

PETALE@CROCUS Analysis and feedback on INDEN

Laboratory for Reactor Physics and Systems Behaviour



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INDEN Consultancy meeting December 2024

EPFL cea

Objective: stainless steel nuclear data

Provide new constraints in the MeV-range and above for stainless steel nuclear data

- Fission: heavy reflectors (GEN-III PWR)
- Fusion: 14 MeV neutrons
- Accelerators: structures activation

Collaboration between CEA & EPFL



EPFL



The CROCUS reactor

Reactor type

- LWR with partially submerged core
- Room T (controlled) and atmospheric P
- Forced water flow (160 l.min⁻¹)

Operation

- 100 W (zero-power reactor)
- i.e., maximum 2.5×10⁹ cm⁻².s⁻¹
- Control: B₄C rods and <u>spillway</u>

Core

- ø60 cm/100 cm, 2-zone
- Inner: 336 UO₂
 1.806 wt%
 1.837 cm
- Outer: 176 U_{met} 0.947 wt% 2.917 cm



U. Kasemeyer *et al.*, "Benchmark on Kinetic Parameters in the CROCUS Reactor," in IRPhE, no. 4440, OECD, Ed. 2007, p. 94 J. M. Paratte *et al.*, "A benchmark on the calculation of kinetic parameters based on reactivity...," Ann. Nucl. Energy, vol. 33, no. 8, pp. 739–748, May 2006

The PETALE program in CROCUS

CEA-EPFL program on stainless-steel heavy reflectors carried out from Sep. to Dec. 2020

- 4 selected materials:
 - Stainless steel 304 L, iron, nickel, and chromium
 - Strong emphasis on estimation of covariances

Neutron transmission experiments

- 21 experiments (one repetition)
- Activation dosimeters between reflector sheets
- Output: dosimeters reaction rates

Reactivity worth experiments

- 5 dedicated experiments: full water, then each material
- Output: effect on criticality of the metallic sheets

Analysis status

- High-fidelity analysis reaching its end
- Collaboration work for **benchmarking** in **ICSBEP** is starting (US DOE funding)
 - with Prof. Siefman @Berkley and C. Percher @LLNL



EPFL

cea



evaluations

Analysis of Spectrometry Data : Dosimetry Setup



- CERVIN platform: 4 HPGe spectrometers
 - Dosimetry platform developed by the CEA for usage at EPFL
 - One fully shielded reference HPGe: Fürggen
 - 3 partially shielded HPGe: Hörnli, Lion & Zmutt

High experimental

- 7 types of activation dosimeters
 - With different energy ranges
- More than 400 dosimeters measured

	differences								
Material	¹¹⁵ In	¹⁹⁷ Au	¹¹⁵ In	⁵⁸ Ni	⁵⁴ Fe	⁵⁶ Fe	²⁷ Al		
Reaction	n, γ	n, γ	n, n'	n, p	n, p	n, p	n, α		
Median Energy of Activation	1.7 eV	5.7 eV	2.0 MeV	3.6 MeV	4.1 MeV	7.6 MeV	8.7 MeV		



Computational Methods

Monte Carlo neutron transport simulation

- Serpent2 and Tripoli-4® in agreement
 - For readability only Serpent2 presented
- Dosimetry using the IRDFF-II library
- Normalization by the 3rd dosimeter (default)
- Reduced χ² statistic in preparation of future work
 - $\chi^2_{\nu} = Res^T \underline{Cov}^{-1} Res / \nu$
- Covariances propagation



 ^{197}Au

PETALE

TRIPOLI-4®

reflector-

Difference [%]

elations

5

-10

 $\chi^2_{\mu} = 0.8$



Core XS uncertainty

Monte Carlo neutron transport simulation

- Perturbed XS:
 - Isotopes: ²⁷AI, ¹H, ¹⁶O, ²³⁵U, ²³⁸U
 - Mt: 2, 4, 18, 102
 - Multiplicity
- Estimated with 66 Serpent2 simulations
- Dosimetry using the IRDFF-II library
- Use larger virtual dosimeters in the reflector
 - Increase in convergence speed

