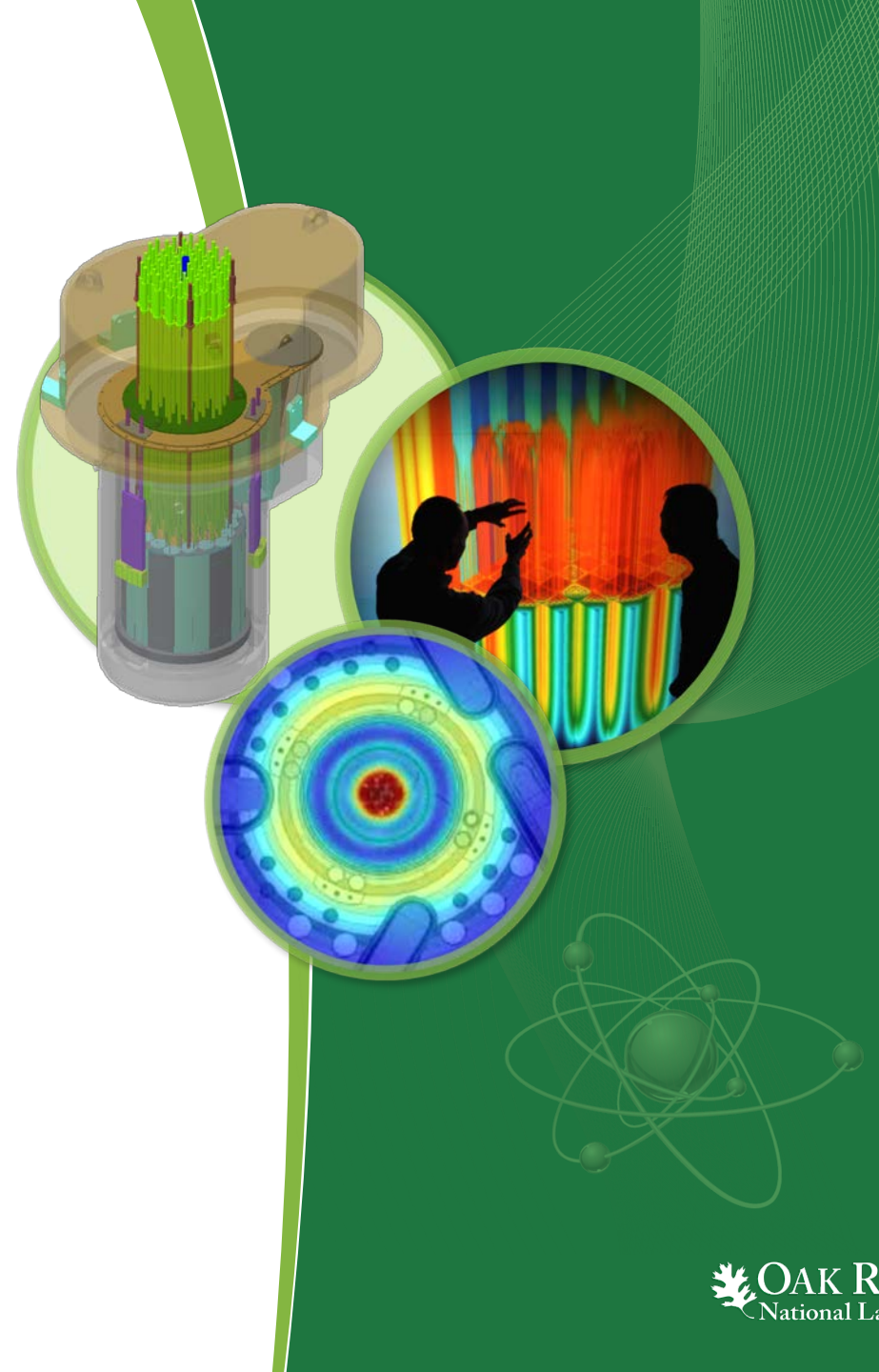


# Decay Heat Uncertainty due to Modeling and Nuclear Data Uncertainties

**Germina Ilas**  
**Henrik Liljenfeldt**

**Oak Ridge National Laboratory**

**SCALE Users' Group Workshop 2017**



# Outline

- Background
- Decay heat analysis methodology
- SCALE validation for spent fuel decay heat analysis
- Uncertainty in BWR spent fuel due to modeling data uncertainties

