1.5%
Structural and auxiliary materials	Al alloys	-	-0.10±1.6%
	Ti alloys	-	-0.17±1.1%
	SS	-	-0.10±1.5%
Total net balance		~14.2 ±0.4%	~5.3±0.5%

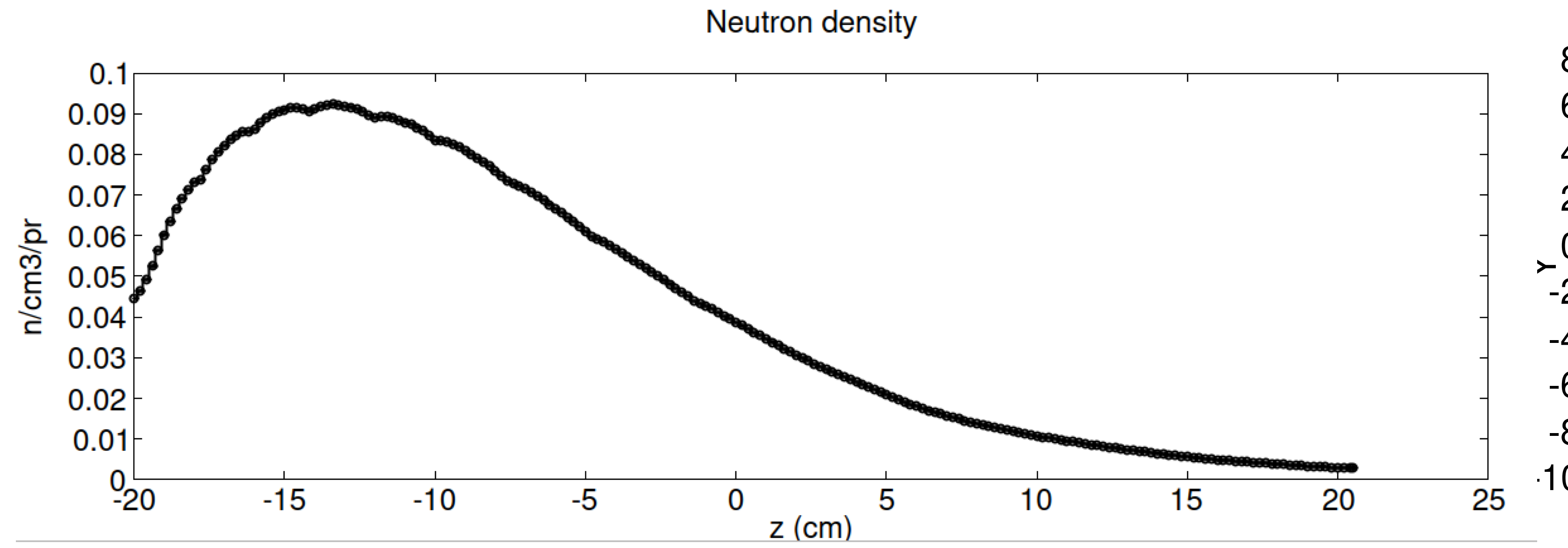
The Neutron balance is the net contribution “<+production -absorption>” of neutrons in each region.

***MixWater is made of 80%D_2O+20%H_2O*

- The active length of the target could be further optimised (possibly shortened)
- This means also possible evaluation of a different thickness and material for the last plate target
- evaluate possible different materials for clad







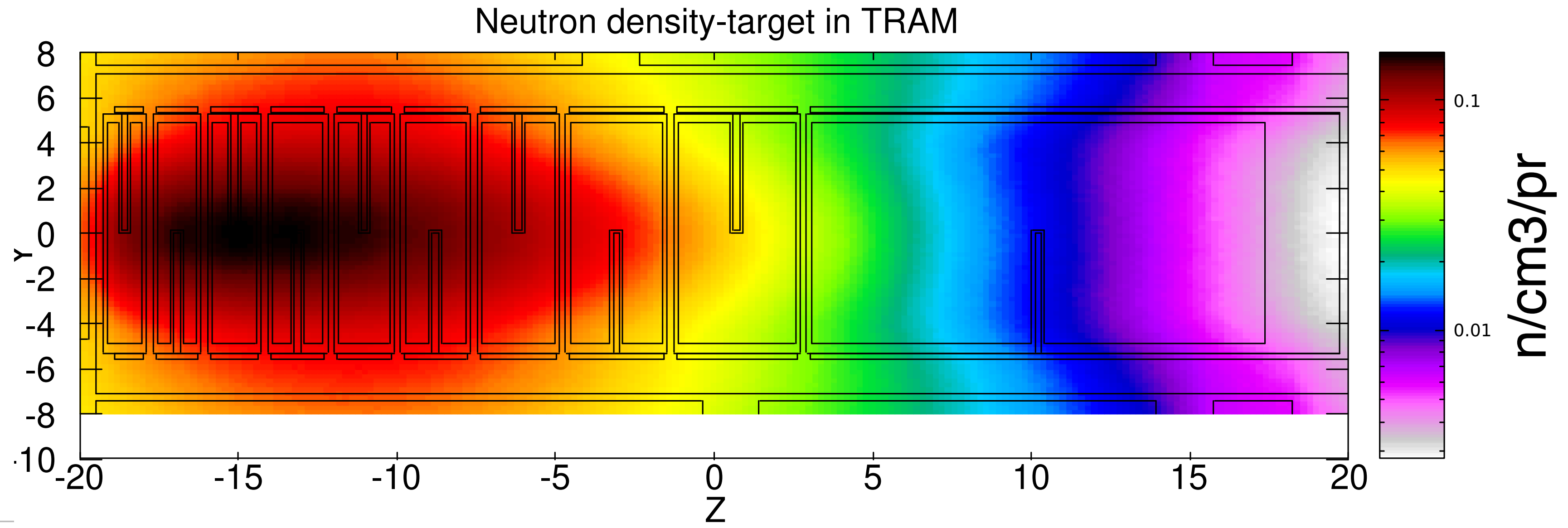
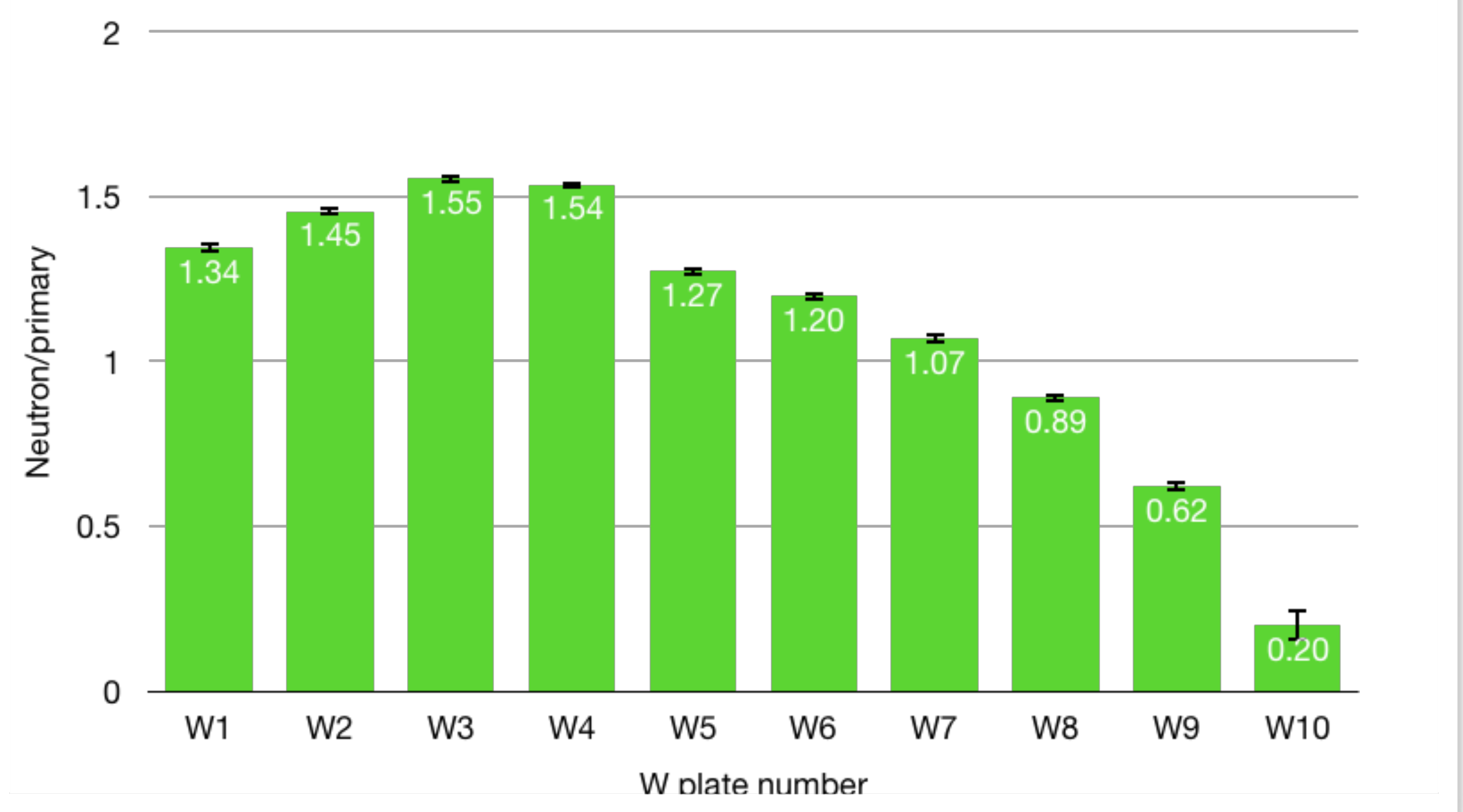
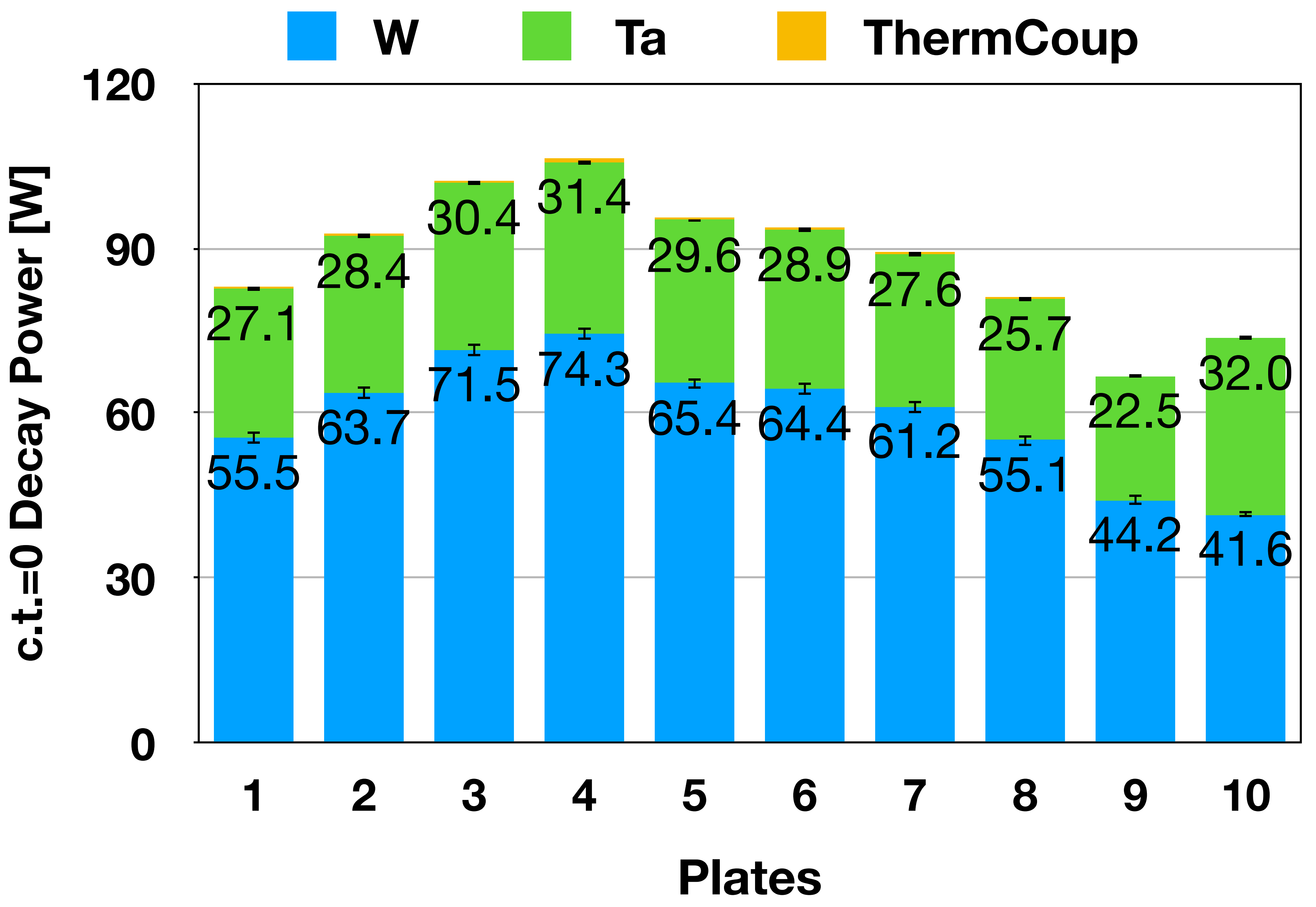


