IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

*Faire avancer la sûreté nucléaire*

# Burn-up impact on nuclear data sensitivity and uncertainty for reactor safety applications

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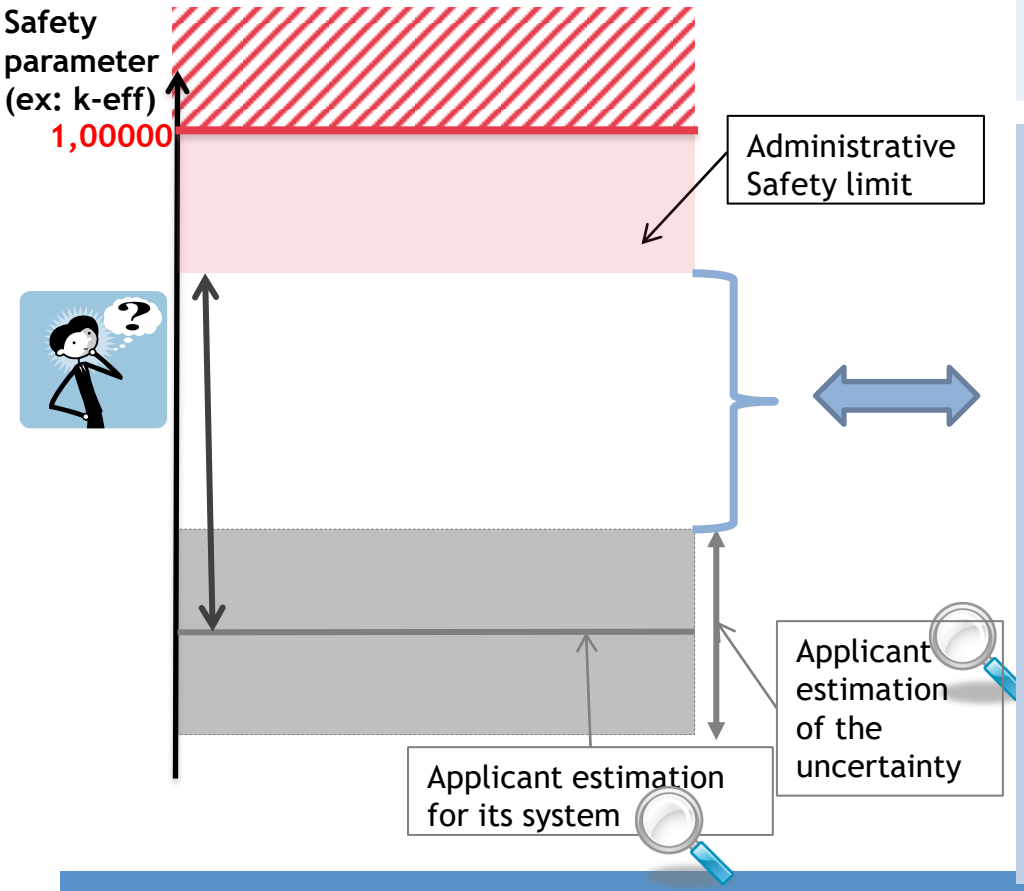
# Outline

- Context
- Methodology
- Burn up impact for PWR
  - Concentrations
  - Nuclear Data Sensitivity
  - Nuclear Data Uncertainty
- Conclusions

# Nuclear data importance for IRSN

- French Institute for Radiological Protection and Nuclear Safety




## Objective:

Assess safety margins provided by designers for the application systems

Safety margin relies on uncertainties due to:

- Manufacturing parameters
  **Explicit source of uncertainties : can be quantified via direct $k_{eff}$ computation**
- Validation of calculation tools:
  - ✓ Modeling and algorithms
    **Minimized by use of highly-accurate criticality tools**
  - ✓ **Nuclear Data**
    **Major inherent unavoidable source of uncertainties. Specific tools/methods are required for its quantification.**

# Nuclear data importance for Burn up applications

- In reactor safety studies, accurate knowledge of the nuclear data (ND) used as input to neutron simulation codes is of the highest importance: necessary to quantify the calculation uncertainty to nuclear data, and especially as a function of irradiation time

- Study the burn-up (BU) effect on ND sensitivities and uncertainties for reactor applications (PWR) for different ND libraries

- GOAL : better understanding of the uncertainties related to the ND impacting the reactor safety studies at IRSN. In the long term it might prompt to propose re-examining existing evaluations and propose new evaluations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# Methodology

# Methodology

- Use of Monte Carlo depletion code (VESTA) to accurately simulate conditions present in reactors
- Sensitivity coefficients calculation at different BU: $S = \frac{\alpha}{k}\frac{dk}{d\alpha}$
  - Calculated in the Monte-Carlo: MORET 5.D.1, MCNP6
  - Using the VESTA concentration results obtained at these BU values
  - Observe the impact of the nuclear data cross sections on $k_\infty$
- Nuclear data uncertainties propagation at different BU: $\sigma^2 = S\ C\ S^T$
  - Tool: TSUNAMI-IP
  - Using the sensitivity coefficients results and the covariance matrices


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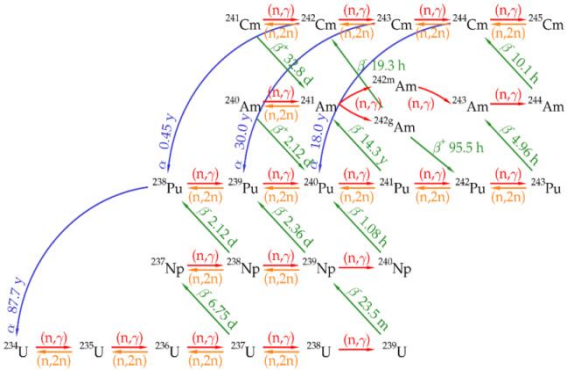
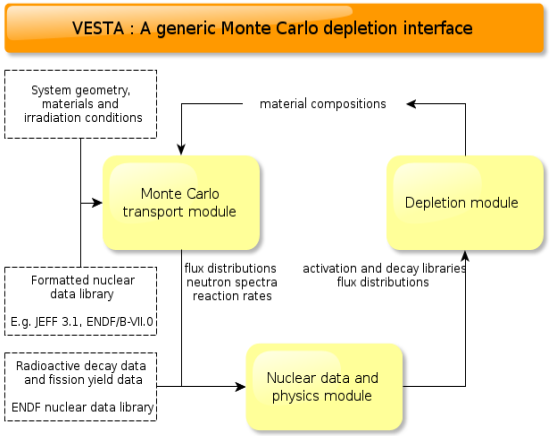
# VESTA: a depletion Monte-Carlo code