Results

- Strong positive correlations in the reflector
 - Expected results
- Negative correlations between core center thermal dosimeters and other dosimeters
 - Mild with core center fast dosimeters
 - Strong with reflector dosimeters





PETALE Results:

- All cases performed with JEFF-3.3
- All mean values
- Position and core XS uncertainties in progress
- Additional simulations with crosssections of JEFF-4T3/INDEN for the reflector





Results : All Reflectorse as April

- XS from JEFF-3.3
- ¹¹⁵In(n,g) dosimeters
 - Median energy of activation ~1.7 eV
- Decreasing trends for nickel and chromium
- No clear trends for iron and steel
- Pattern due to the spectrum hardening and dosimetry XS covariances







- XS from JEFF-3.3
- ¹⁹⁷Au(n,g) dosimeters
 - Median energy of activation ~5.7 eV
- Decreasing trends for nickel
- Thickness effect for chromium
- Good agreement for iron and steel





- XS from JEFF-3.3
- ¹¹⁵In(n,n') dosimeters
 - Median energy of activation ~2 MeV
- Opposing trend between iron and the other alloy component
 - Over-reflection of the neutron for nickel and chromium
 - Over-transparency of the iron
 - Mild over-transparency for stainless steel (304L)





- XS from JEFF-3.3
- ⁵⁸Ni(n,p) dosimeters
 - Median energy of activation ~3.6 MeV
- Discrepancy between Serpent2 and Tripoli4®
 - Serpent 2.1.21 has an issue interpreting some unexpectedly defined XS
 - Corrected in later release





- XS from JEFF-3.3
- ⁵⁸Ni(n,p) dosimeters
 - Median energy of activation ~3.6 MeV
- Discrepancy between Serpent2 and Tripolio VED
- Border effect for nickel
- Over-transparency of iron and steel 304L
- Strong over-reflection for chromium





Simulations of the transmission experiments

- XS from JEFF-3.3
- ⁵⁶Fe(n,p) dosimeters
 - Median energy of activation ~7.6 MeV

Unexpected behaviour

Sudden drop of the C/E at the end of the reflector





- XS from JEFF-3.3
- ⁵⁶Fe(n,p) dosimeters
 - Median energy of activation ~7.6 MeV
- Unexpected behaviour SOLVED
 - Effect of ⁵⁵Mn impurities (5.8 ppm)
 - Overestimation of the experimental reaction rates
 - Up to 20% difference at the end of the block!





- XS from JEFF-3.3
- ⁵⁶Fe(n,p) dosimeters
 - Median energy of activation ~7.6 MeV
- Unexpected behaviour due to ⁵⁵Mn COLVED
- Nickel, chromium, iron and steel
 - Over-transparency
 - And thickness effect
 - Steel shows the strongest trend





- XS from JEFF-3.3
- ²⁷Al(n,a) dosimeters
 - Median energy of activation ~8.7 MeV
- Nickel and steel
 - Over-transparency
 - And thickness effect
- Good agreement of the iron and chromium





Feedback on JEFF-4T3: 304L Reflectors

Simulations of the stainless steel 304L transmission experiments

- XS from JEFF-3.3 and JEFF-4T3
 - Minor alloy elements and impurities included
- Both evaluations are in agreement with the experiments
 - Flat C/E
 - χ^2_{ν} also in agreement







Feedback on JEFF-4T3: 304L Reflectors

Simulations of the stainless steel 304L transmission experiments

- XS from JEFF-3.3 and JEFF-4T3
 - Minor alloy elements and impurities included
- JEFF-4T3 flattens the previous trends in the fast neutron range
 - Especially for ¹¹⁵In(n,n') and ⁵⁸Ni(n,p) dosimeters
 - Some over-transparency still visible at higher energy