Figure 4: TRAM case: *neutron production in W plate*





Cladding material: Densimet and TZM

MATERIAL	densimet			#:		ρ:	18.
Z:		Am:		A:		dE/dx:	▾
COMPOUND	densimet ▾			Mix:	Mass ▾	Elements:	4..6 ▾
f1:	0.95	M1:	TUNGSTEN ▾	f2:	0.025	M2:	NICKEL ▾
f3:	0.025	M3:	IRON ▾	f4:		M4:	▾

Advantages of DENSIMET® and INERMET®:

- High density of 17.0 to 18.8 g/cm3 (similar to pure tungsten)
- Better machinability compared to pure tungsten
- Cost-efficient manufacture of complex products and components
- High modulus of elasticity and excellent mechanical properties
- High absorption capacity for X-rays and gamma rays
- Safe for human health and the environment

DENSIMET® is also characterized by its excellent strength and ductility, while another clear advantage of INERMET® lies in its non-magnetic characteristics.

..Anyway no many data are available about corrosion/erosion and possibly dedicated studies will be needed

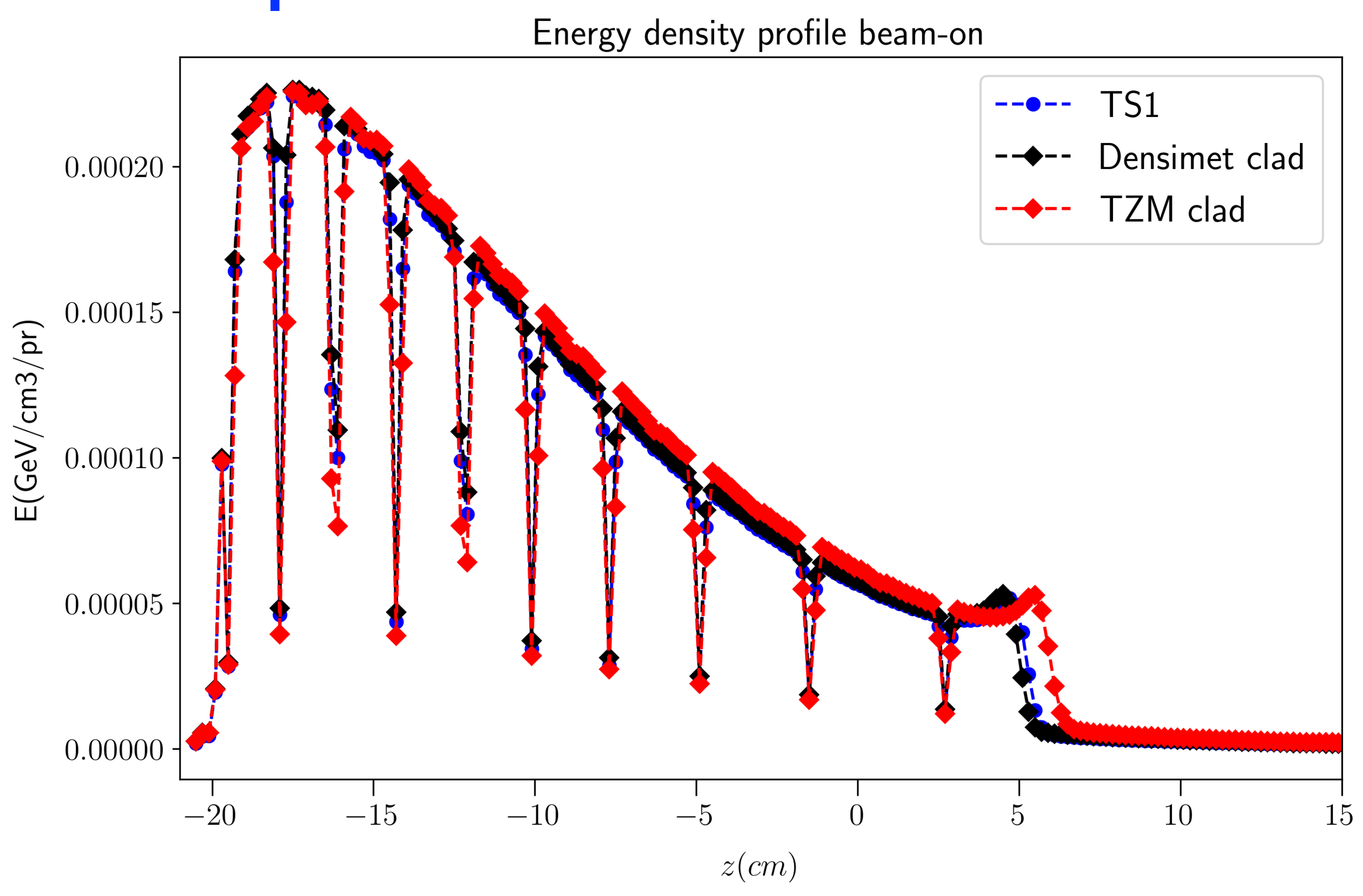
MATERIAL	TZM			#:		ρ:	10.22
Z:		Am:		A:		dE/dx:	▾
COMPOUND	TZM ▾			Mix:	Mass ▾	Elements:	7..9 ▾
f1:	0.994	M1:	MOLYBDEN ▾	f2:	0.005	M2:	TITANIUM ▾
f3:	0.0008	M3:	ZIRCONIU ▾	f4:	0.002	M4:	CARBON ▾