- Goal : simulate material composition under irradiation very accurately
- Applications : criticality safety, reactor safety studies (PWR, BWR, research reactors, fusion systems, ..), cycle (transport, scenario ..), waste characterization, material activation ..
- VESTA philosophy : a generic interface customisable to a user's needs :
  - Monte Carlo code: MCNP(X/6), MORET 5
  - Depletion module: ORIGEN 2.2, PHOENIX, FISPACT, etc.
  - Nuclear data libraries : JEF2.2, JEFF-3.1, JEFF-3.1.1, JEFF-3.2, JEFF-3.3, JENDL, ENDF/B-VII.0, ENDF/B-VII.1 at different temperatures
- VESTA 2.1.5 has been validated for 65 isotopes on 96 radiochemical assay and decay heat measurements using JEFF-3.1 and ENDF/B-VII.0






**VESTA 2.1.5 is distributed by the NEA Databank and RSICC (more than 100 users worldwide)**

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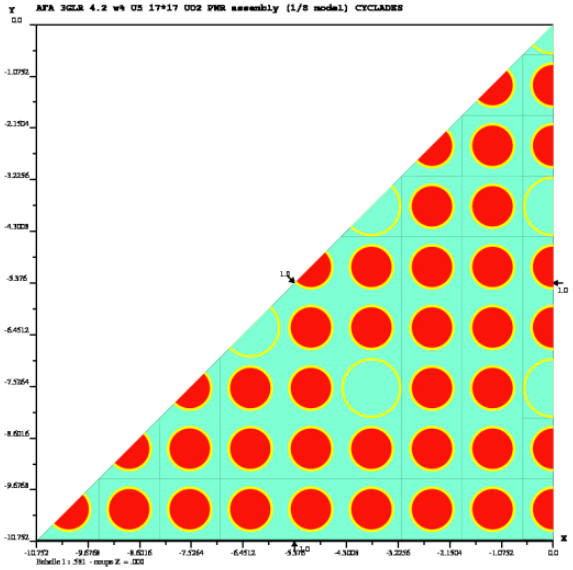
# PWR simulations

- Four different French PWR fuel operations with different enrichments were used:

  3.1%, 4%, 4.2% and 4.5% $^{235}U$

- Simulation Parameters (ALCADE):
  - 17 x 17
  - Fuel: UOX ($^{235}U$ : 4.0%)
  - Burn-up = 49 GWd/t
  - 1/8 of an assembly
  - 1 m active height
  - 700 ppm Boron
  - Burn-up step = 1 GWd/t (without Gd)