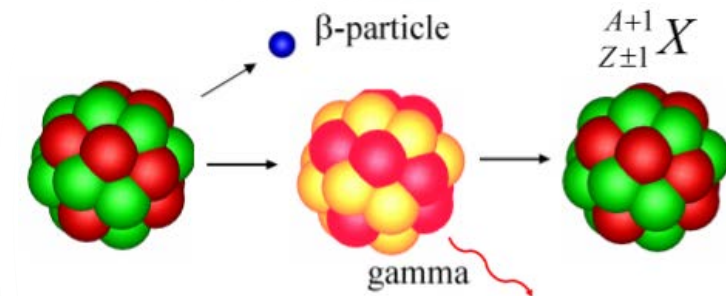
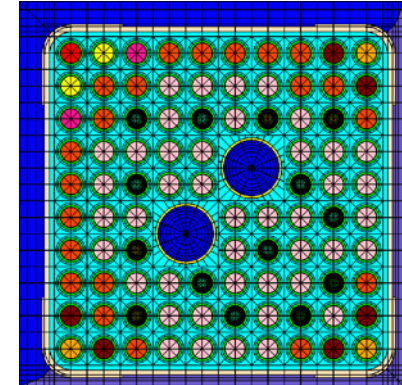
# Relevance



- Decay heat in spent fuel is critical for the design, safety, and licensing analyses of spent nuclear fuel storage, transportation, and repository systems
- Estimation of decay heat relies in general on code predictions and on available measurements
- Decay heat measurements can be expensive or impractical for covering the multitude of existing fuel designs, operating conditions, and specific application purposes
- Gap of knowledge is heavily supplemented through computer simulations
- Well-validated codes and uncertainty analysis are essential

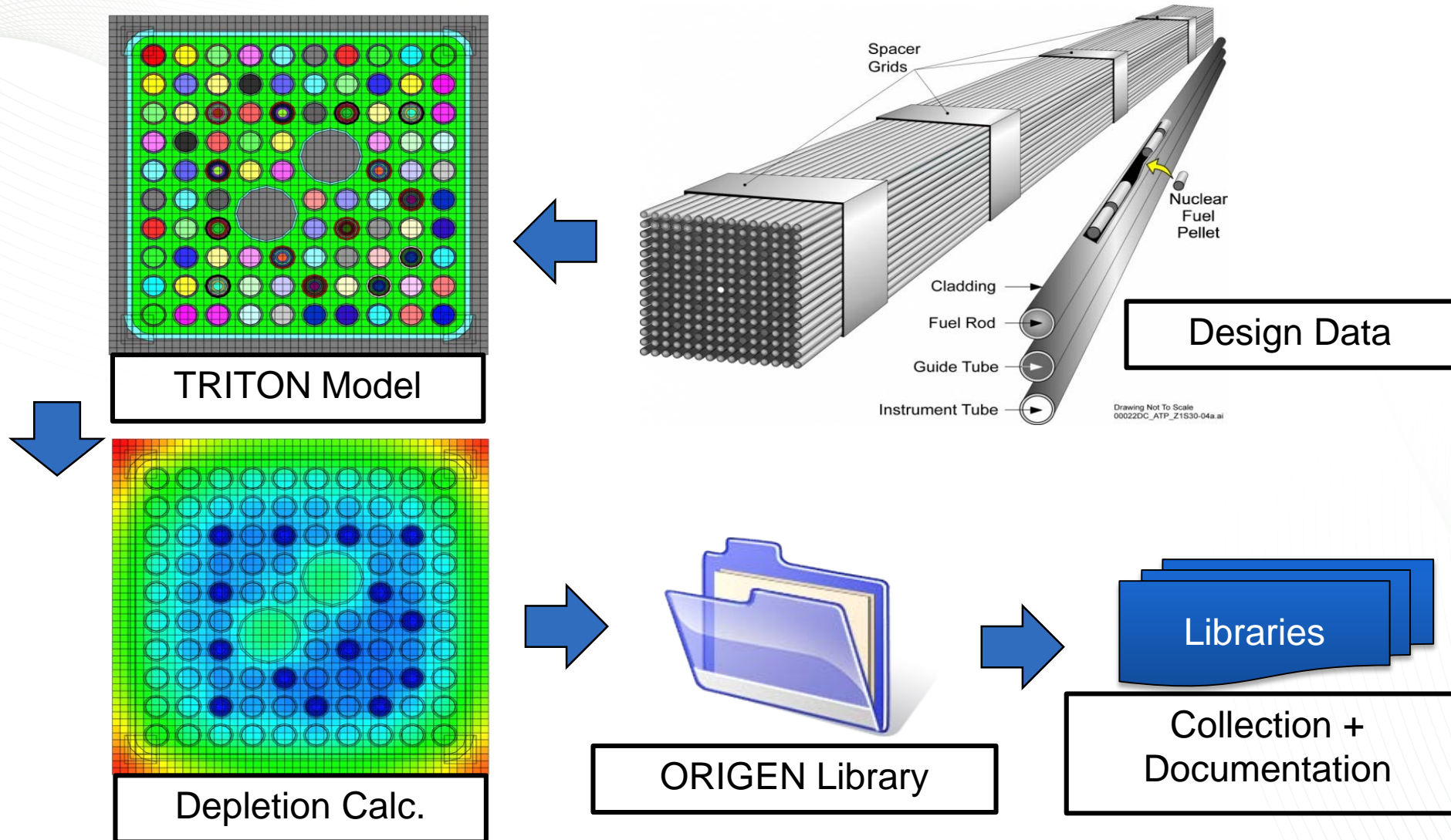
# What is Residual Decay Heat?