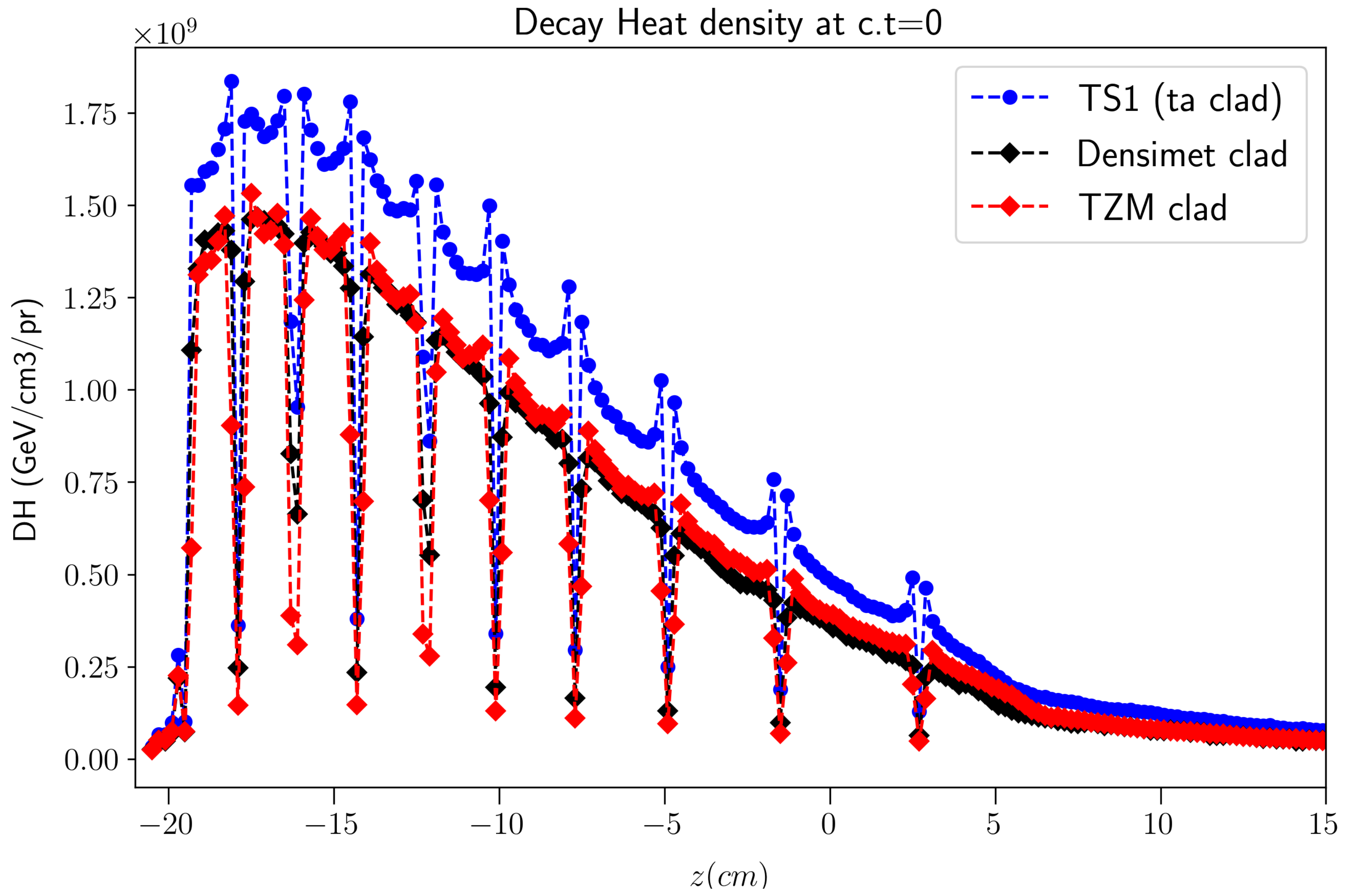
TZM is a molybdenum alloy with titanium and zirconium.

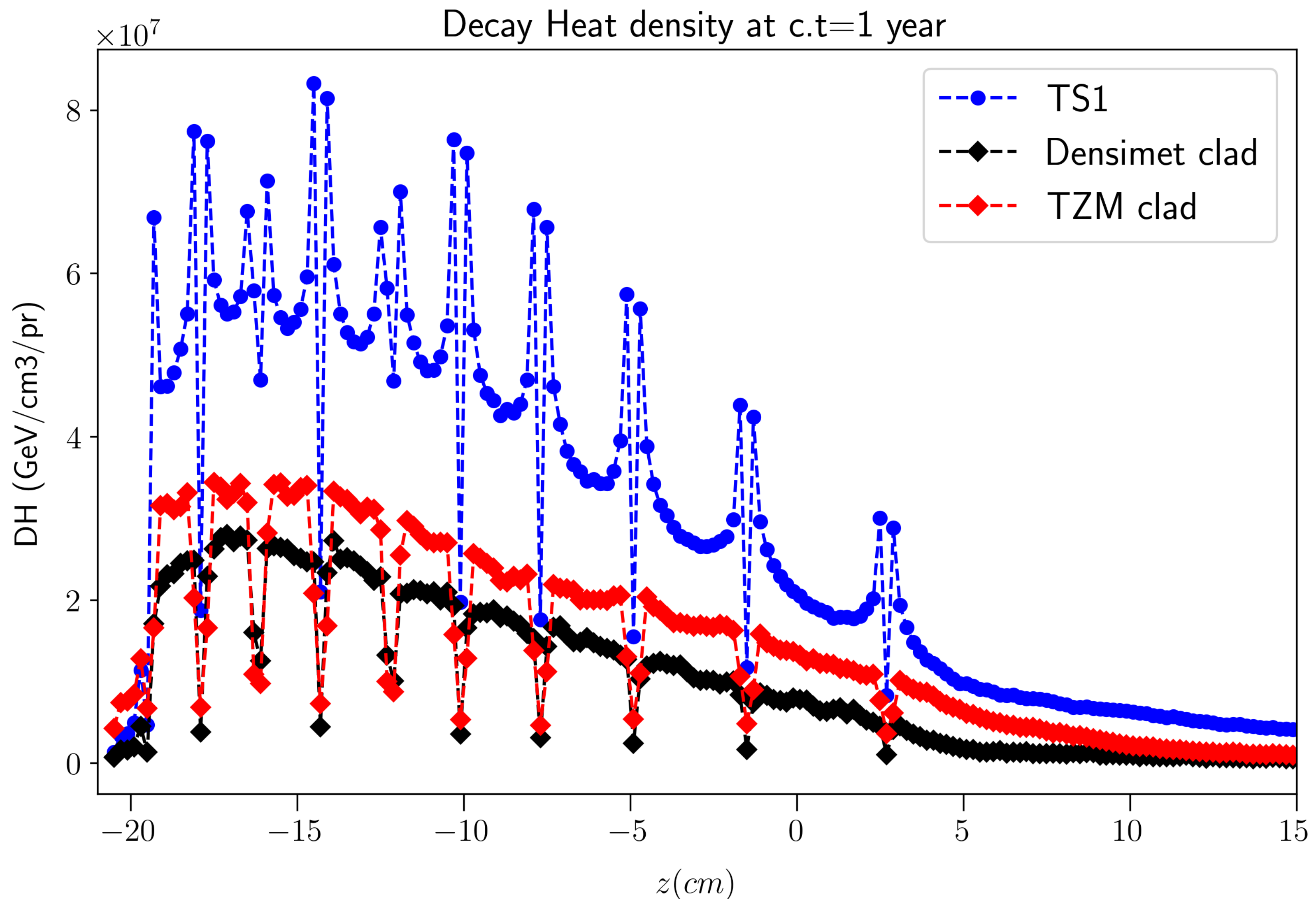
For further details refer to Alan Prothero talk

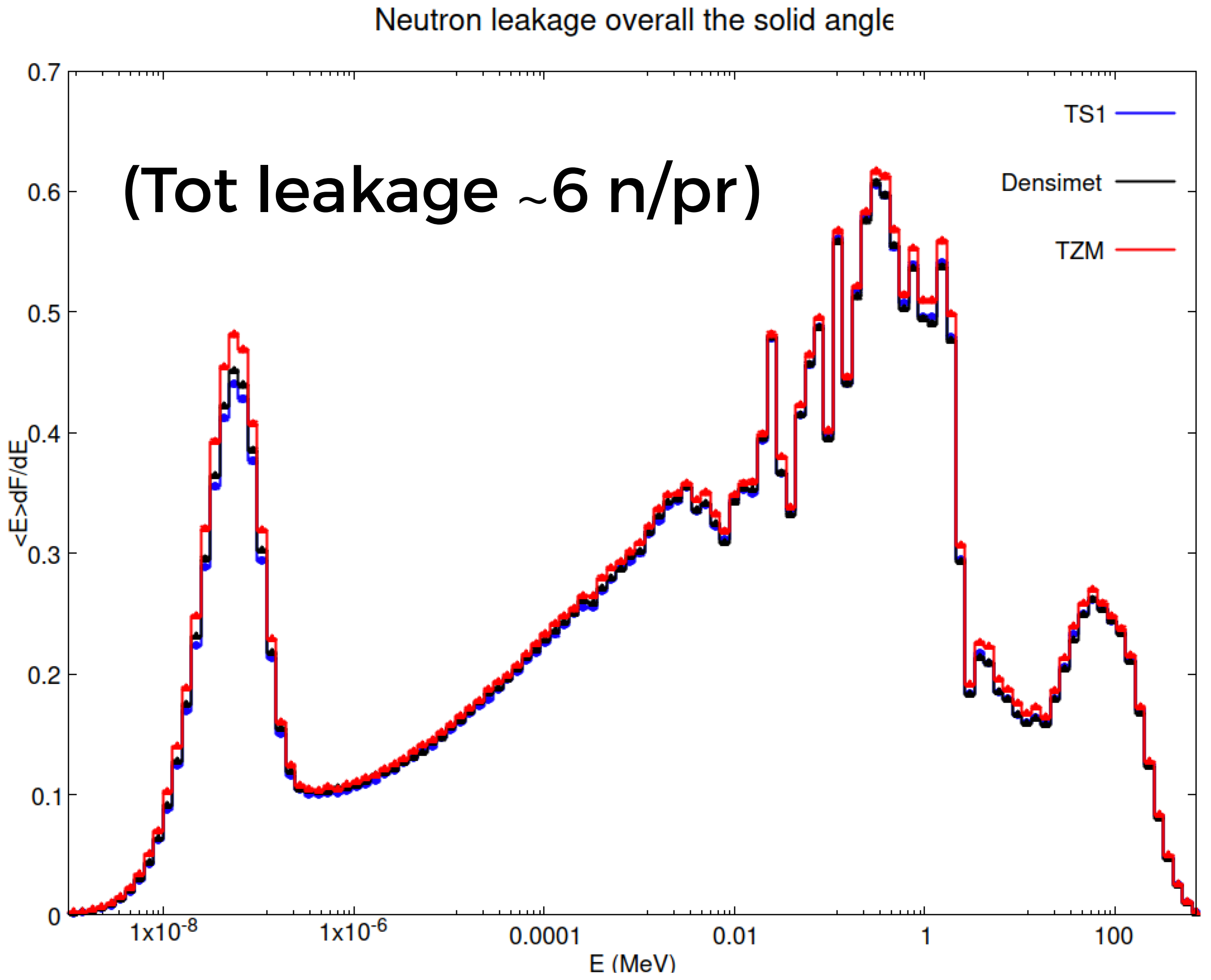
Comparing different materials for cladding