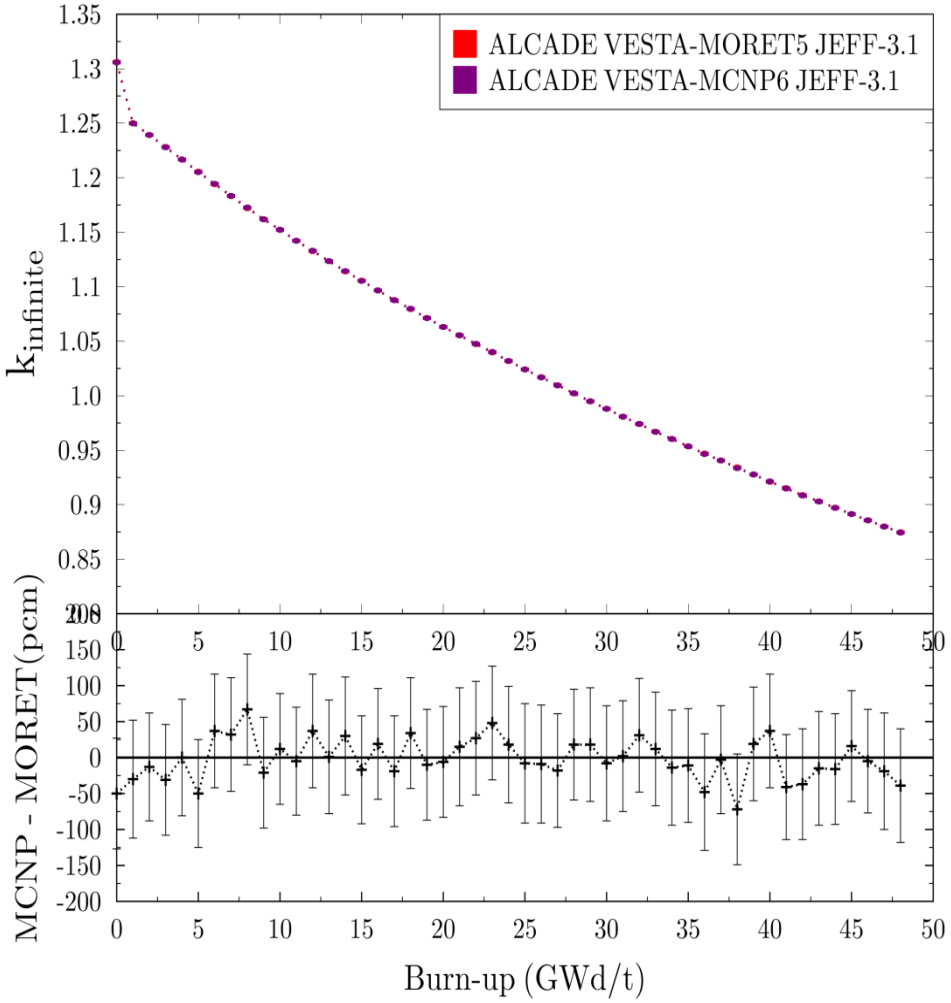


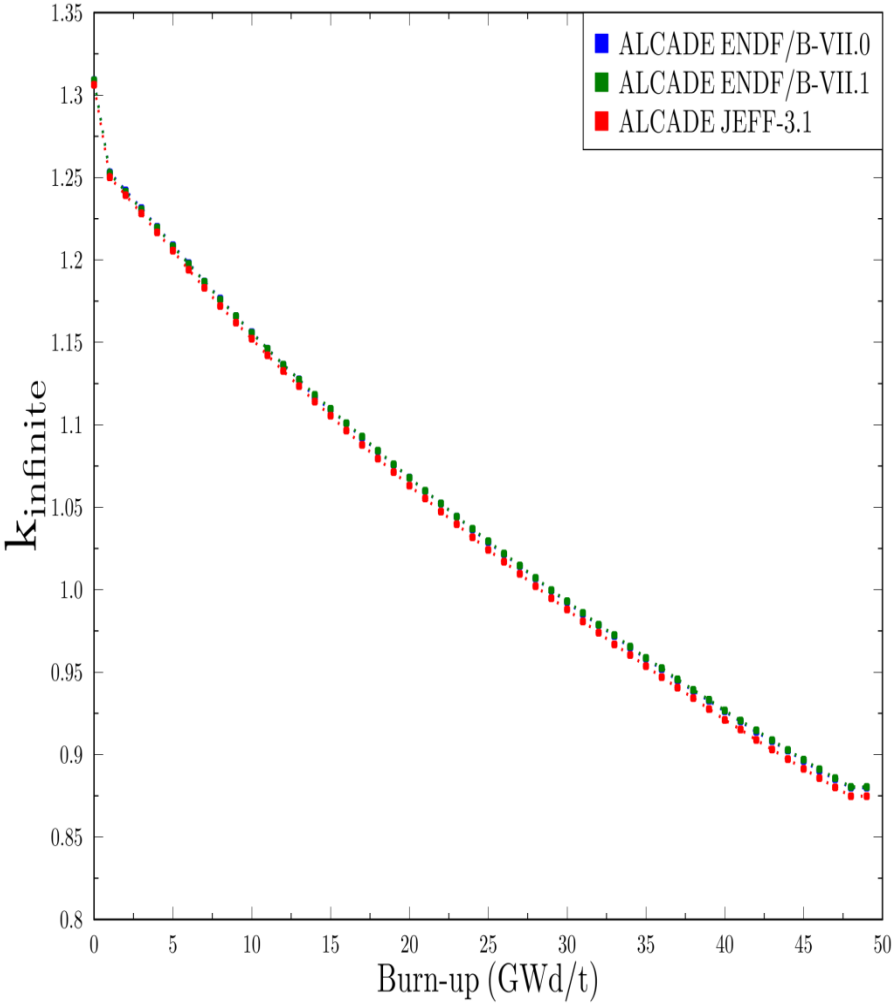
- Irradiation history has to be known with precision

$$P = \frac{BU \cdot M_{HMi}}{\Delta t}$$

- Nuclear Data: ENDF/B-VII.0, ENDF/B-VII.1 and JEFF-3.1 libraries

# $K_\infty$ results

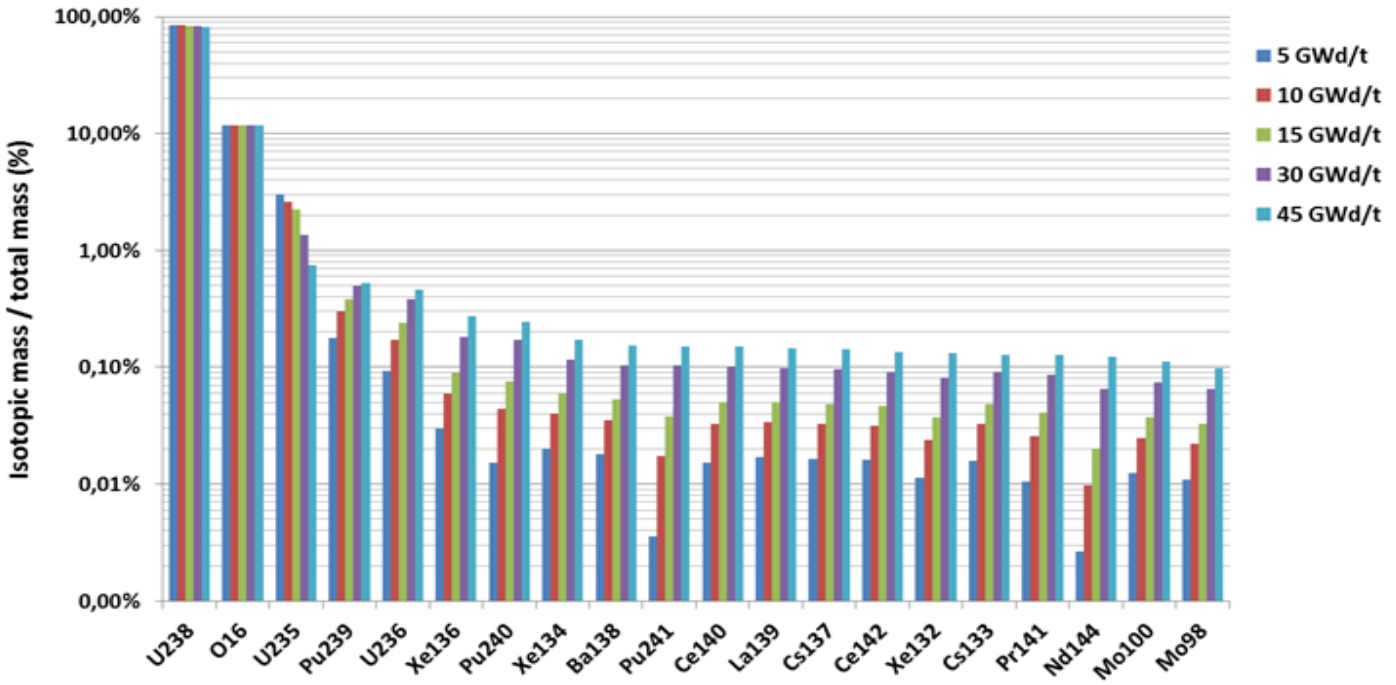


# BU impact on PWR

# BU impact on concentration (ENDF/B-VII.1)

- The results obtained for the different operations and using different libraries don't show any significant differences
- The list is representative of the isotopic concentration of a French UOX-fuel PWR (without Gd)