Feedback on INDEN: Iron Reflectors

- XS from JEFF-3.3 and INDEN
 - All available isotopes
- ¹¹⁵In(n,g) is slightly less consistent
 - χ^2_{ν} from 3.3 to 6.1
- ¹⁹⁷Au(n,g) in agreement with the experimental data
 - Flat C/E







Feedback on INDEN: Iron Reflectors

- XS from JEFF-3.3 and INDEN
 - All available isotopes

- The INDEN evaluation is in good agreement with the experiments around 2 MeV and 3.6 MeV
 - The previous trend is flattened







Feedback on INDEN: Iron Reflectors

- XS from JEFF-3.3 and INDEN
 - All available isotopes

- At higher energy the trend is slightly stronger than before
 - Slight increase in trend (statistically significant)







Feedback on INDEN: Chromium Reflectors

- XS from JEFF-3.3 and INDEN
 - Here the older INDEN only includes Cr-52

- A trend appeared in the near thermal range for chromium
 - Visible with both experiments
 - Degraded χ^2_{ν}







Feedback on INDEN: Chromium Reflectors

- XS from JEFF-3.3 and INDEN
 - Here the older INDEN only includes Cr-52
- The discrepancies around 2 MeV are reduced with INDEN
 - A clear trend is still visible
- The Ni dosimeter trend is preserved
 - But the activation profile is different







Feedback on INDEN: Chromium Reflectors

- XS from JEFF-3.3 and INDEN
 - Here the older INDEN only includes Cr-52

- The trends at higher energy (⁵⁶Fe(n,p) and ²⁷Al(n,α) dosimeters) are mostly preserved
 - No significant differences are observed in the C/E observed
 - Observed small differences maybe from calculation statistics







Feedback on TENDL: Nickel Reflectors

- XS from JEFF-3.3 and Tendl-23/24
 - Tendl-23 from JEFF-4T3 ace files
 - Tendl-24 from JEFF-4T4 ace files

- Magnified drops at the edges of the reflectors
- A gradual increases of the C/E appears after a few sheets







Feedback on TENDL: Nickel Reflectors

- XS from JEFF-3.3 and Tendl-23/24
 - TendI-23 from JEFF-4T3 ace files
 - TendI-24 from JEFF-4T4 ace files

- TendI-24 close to JEFF-3.3
 - TendI-23 has slightly stronger trend with In(n,n') and Ni(n,p)





Comparison to JEFF-4T3

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1.3

- Simulation with INDEN/JEFF-4T3 shows mixed results with respect to JEFF-3.3
 - Reduced χ^2 are lower and trends are flattened in most cases for iron and stainless steel
 - New trends and effect appeared for nickel and chromium

						01						
	JEFF-3.3 (JEFF-3.1.1 for Cr fast neutron dosimeters)					INDEN/TendI-24						
	¹¹⁵ In(n,γ)	¹⁹⁷ Au(n, γ)	115 In(n, n')	⁵⁸ Ni(n, p)	⁵⁶ Fe(n, p)	²⁷ Al(n, a)	115 In(n, γ)	197 Au(n, γ)	115 In(n, n')	⁵⁸ Ni(n, p)	⁵⁶ Fe(n, p)	²⁷ Al(n, a)
	1.7 eV	5.7 eV	2.0 MeV	3.6 MeV	7.6 MeV	8.7 MeV	1.7 eV	5.7 eV	2.0 MeV	3.6 MeV	7.6 MeV	8.7 MeV
Cr	9.7	2.81	37.8	35.7	5.4	0.8	14	11	21	37.5	7.9	2
Ni	5.7	3.3	10.9	7.7	5.8	7.2	32.8	20	23.5	5.2	2.9	-
Fe	3.25	0.88	13.7	26.7	8.9	1.3	6.1	1.5	2	2.6	12.4	3
04L	1.3	1.1	6.5	28.3	13.5	10.9	0.4	1	4.7	3.9	6.4	-