We compare the ISIS-TS1 target in TRAM with two notional target in TRAM: Densimet and TZM —> low neuton absorption XS









- Notional calculations of ISIS-TS1:
  - W core and W_core/Densimet_clad
  - W_core/TZM_clad
- Results show that the neutron yield remain unaffected whilst the decay is largely reduced

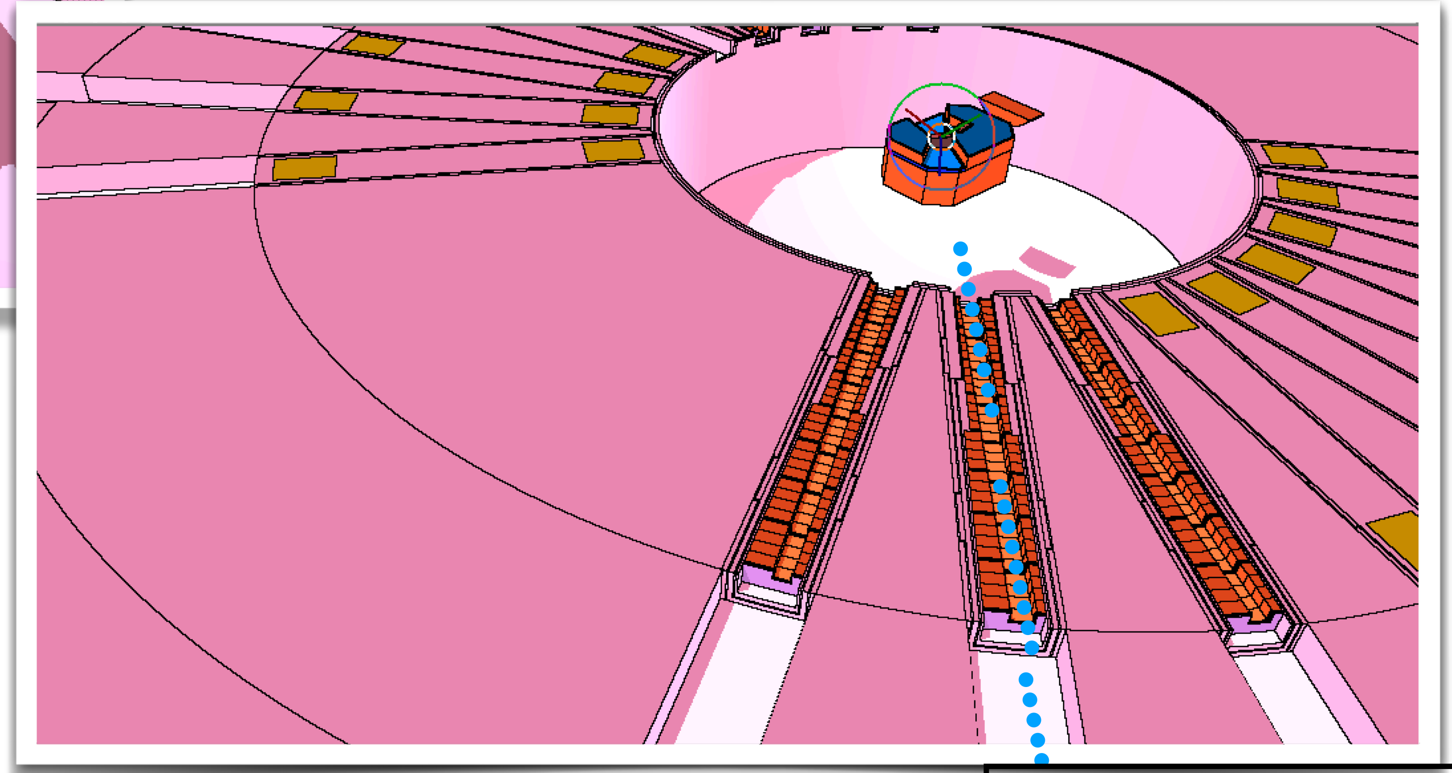
Neutron leakage:

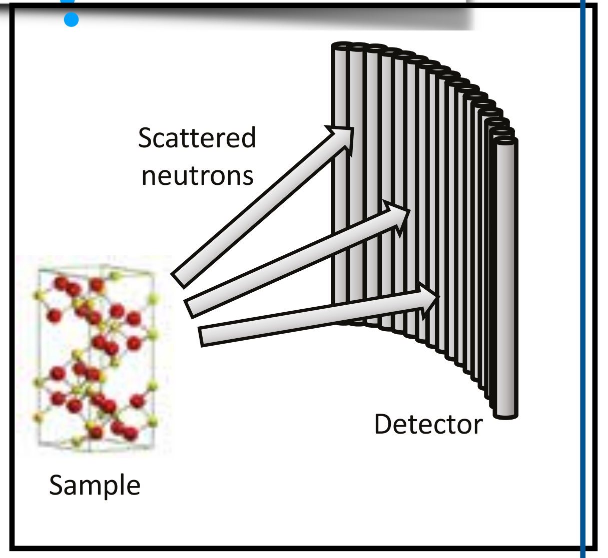
Optimization of the target/reflector/moderator coupling

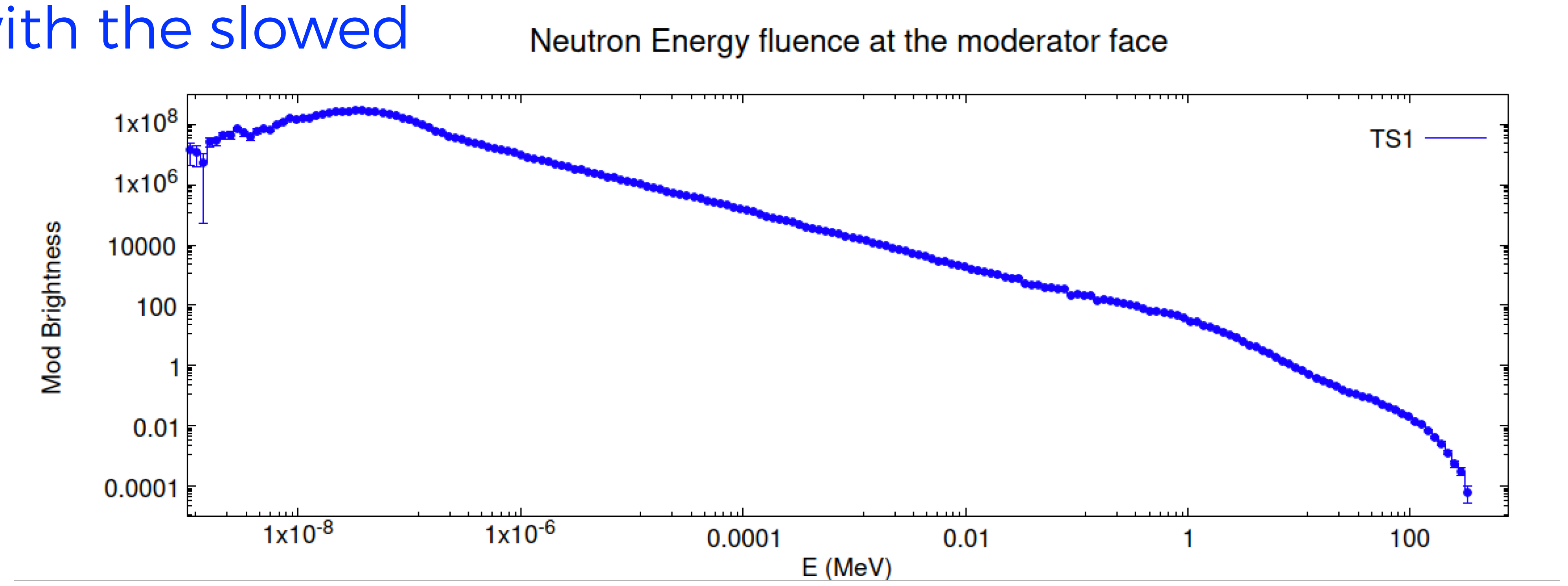
Valuable figures of merit are the moderator brightness ad pulse shape at the instrument