# BU impact on sensitivity (ENDF/B-VII.1)

- Sensitivity coefficient represents the variation of the *k* value of a system due to a given parameter (α), like an isotope cross-section. The sensitivity coefficient is defined as: $S = \frac{\alpha}{k} \frac{dk}{d\alpha}$

- Using MORET 5 :
  - In MORET 5.D.1: a continuous-energy sensitivity coefficients calculation has been recently implemented

    *A. Jinaphanh, N. Leclaire, B. Cochet and B. Quaghebeur, "Validation of continuous energy sensitivity coefficients calculations in the MORET 5 code", Proc. ICNC 2015, Charlotte, (2015).*

  - Relies on the differential operator method and the estimation of the adjoint source using the Iterated Fission Probability (the one implemented in both MCNP6 and SCALE)
  - The energy-dependent sensitivity calculations are stored into the 238 SCALE energy binning in a sensitivity data file (SDF)
  - Calculations performed for different ND libraries and for 4 different BU values (5, 15, 30 and 45 GWd/t), using the concentration results of the VESTA simulations

# BU impact on sensitivity (ENDF/B-VII.1)

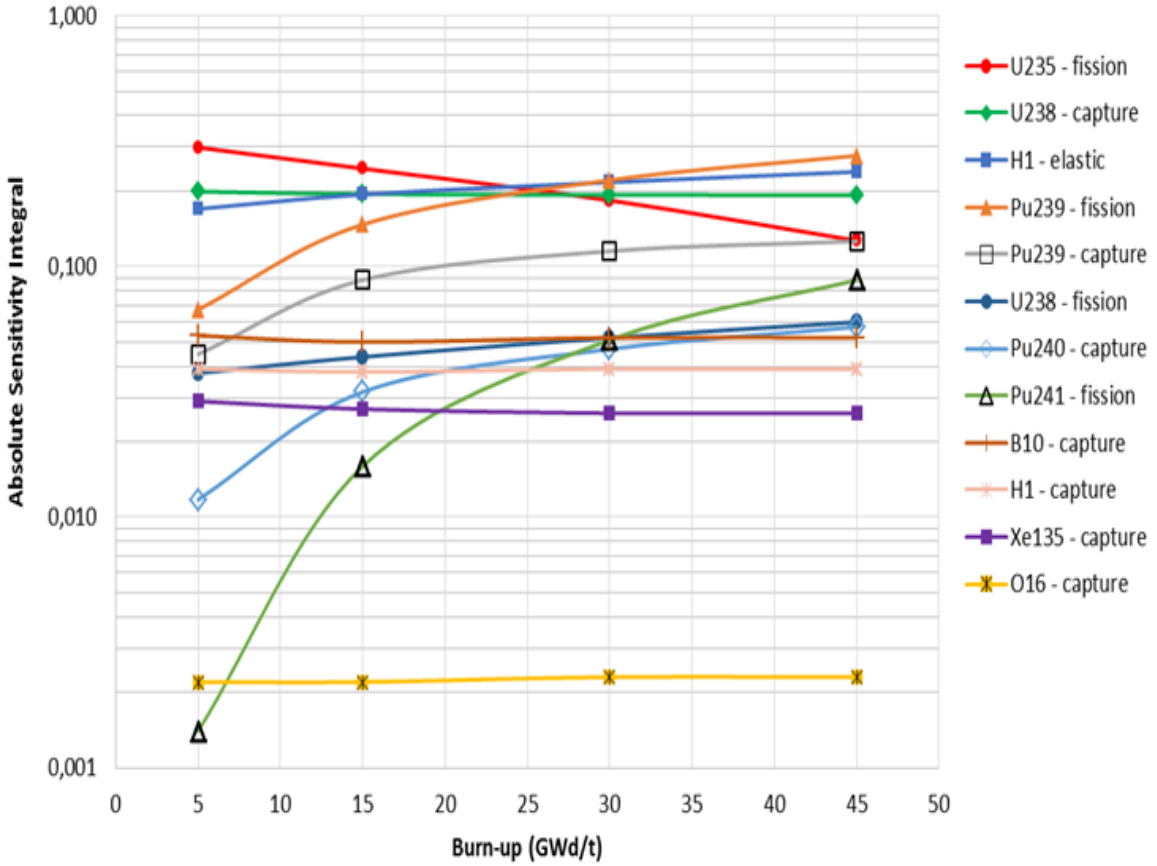
- $K_\infty$ integrated sensitivity coefficients from MORET 5.D.1 at 5, 15, 30, and 45 GWd/t:

| 5 GWd/t | | 15 GWd/t | | 30 GWd/t | | 45 GWd/t | |
|---|---|---|---|---|---|---|---|
| Data | S | Data | S | Data | S | Data | S |
| $^{235}$U nubar | 0.784 | $^{235}$U nubar | 0.591 | $^{239}$Pu nubar | 0.424 | $^{239}$Pu nubar | 0.500 |
| $^{235}$U fission | 0.299 | $^{239}$Pu nubar | 0.302 | $^{235}$U nubar | 0.396 | $^{239}$Pu fission | 0.277 |
| $^{238}$U capture | -0.199 | $^{235}$U fission | 0.246 | $^{239}$Pu fission | 0.221 | $^{235}$U nubar | 0.250 |
| $^{1}$H elastic | 0.169 | $^{238}$U capture | -0.194 | $^{1}$H elastic | 0.216 | $^{1}$H elastic | 0.238 |
| $^{239}$Pu nubar | 0.145 | $^{1}$H elastic | 0.193 | $^{238}$U capture | -0.193 | $^{238}$U capture | -0.192 |
| $^{235}$U capture | -0.109 | $^{239}$Pu fission | 0.147 | $^{235}$U fission | 0.183 | $^{241}$Pu nubar | 0.152 |
| $^{238}$U nubar | 0.067 | $^{239}$Pu capture | -0.088 | $^{239}$Pu capture | -0.115 | $^{235}$U fission | 0.127 |
| $^{239}$Pu fission | 0.067 | $^{235}$U capture | -0.078 | $^{241}$Pu nubar | 0.093 | $^{239}$Pu capture | -0.126 |
| $^{10}$B capture | -0.053 | $^{238}$U nubar | 0.073 | $^{238}$U nubar | 0.082 | $^{238}$U nubar | 0.090 |
| $^{239}$Pu capture | -0.044 | $^{10}$B capture | -0.051 | $^{10}$B capture | -0.052 | $^{241}$Pu fission | 0.088 |

- A strong impact of burn-up on the $k_\infty$ integrated sensitivity results is observed

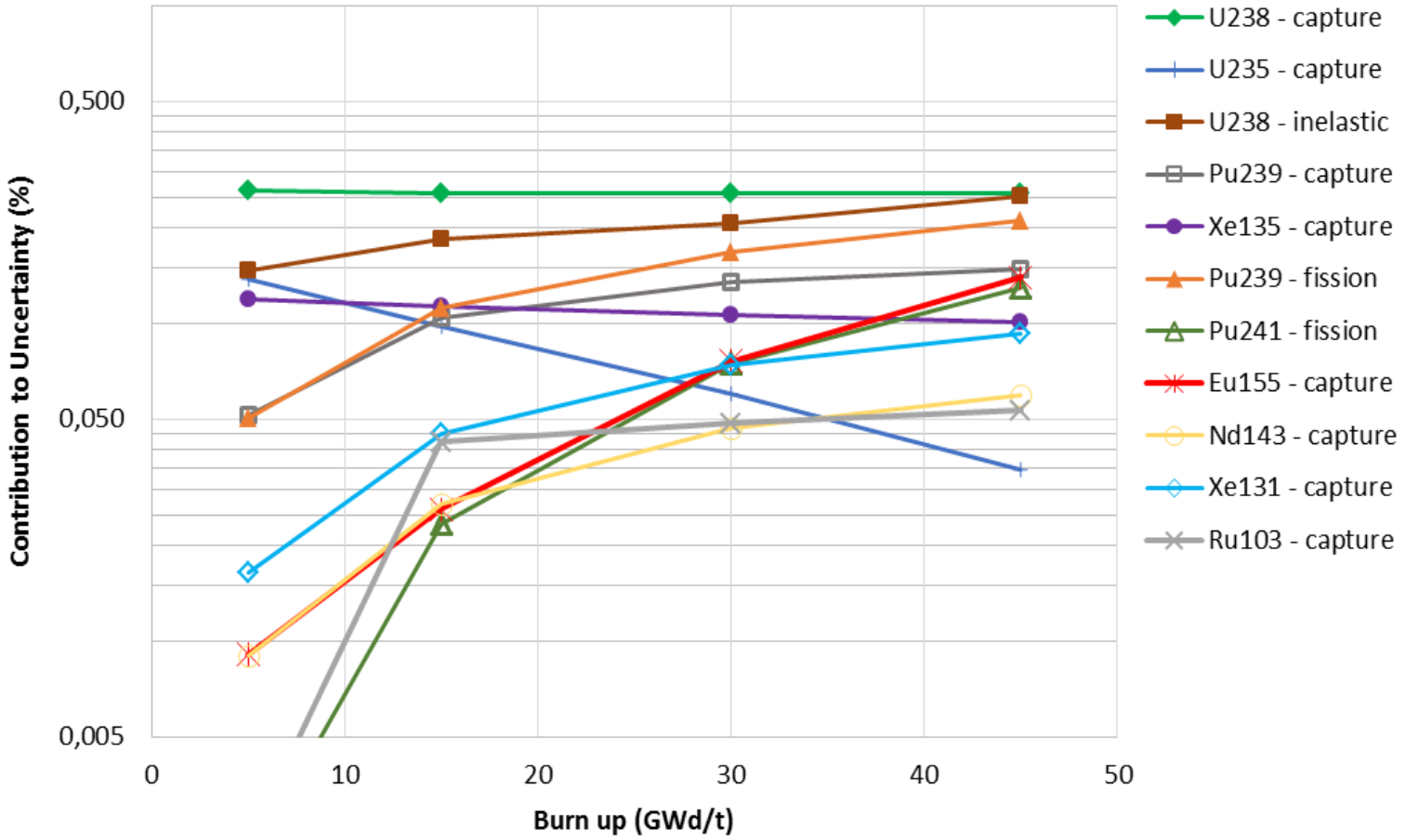
# BU impact on sensitivity (ENDF/B-VII.1)

- As BU increases, sensitivity of certain isotopes increases due to their increase in concentration
- Main example: $^{239}$Pu macroscopic fission cross-section, to which the integral $k_\infty$ sensitivity value increases from 7 % at 5 GWd/t to 30 % at 45 GWd/t
- Same behavior observed for $^{239}$Pu capture, $^{240}$Pu capture and $^{241}$Pu fission cross-sections
- The inverse is also true: the $k_\infty$ sensitivity to $^{235}$U fission cross-section is decreasing from 30 % at 5 GWd/t to less than 13 % at 45 GWd/t



# BU impact on ND uncertainty (ENDF/B-VII.1)

TSUNAMI-IP results using the sensitivity coefficients from MORET and the SCALE-6.2 56 groups ENDF/B-VII.1 covariance library. Propagated uncertainty values on *k* multiplication factor given as dk/k (%):