Conclusion

- The PETALE experiment was conducted end of 2020
 - The high-fidelity analysis is nearing its end
 - The benchmarking work is starting
- High-fidelity analysis for the transmission experiments is nearing completion
 - All C/E with JEFF-3.3
 - C/E and EPFL agree on the observed trend
 - Cr reflector discrepancies source is identified and resolved using JEFF-3.1.1
 - The reasons for the drop in ⁵⁶Fe dosimeter was due to ⁵⁵Mn impurities
 - Core XS-related uncertainties are being added
- Comparison of C/E between INDEN and JEFF-3.3 evaluations
 - INDEN shows overall better results for iron
 - Especially in the range of ⁵⁸Ni and ¹¹⁵In(n,n') dosimeters
 - INDEN shows better results for chromium around 2 MeV
 - Higer energies are not affected on average
 - Different trends appeared at lower energy
 - JEFF-4T3 shows overall better results for stainless-steel 304L
 - Different trends appeared in the thermal range for the nickel reflector

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EPFL OUTLOOK: HARVEST-X reproducibility

Production and analysis of new experimental results allowing to tackle biases

- Reproduction with other systems
 - Experiments in accelerator facility
 - Experiments in **reference fields**
- Reproduction with other methods
 - Pile-oscillation experiments in CROCUS: BLOOM

BLOOM

- Running since Fall 2024 up to February 2025
- 25 materials (with samples directly cut from PETALE spares)
- Local and Global Flux measurement

SAFFRON Global & **local** measurements







Merci

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Questions ?

















Reflector: 304L, Dosimeters: ⁵⁸Ni(n,p)




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Normalized Cumulative Reaction Rate



Energy Me











■ INDEN Consultancy meeting: Analysis of PETALE and feedback on new evaluations

















Normalized Cumulative Reaction Rate



























































Reflector: Nickel, Dosimeters: ⁵⁸Ni(n,p)











EPFL Objective: stainless steel nuclear data

Provide new constraints in the MeV-range and above for stainless steel nuclear data

- Fission: heavy reflectors (GEN-III PWR)
- Fusion: 14 MeV neutrons
- Accelerators: activation



Collaboration between CEA & EPFL



Iron inelastic scattering cross section data (JANIS)

Cea



evaluations

meeting: Analysis of PETALE and feedback

INDEN Consultancy

Experimental design

Program in CROCUS* on elemental-type reflector experiments, for new constraints in the MeV-range on stainless steel nuclear data

- Separate study of s. steel (304L), Fe, Ni and Cr
 - · Reactivity worth of reflectors
 - Transmission using activation dosimetry

Collaboration between CEA & EPFL







¹ A. Laureau et al., "Uncertainty propagation for the design study of the PETALE experimental programme in the CROCU reactor." EPJ Nucl. Sci. Technol., vol. 6, p. 9, 2020. ² V. Lamirand et al., "An Experimental Programme optimized with Uncertainty Propagation: PETALE in the CROCUS Reactor," EPJ Web Conf., vol. 211, p. 03003, Jun. 201962



Experimental design by uncertainty propagation

Relating XS uncertainty distribution with measured reaction rates using Total Monte Carlo and Correlated Sampling^{1,2}



× N full core Monte Carlo calculations
 ⇔ 1 node week



¹ <u>A. Laureau et al., "Uncertainty propagation for the design study of the PETALE experimental programme in the CROCUS reactor," *EPJ Nucl. Sci. Technol.*, vol. 6, p. 9, 2020. ² <u>V. Lamirand *et al.*, "An Experimental Programme optimized with Uncertainty Propagation: PETALE in the CROCUS Reactor," *EPJ Web Conf.*, vol. 211, p. 03003, Jun. 2019**63**</u></u>



Experimental design by uncertainty propagation

Relating XS uncertainty distribution with measured reaction rates using Total Monte Carlo and Correlated Sampling¹

Dosimeters selection + target uncertainty



Ratios between RR distributions and activity uncertainties for the iron reflector



Correlations between reactions for each dosimeters' locations, in the case of the iron reflector



High resolution model

- From design model to high resolution
 - Model with structural elements
 - Fully voxelated reflectors

CROCUS

Estimation of correction factors and uncertainties

Case

Sheet

- Preparation for the benchmark
- Simulation with Serpent2 (EPFL)...