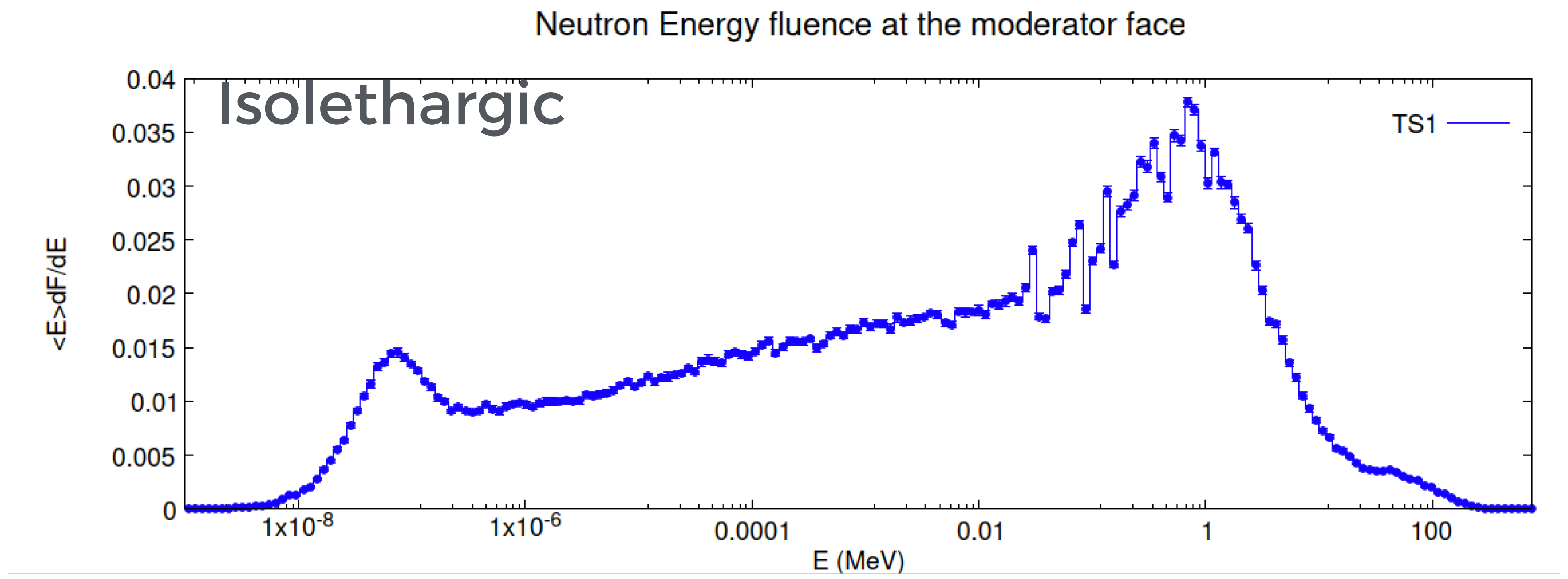
Moderator brightness and pulse at instrument inlet

Moderators are intended to be the actual source that feeds the instrument with the slowed neutrons as needed for neutron scattering experiment

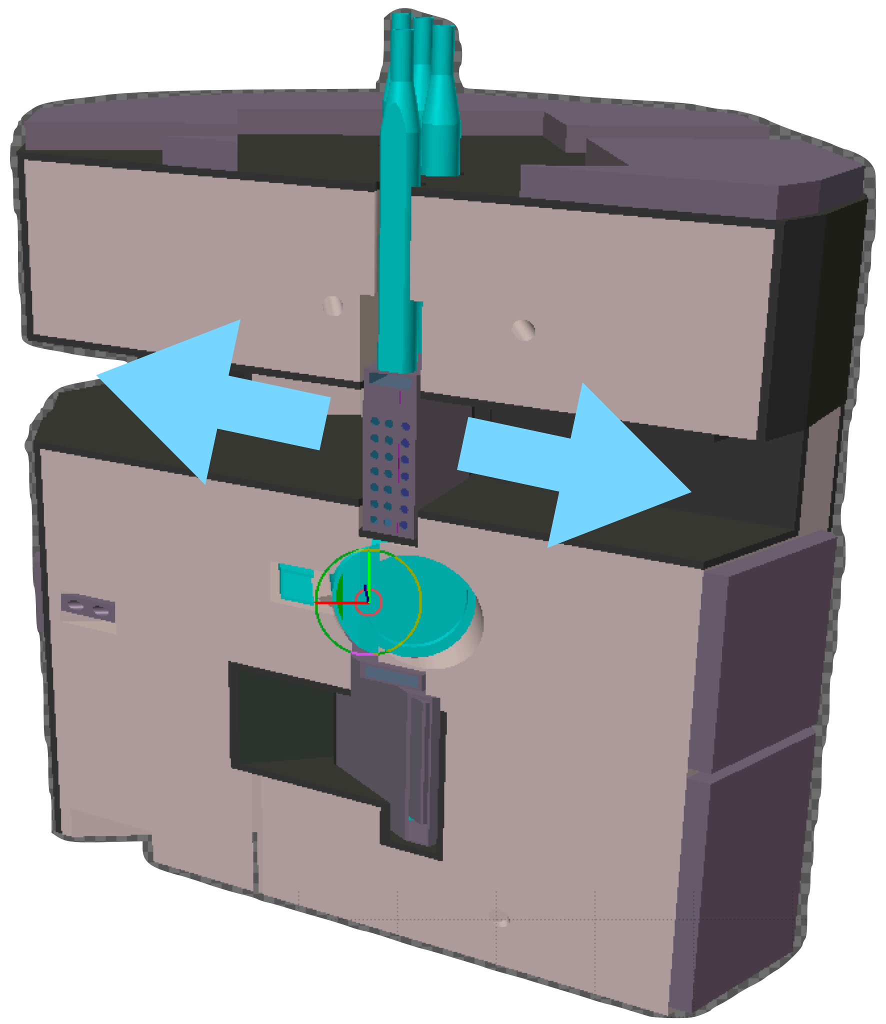






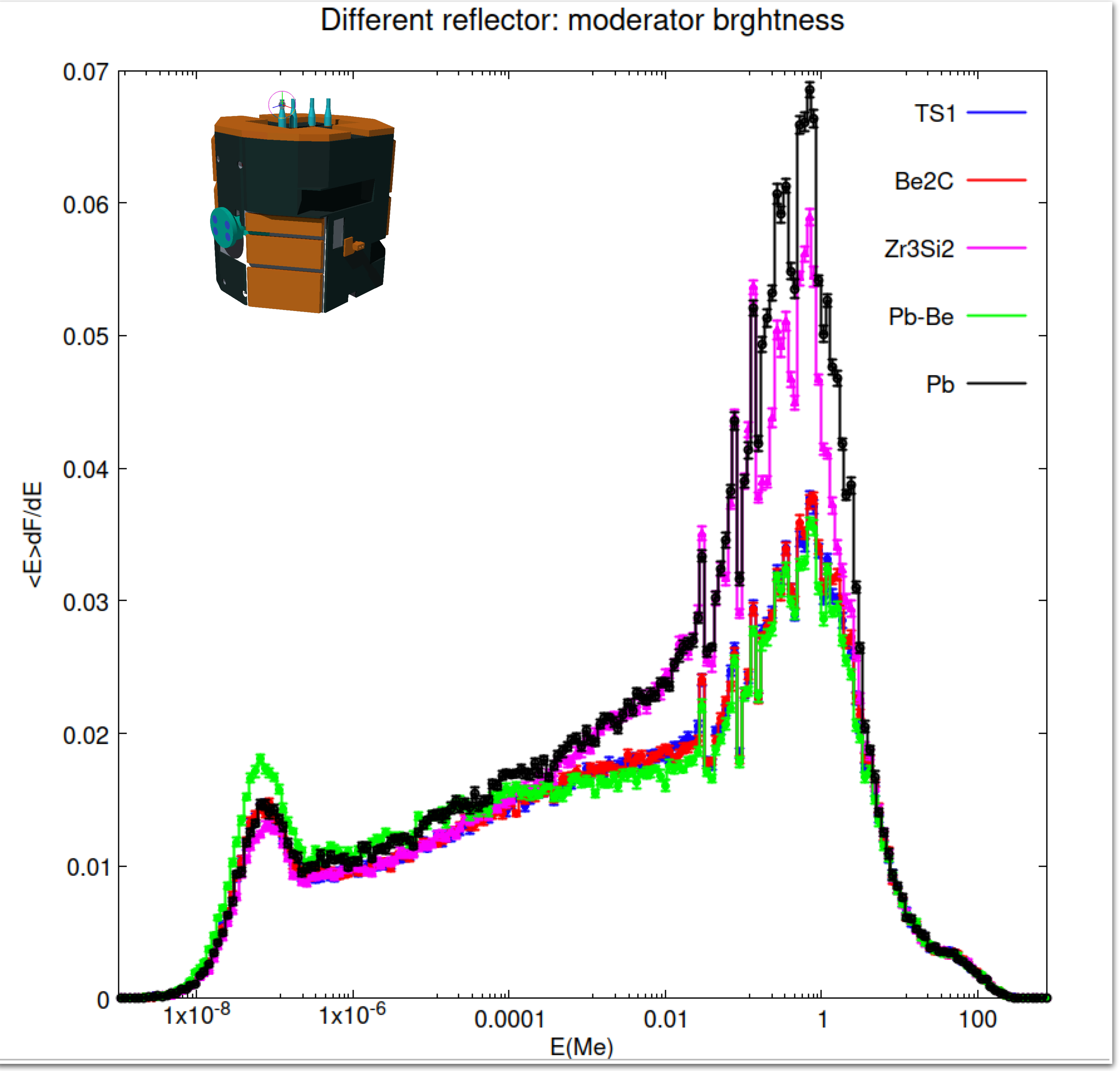


coupling FLUKa/McStas with different and independent approach wrt MCNPx/McStas—> validation in progress



Comparing different materials for Reflector

We compare the ISIS-TS1 target in TRAM with two notional target in TRAM: W_core/Densimet_clad & W_core/TZM_clad



Material	Density (g/cm3)
Be/BeO	1.8
Be2C	2.4
Zr3Si2	5.86
Pb	11
Pb/Be	6.4

ORNL/TM-2023/3011

Be2C

High moderating efficiency and low absorption cross section. It could serve as moderator alternative to graphite (greater slowing power) and much better radiation damage characteristics.