# BU impact on ND uncertainty (ENDF/B-VII.1)

- TSUNAMI-IP results using the sensitivity coefficients from MORET and the SCALE-6.2 56 groups ENDF/B-VII.0 covariance library: propagated uncertainty values on *k* multiplication factor given as dk/k (%) and a contribution in uncertainty on *k* by individual isotope/reaction.

| Burn-up value (GWd/t) | $k_\infty$ | % $dk_\infty/k_\infty$ | Individual contribution | |
|---|---|---|---|---|
| 5 | 1.20840 ± 0.00014 | 0.47920 ± 0.00066 | $^{238}$U capture | 0.25503 ± 0.00003 |
| | | | $^{235}$U nu-bar | 0.22228 ± 0.00001 |
| | | | $^{238}$U inelastic | 0.14723 ± 0.00047 |
| | | | $^{239}$Pu nu-bar | 0.14676 ± 0.00001 |
| | | | $^{235}$U capture | 0.14564 ± 0.00001 |
| 15 | 1.10940 ± 0.00014 | 0.54700± 0.00071 | $^{239}$Pu nu-bar | 0.30886 ± 0.00003 |
| | | | $^{238}$U capture | 0.24921 ± 0.00002 |
| | | | $^{238}$U inelastic | 0.17143 ± 0.00052 |
| | | | $^{235}$U nu-bar | 0.16677 ± 0.00001 |
| | | | $^{135}$Xe capture | 0.11459 ± 0.00001 |
| 30 | 0.99297 ± 0.00014 | 0.65360 ± 0.00087 | $^{239}$Pu nu-bar | 0.43580 ± 0.00006 |
| | | | $^{238}$U capture | 0.24783 ± 0.00002 |
| | | | $^{238}$U inelastic | 0.20752 ± 0.00064 |
| | | | $^{239}$Pu fission | 0.16715 ± 0.00002 |
| | | | $^{239}$Pu capture | 0.13218 ± 0.00001 |
| 45 | 0.89706 ± 0.00013 | 0.74210 ± 0.00151 | $^{239}$Pu nu-bar | 0.51435 ± 0.00008 |
| | | | $^{238}$U capture | 0.24881 ± 0.00002 |
| | | | $^{238}$U inelastic | 0.23089 ± 0.00072 |
| | | | $^{239}$Pu fission | 0.21061 ± 0.00001 |
| | | | $^{239}$Pu capture | 0.14702 ± 0.00001 |

The last column shows the nuclear data uncertainty main contributions. The relative standard deviation in $k_\infty$ is computed from the individual values by applying a quadratic sum.

# BU impact on nuclear data S/U

| Top contributors to both sensitivity and uncertainty | |
|---|---|
| Low BU | High BU |
| $^{235}$U nubar | $^{239}$Pu nubar |
| $^{235}$U fission | $^{238}$U capture |
| $^{235}$U capture | $^{239}$Pu fission |
| $^{238}$U capture | $^{239}$Pu capture |

- ND contributions to the final uncertainty are correlated to the burn-up
- There is a clear dependency between concentrations, sensitivities and uncertainties
- FP also highly contribute to uncertainty, such as, $^{143}$Nd, $^{103}$Ru and $^{155}$Eu which have both a high sensitivity and high uncertainty contribution value
- But for some cases the contribution to uncertainty is huge even if the $k_\infty$ sensitivity is not significant. In that case, the final ND uncertainty directly comes from the covariance data. Ex: $^{238}$U inelastic, $^{155}$Eu capture
- On the contrary: the sensitivity to $^{1}$H elastic is huge, while its uncertainty contribution is low due to the low covariance matrix uncertainty.

# Conclusion

- The three distinct nuclear data libraries showed very similar concentration and sensitivity results as a function of BU. The different PWR operations simulated showed likewise very similar results for the isotopic concentration, as well as for the $k_\infty$ sensitivity and uncertainty results as a function of BU

- A strong BU impact on the ND sensitivity and uncertainty was observed on the PWR simulations results. A short list of ND sets showing high $k_\infty$ sensitivity and uncertainty (at 1$^{st}$ order perturbation theory), using ENDF/B-VII.1 and ENDF/B-VII.0 covariance matrices, has been presented for different BU values

- These results indicate that special attention should be paid on ND uncertainties for systems that evolve with irradiation time

- Results to be confronted with benchmarks (TSURFER and/or MACSENS currently under development at IRSN)

- ND uncertainty on the concentration results has also to be estimated !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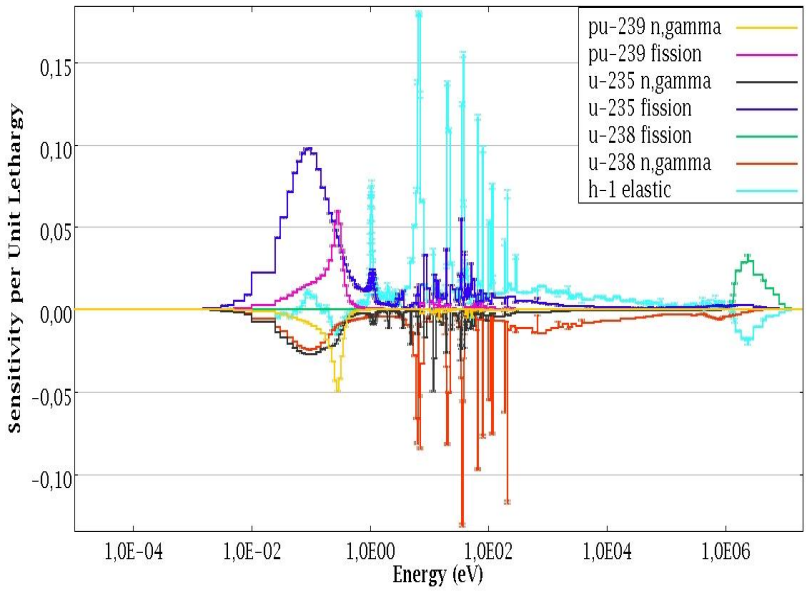
# Back-up