Water

10 20 cm

U_{met}

 UO_2



Simulation with custom SERPENT2 solver

3D Monte-Carlo transport code

- Modified build of Serpent 2.1.21^{1, 2}
 - Dosimeter tally with IRDFF-II library³
 - Variance reduction method
 - Correlated sampling
 - ND uncertainty propagation
 - Sampled XS: neutrons with multiple weights
 - Multiple results at once
 - More information tomorrow at 10:54 with Axel Laureau in Session Tu2T2
 - With openMC
 - Works with surface tracking
 - Not implemented in delta tracking
 - Better convergence of thin surfaces

1. J. Leppänen, et al., "The serpent monte carlo code: Status, development and applications in 2013,"

2. A. Laureau, et al., "Monte-carlo development for ND assimilation and experiment optimisation.".

3. A. Trkov, et al., "IRDFF-II: A New Neutron Metrology Library. Special issue of Nuclear Data Sheets", Vol. 163, pp. 1-108 (2020)

Variance reduction







Model constraint: uncertainties on position

Monte Carlo estimation of position uncertainties

- Results obtained through perturbed geometries calculation
- All elements can move with respect to their mechanical clearance
- The box itself can move with respect to position uncertainties
- Uncertainties and correlations included in the final C/E
- Expensive in computational power





Model constraint: uncertainties on position

INDEN Consultancy meeting: Analysis of PETALE and feedback on new evaluations





EPFL cea

INDEN Consultancy meeting: Analysis of PETALE and feedback on new evaluations

Backup Computational Methods

Monte Carlo neutron transport simulation

Core uncertainties



Fig. 9. Propagated nuclear data uncertainty on the dosimeter reaction rate using ENDF/B-VII.1 (left), ENDF/B-VIII.0 (middle) and JEFF-3.3 (right). The top plots are the standard deviation (1σ) for the different dosimeters and reactions on the x-axis. The bottom matrices are the correlation matrices associated with the standard deviation.



Backup: TMC

Correlated Sampling technics?

Principle

- Objective: replace 2 "close" calculations by a single one
 - \rightarrow calculation speed-up only 1 run
 - \rightarrow variance reduction same neutron path
 - \rightarrow no first order assumption
- Neutron weight modification
 → ratio of probabilities between the two systems
- Different application fields
 - → surface displacement
 - → element concentration / density modification
 - → Doppler effect
 - → ... nuclear data uncertainty

Drawbacks

- Needs probabilities different from zero and infinity
 → can not make isotope appears from scratch
- If the systems are too different the neutron weight is too different
 → bad convergence









Backup: TMC

Correlated Sampling with multiple Cross Sections: TMC-CS

Principle

- Each set of cross sections corresponds to a different system
 → different probabilities during the transport
- Neutron weight modification for each XS set
- Multiple "isotopes" and "mt" all together
 → ratio of probabilities between the two systems

Nuclear Data cross sections

- "Classic" TENDL cross section
 → sampling on the nuclear data parameters
- "Extended" TENDL EUROfusion ("to fill the gap")
 → sampling on the nuclear models themselves (more challenging)





256 random TENDL ⁵⁶Fe cross sections





Backup: TMC

Principle of the Bayesian Monte Carlo (BMC)

- Step 1: generation of random cross sections (XS) in agreement with the prior experimental knowledge
 → e.g. TENDL, JEFF+NUSS
- Step 2: Total Monte Carlo (TMC) uncertainty propagation
 prior calculated "C" value for each set of cross sections
- Step 3: Comparison with experimental "E" results and XS-weighting in the BMC process
 → reduced posterior uncertainty using w_x = exp (- Res^TCov⁻¹Res



► C-E

Hypothesis : ther is no slope in the C/E

 $\chi^2 = ResTCov^{-1}Res$




Backup: BMC



'Res' is supposed to be the 'Calculation' vs 'Experiment' difference -> average C value used instead for BMC testing