Zr3Si2

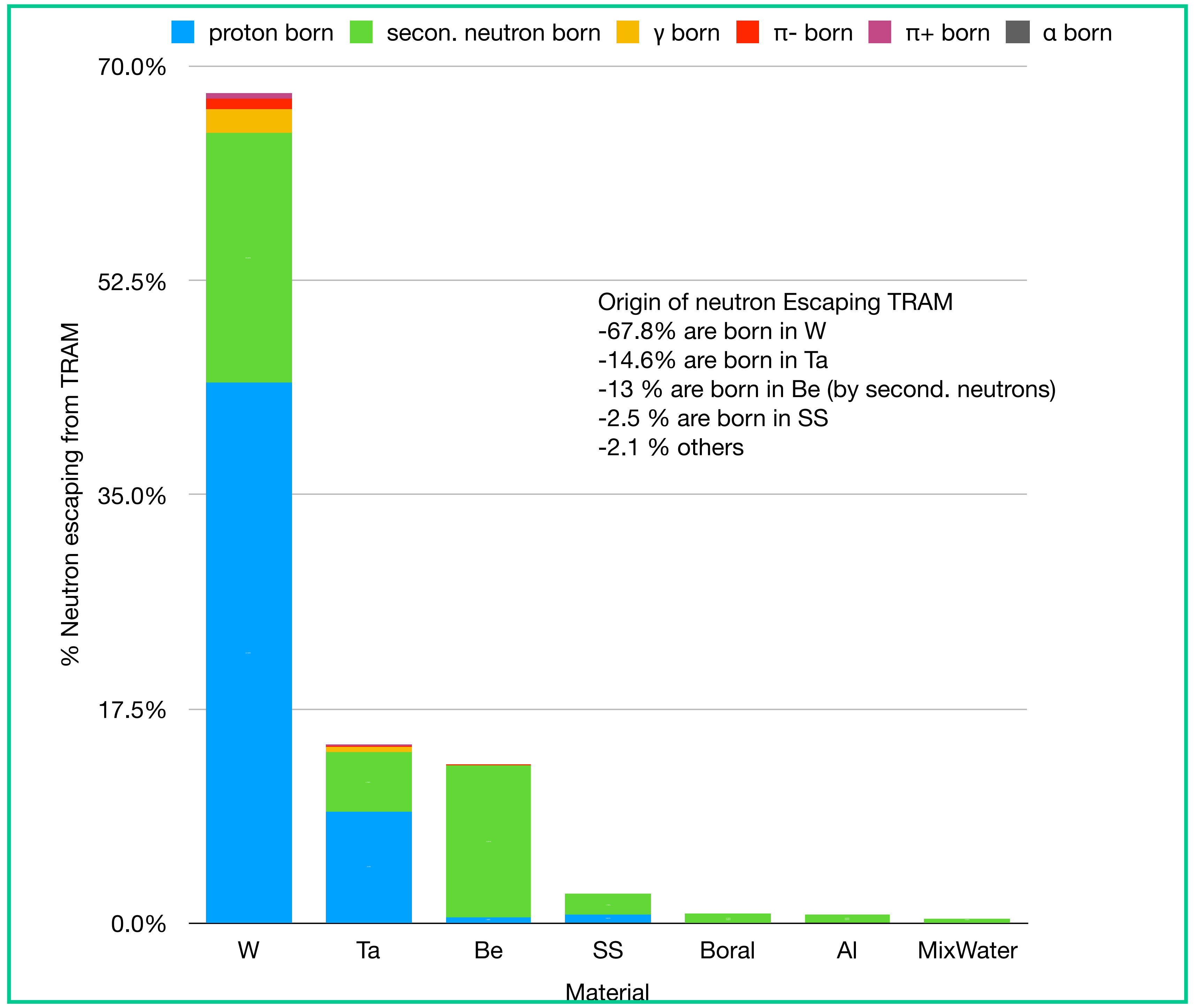
It is a heavy reflector material with promising application for high temperature nuclear gas reactor

Analysis of Background

gamma+ delayed neutrons+(high energy neutrons)

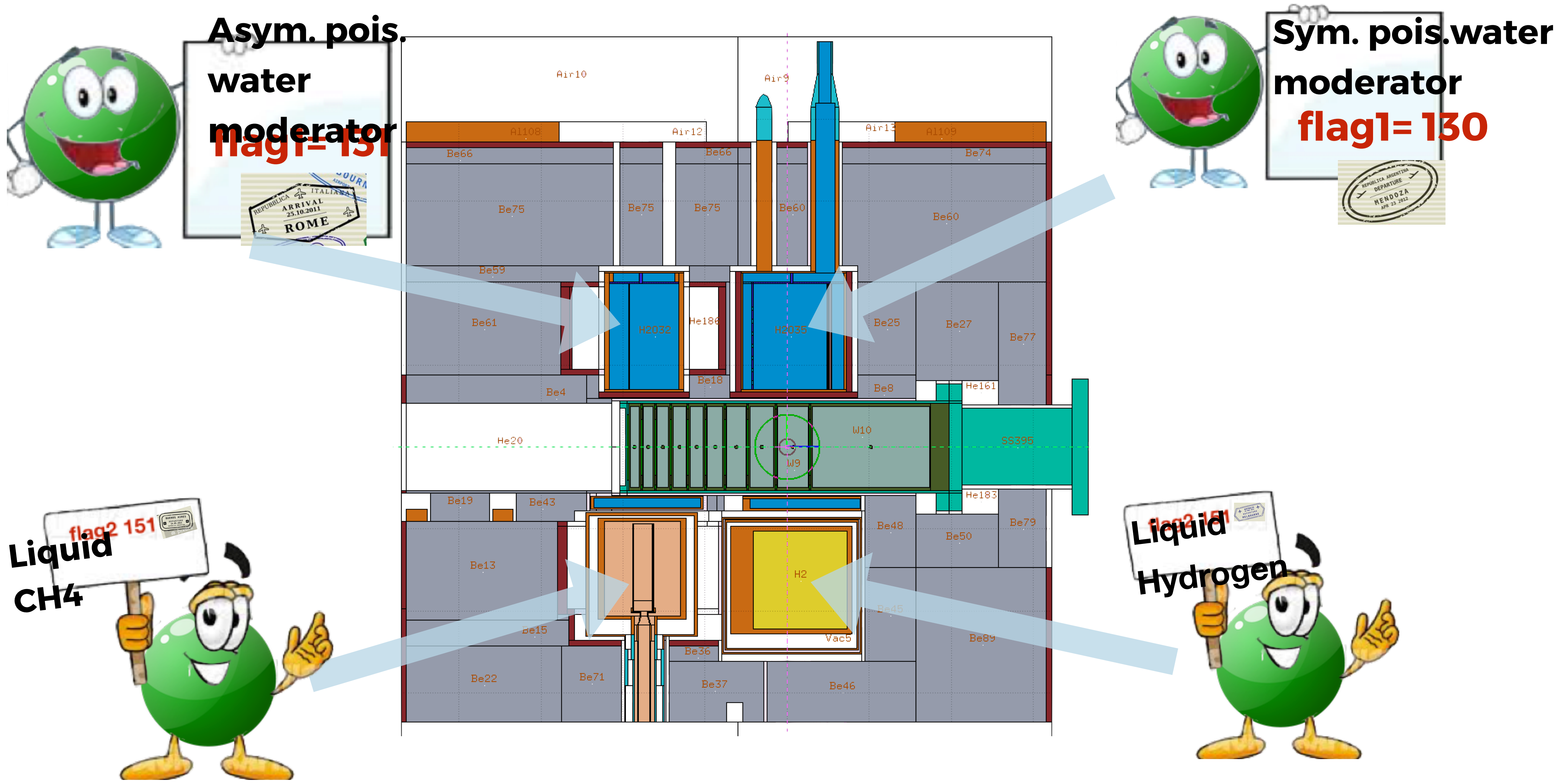
Escaping neutrons: where are they coming from?

By running FLUKA with suitable linked executables (from advanced user routines) it is possible to estimate and record for each escaping neutron the region where the neutrons themselves have been generated and info about parent particles



Materials where *TRAM* escaping neutrons originated

Origin	Neutron Escaping [%]
W	67.8
Ta	14.6
SS	13.0
Be	2.5
Boral	0.8
Al-alloys	0.7
MixWater	0.4
Others	0.2



Flagged neutrons trough moderators

Neutrons born in W and Ta are originated mainly by direct proton spallation, while the second relevant contribution (almost half of the former one) is coming from secondary neutrons.