# BU impact on sensitivity (ENDF/B-VII.1)

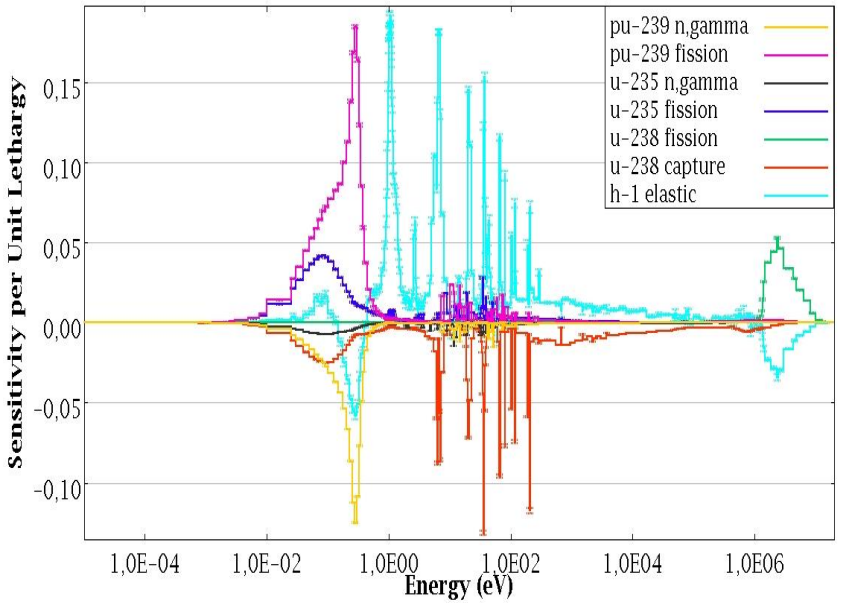
- Energy dependent sensitivity profiles obtained from MORET 5 for the top contributors at 5 GWd/t (left) and 45 GWd/t (right)

- Points out the impact of burn-up on the main isotopic energy dependent sensitivities.

5 GWd/t

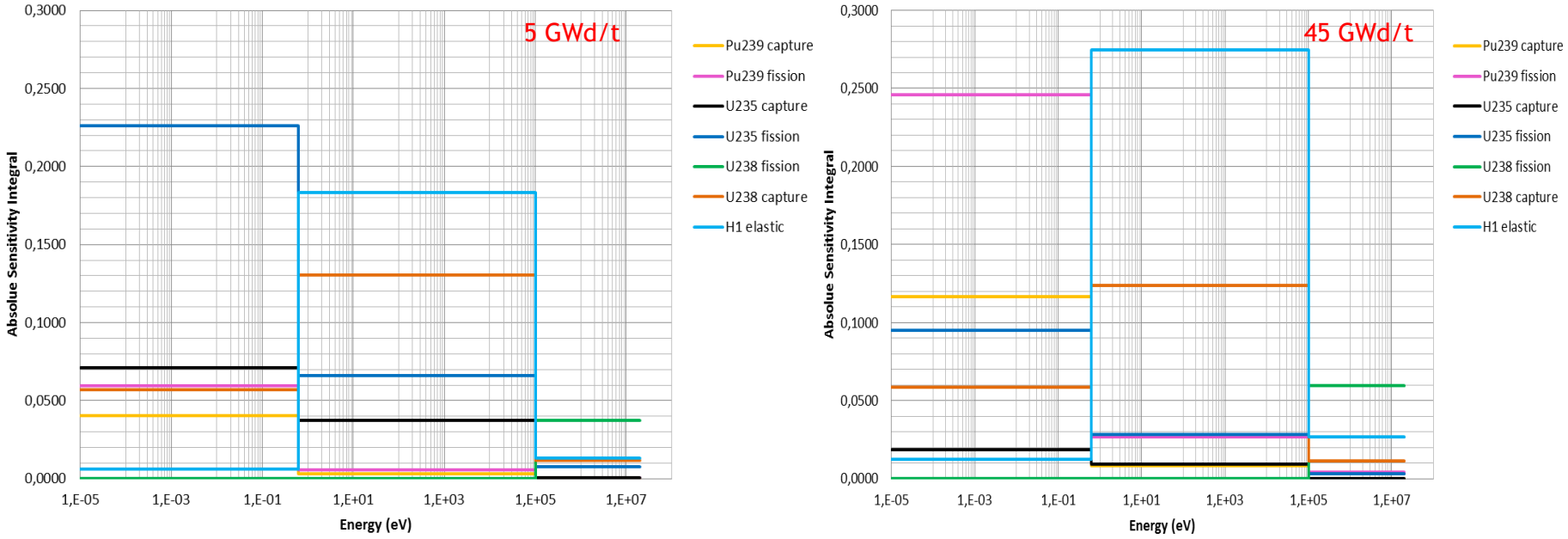



45 GWd/t

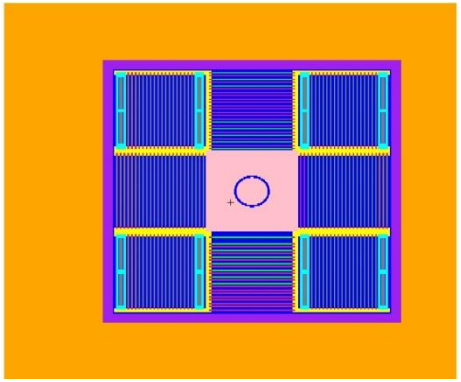


# BU impact on sensitivity (ENDF/B-VII.1)

- Sensitivity coefficients have been integrated in the thermal (≤ 0.625 eV), epithermal (0.625 eV < E < 100 keV) and fast (≥ 100 keV) energy intervals
- At 5 GWd/t sensitivity to $^{235}U$ fission reaches 23 % in the thermal energy range while it is decreased to around 10% at 45 GWd/t, whereas sensitivity to $^{239}Pu$ fission is increased to almost 25 %