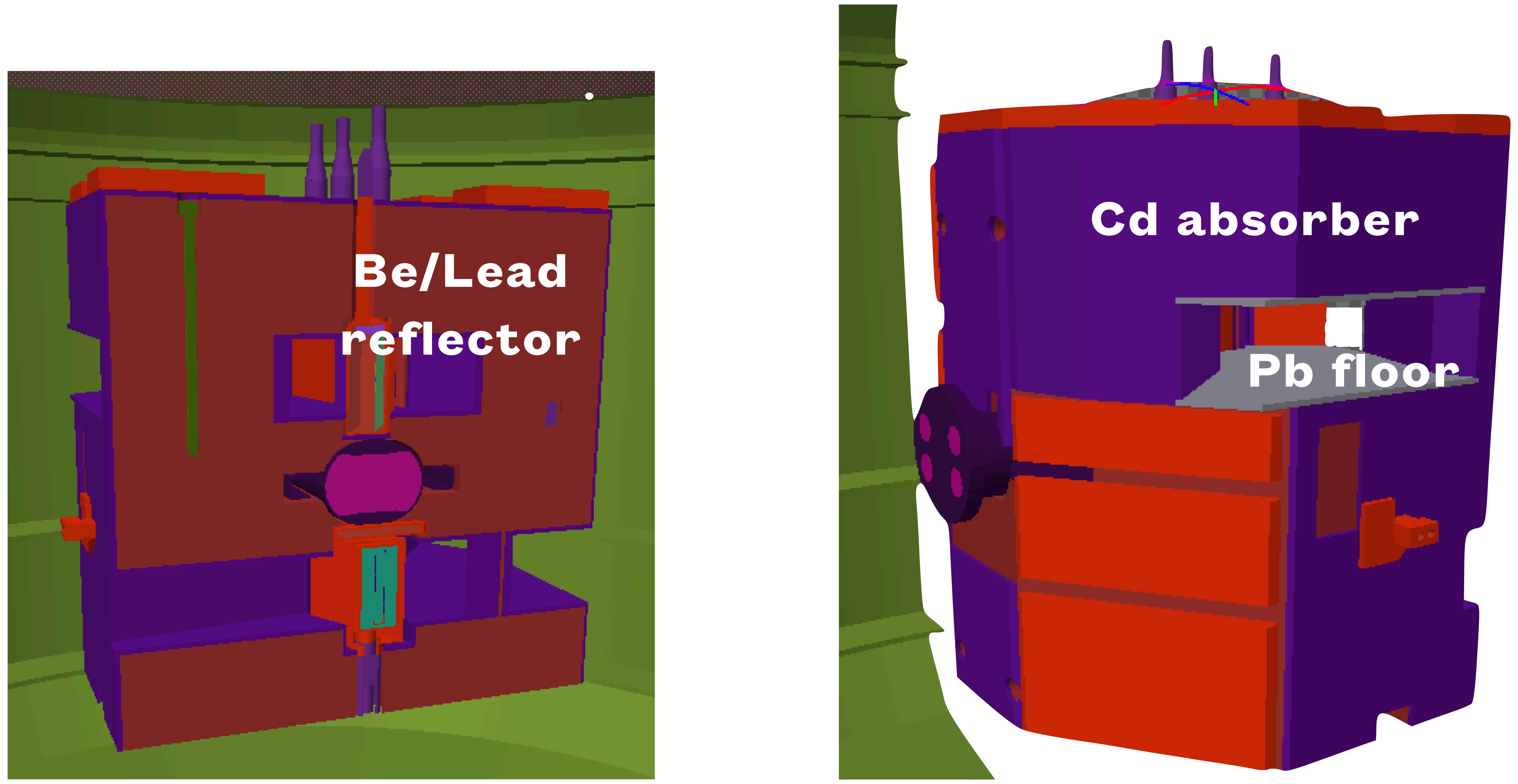
The reverse is happening in Be, SS, and other auxiliaries materials (Al, MixWater, etc) where neutrons are produced quite exclusively by secondary neutrons.

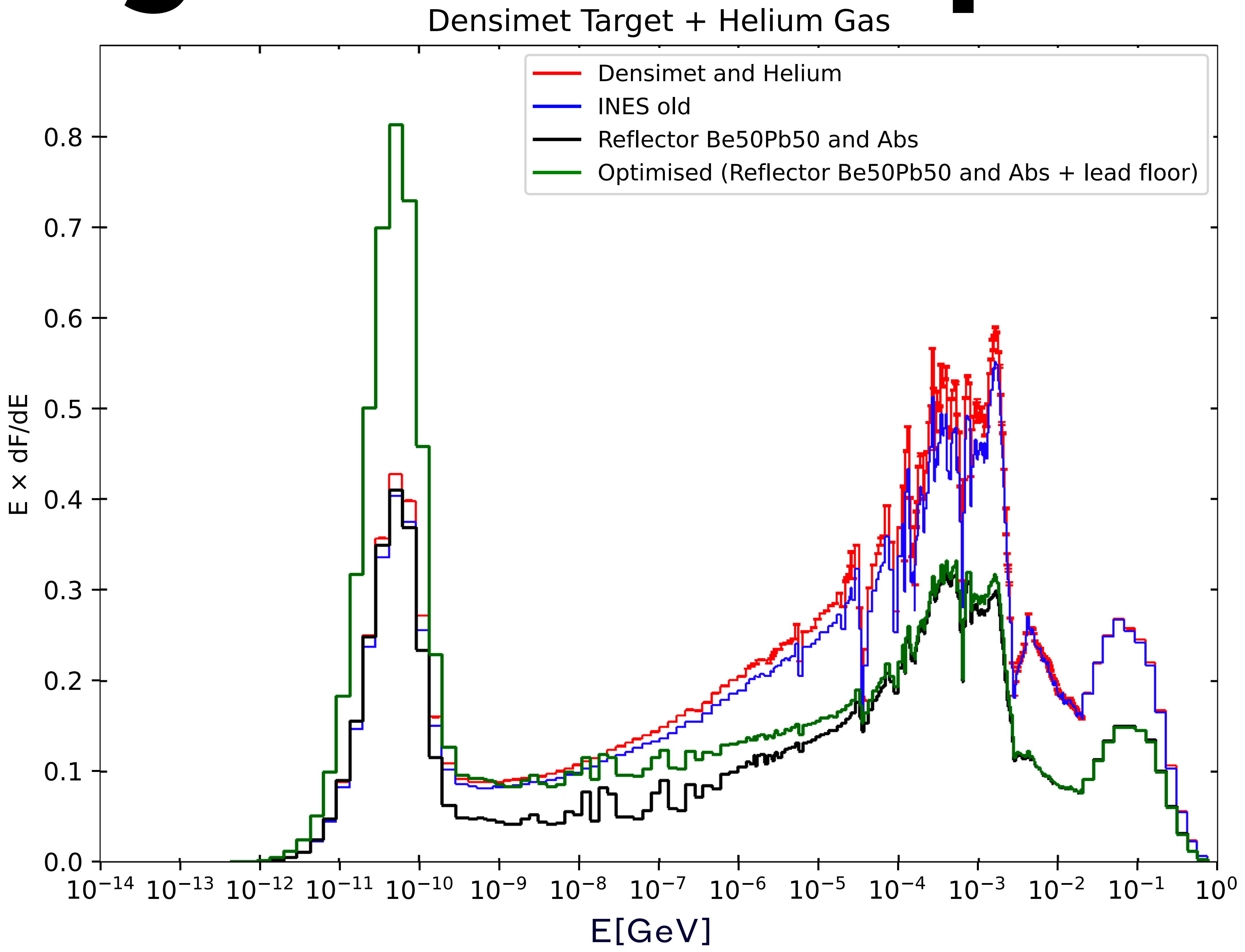
This kind of analysis has required to flag neutrons and latch them to their parents in the regions where they are generated.
This has been accomplished by suitably coding the mgdraw.f and suprf.f advanced routines

The results below refer to the reference scenario: 800 MeV protons onto the present operating TRAM. The same kind of analysis can be carried out for more finalised target in order to optimise the final design in the frame of suitable coupling of target with moderators and reflector

Reducing HE n and increasing the thermal peak

1. Focus on reducing high energy neutron and gamma contributions
2. Use advanced MC features for more efficient TRAM design: "latching" and "flagging" methods
3. Consider new reflector and absorber materials:
   - CdInAg instead of Boral
   - 50% Be / 50% Pb reflector instead of all Be
   - Pb layer instead of Boral in beam aperture toward water moderators





Reflectors and Absorbers for Neutron and Gamma Suppression

- Be/Pb reflector and Cd-In-Ag absorber suppress high energy neutrons
- Lead floor/wall in beam line aperture inside reflector increases thermal peak
- Green and black cases use 50% Pb and 50% lead reflector
- In-Cd-Al more efficient at suppressing epithermal and fast neutrons due to resonances in capture cross section

Conclusion

- The FLUKA code features as a valuable tool for optimizing neutron source facilities by enabling comprehensive tracking of neutrons from the target to the sample

- The use of a validated model provides a reliable framework for addressing key design choices within the ISIS-2 project (using it as notional tool for having evaluations about changes in the relevant nuclear parameters).

- We are now in the phase of finalising the coupling between FLUKA model of TS1 and MCStas instrument

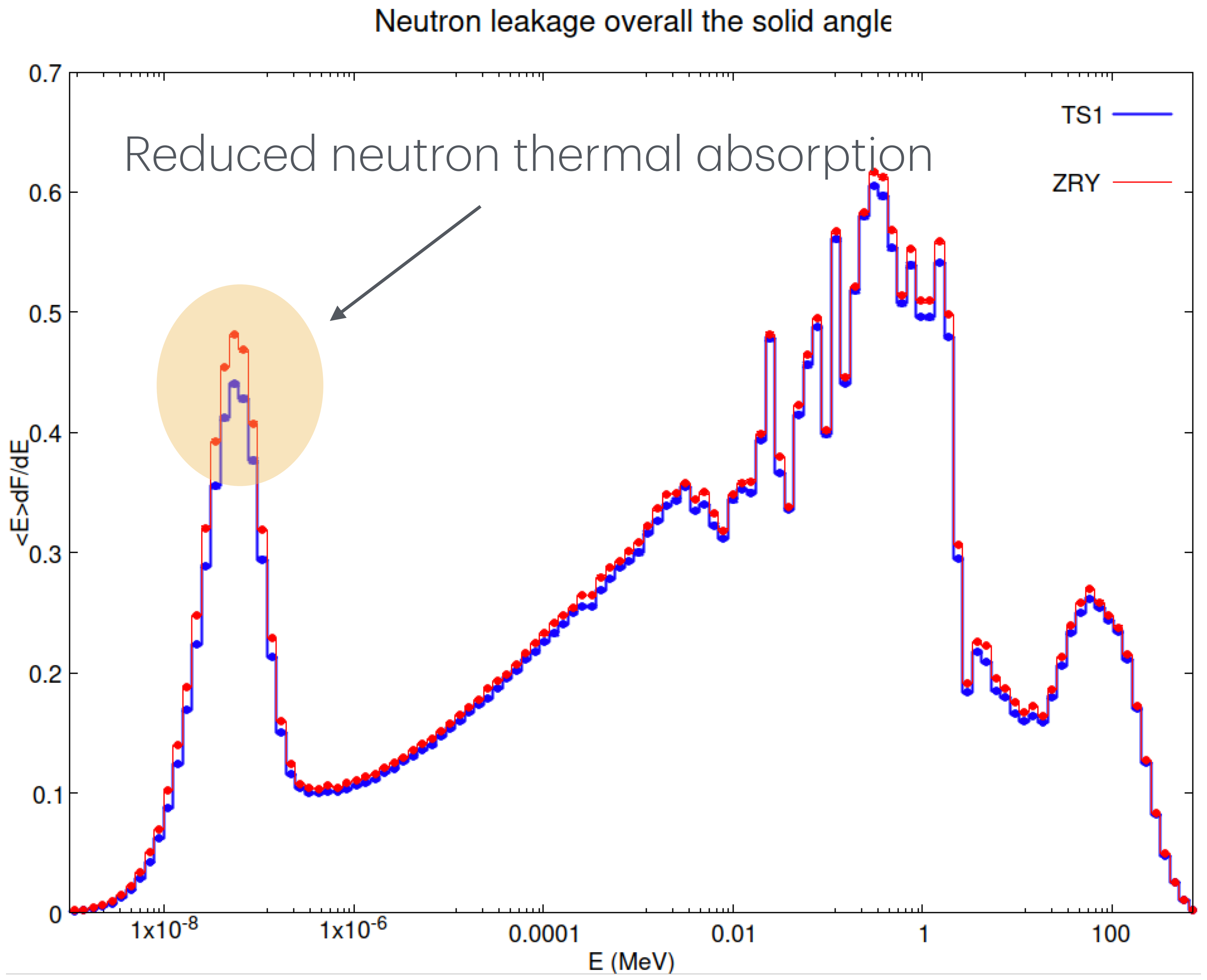
- Successful implementation requires some advanced features and the development of an appropriate interface between the FLUKA model and optical simulation codes like McStas, which are used to simulate instruments.

- In the design of ISIS-2, a parallel research effort should focus on reducing neutron losses while striving to increase power, to ensure both enhanced performance and efficiency.

Spares

Comparing different material for target vessel

We compare the ISIS-TS1 target in TRAM with two notional target in TRAM: zircaloy vessel



DELAYED NEUTRONS

1. Delayed neutrons are emitted by neutron-rich (fission or spallation) fragments that are called delayed neutron precursors.
2. These precursors usually undergo beta decay, but a small fraction of them are excited enough to undergo neutron emission.
3. The emission of neutrons happens orders of magnitude later compared to the emission of the prompt neutrons.

Relevance in Nuclear reactors

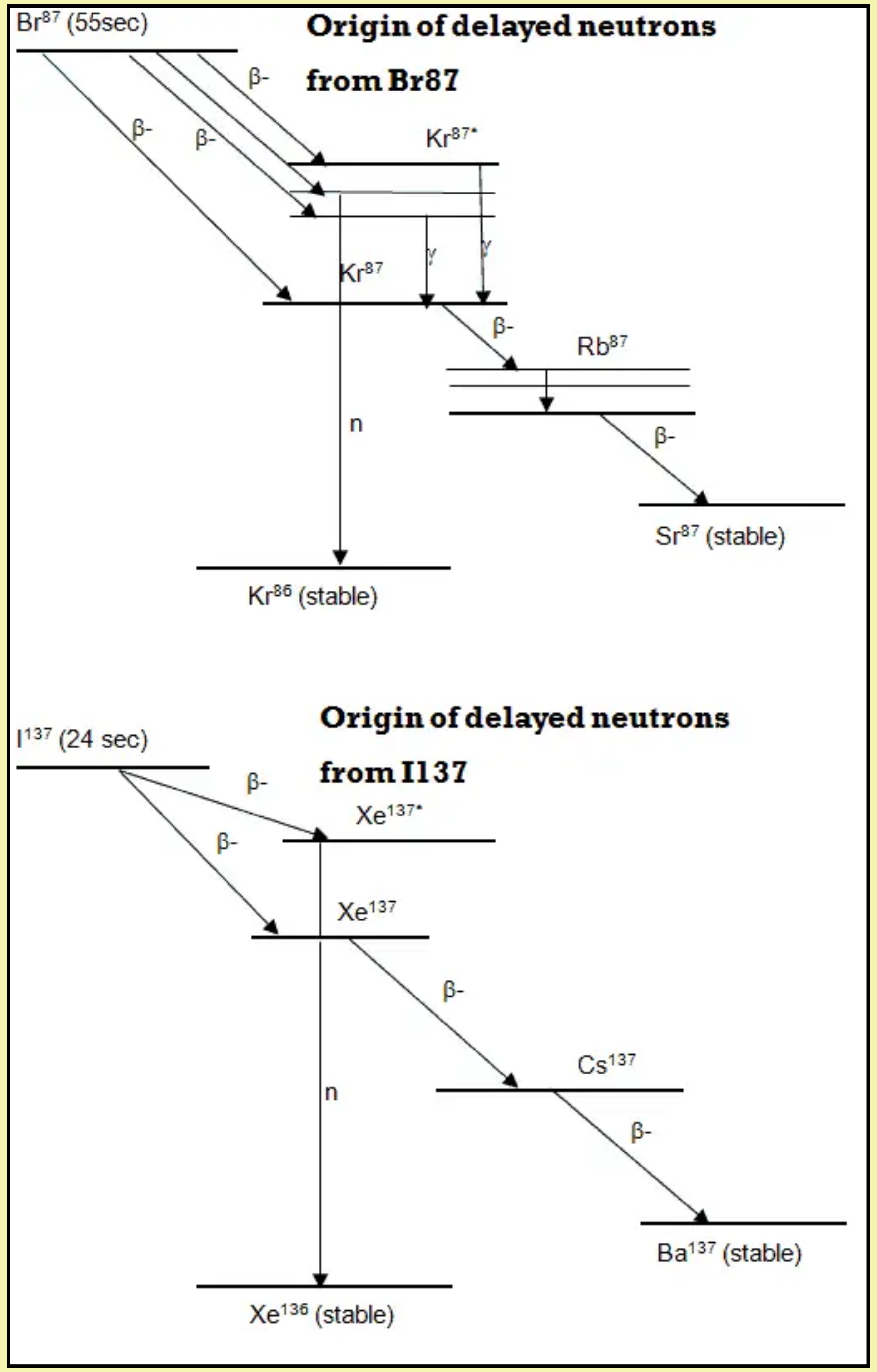
Most of the neutrons produced in fission are prompt neutrons,

"Delayed" neutrons are emitted with half-lives ranging **from few milliseconds up to 55 s** for the longest-lived precursor (87Br)

The presence of delayed neutrons is perhaps the most important aspect of the fission process from reactor control:

Neutron balance for CANDU reactors

Neutrons	Contribution
Prompt Neutrons	99,470,000,000,000
Delayed Neutrons	500,000,000,000
Photoneutrons	30,000,000,000
Spontaneous Fission	1
Total (10^{14} n cm^{-2} s^{-1})	100,000,000,000,000



Neutronic background in Spallation Facilities

Delayed neutrons from Bromine and Rubidium are produced as a results of spallation process.

Neutrons coming from(alpha, n) reactions with high energy alpha (> 4 MeV) coming from short life alpha decay radionuclides

Photoneutron produced in coolant or Be when the target is not irradiated by proton but still kept in loco for cool down purposes

Delayed neutron precursor's activity at EOI @ ISIS

Z	A	RN	Activity [Bq]	T1/2
35	86	Br86	5.06E+09	54-sec
35	87	Br87	1.27E+09	55-sec
35	88	Br88	4.43E+09	15.5 sec