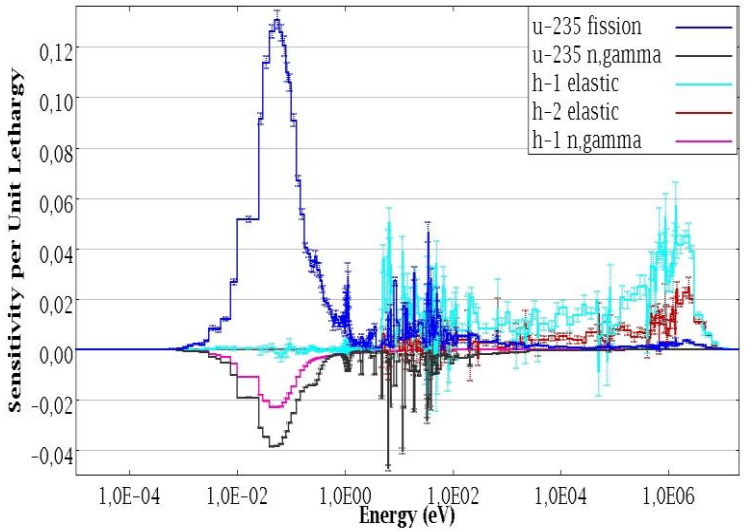
# ORPHEE reactor



- A research reactor case is studied to observe the impact of a higher fuel enrichment on the composition, sensitivity coefficients and uncertainties results.

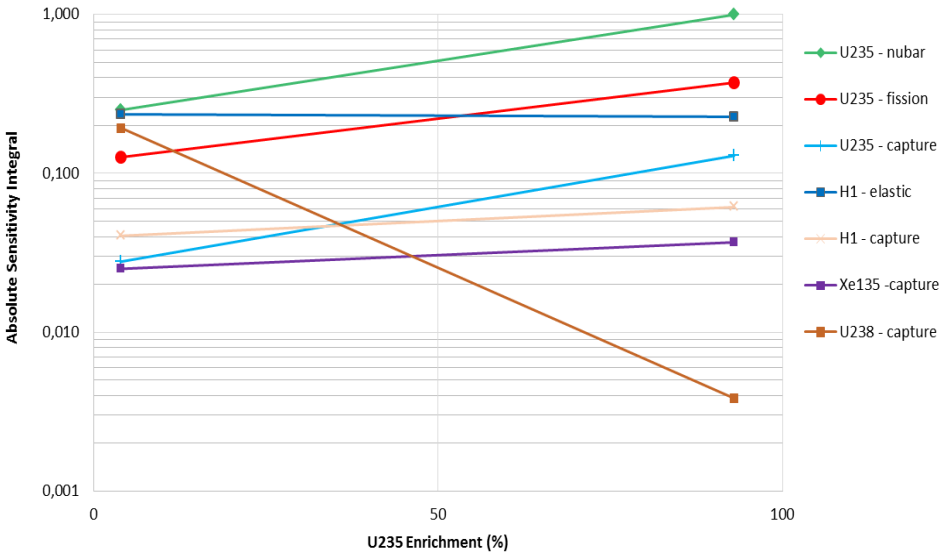
- The core consists of 8 assemblies of fuel parallel plates made of aluminium and uranium alloy (UAl), with an enrichment of 93 % inside a heavy water tank and that are arranged around a central beryllium reflector.

- Due to the reactor's significantly higher enrichment (93 % $^{235}U$), the sensitivity to $^{235}U$ nuclear data remains the most significant through irradiation.

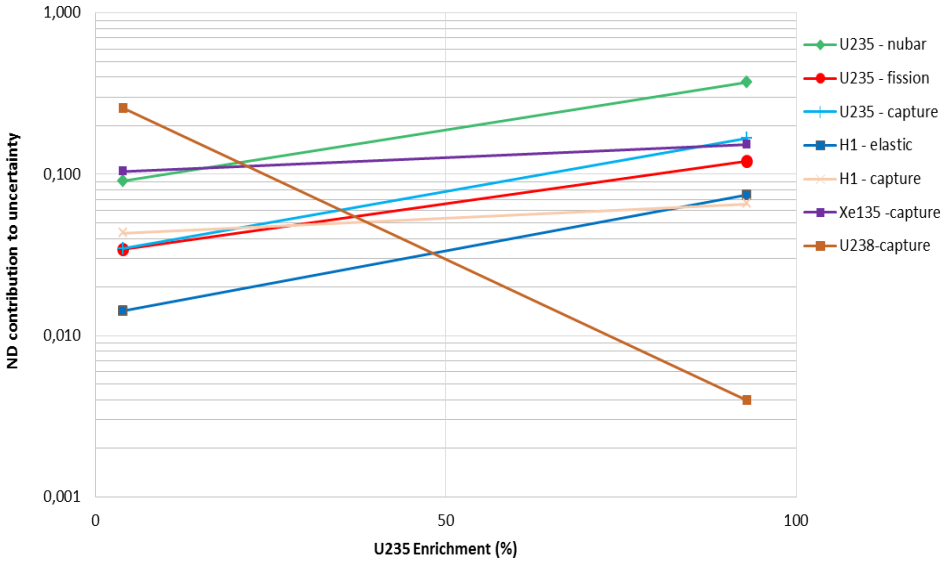


# ORPHEE reactor

- Comparison with the PWR sensitivity coefficients results at 45 GWd/t :




- Comparison with the PWR ND uncertainty contributions at 45 GWd/t :




| $k_\infty$ | % $dk_{eff}/k_{eff}$ | Individual contribution | |
|---|---|---|---|
| 0.99588 ± 0.00016 | 0.54300 ± 0.00127 | $^{235}$U nubar | 0.37210 ± 0.00015 |
| | | $^{235}$U capture | 0.16872 ± 0.00002 |
| | | $^{16}$O elastic | 0.17452 ± 0.00086 |
| | | $^{135}$Xe capture | 0.15337 ± 0.00002 |
| | | $^{2}$H elastic | 0.13267 ± 0.00035 |