- Decay heat generated in spent nuclear fuel = all contributions of recoverable energy released from the decay of radionuclides in fuel after its discharge from the reactor
- Decay heat is driven by the isotopic composition in fuel at the end of irradiation
- Decay heat varies with the decay time after discharge (cooling time)
- Calculation of decay heat can be performed with computational tools that simulate
  - the nuclide transmutations and decay processes during fuel irradiation in the reactor
  - the decay from discharge to a designated cooling time



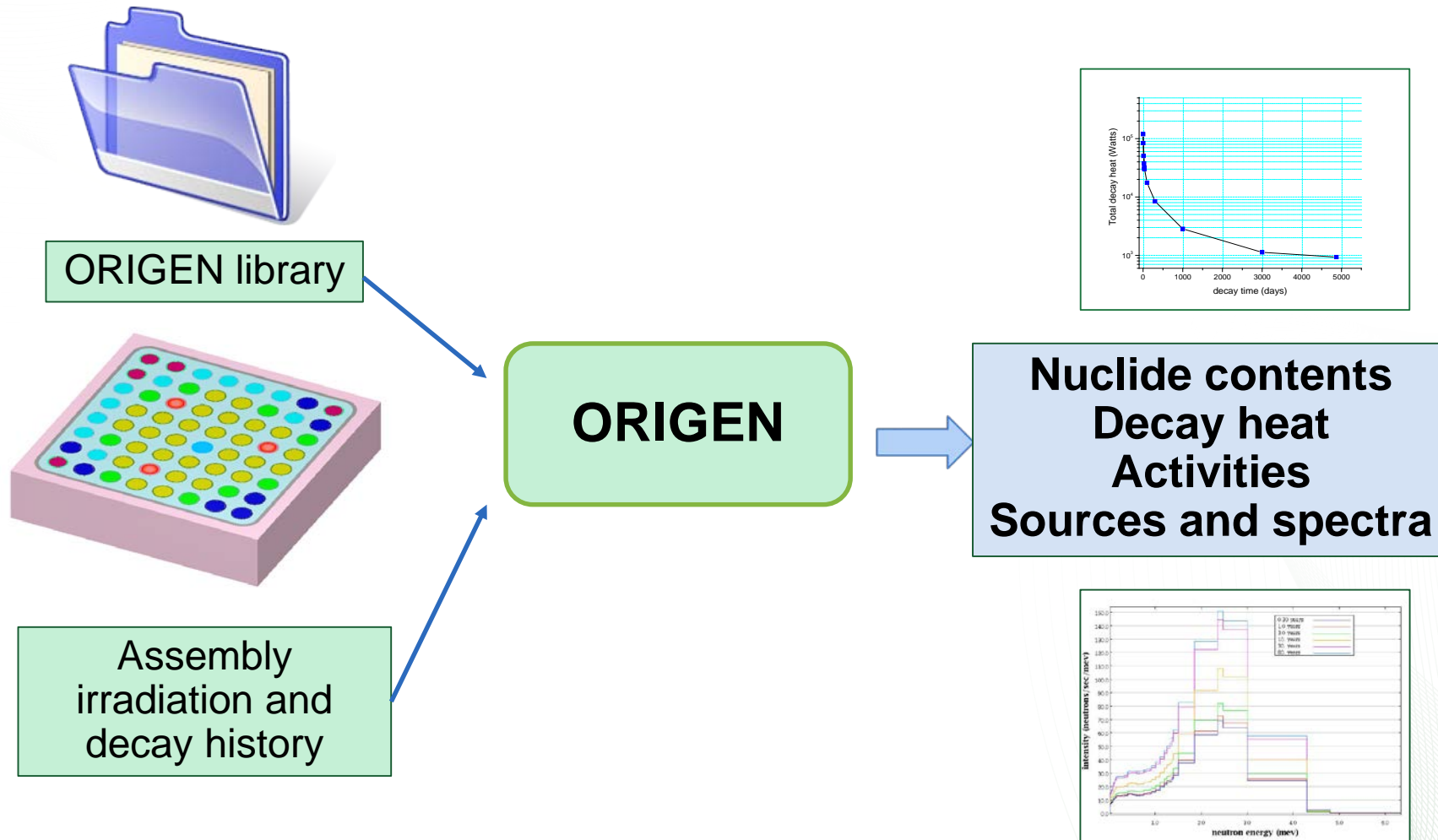
# Methodology for Decay Heat Validation

## Step 1 – Generation of ORIGEN cross-section libraries



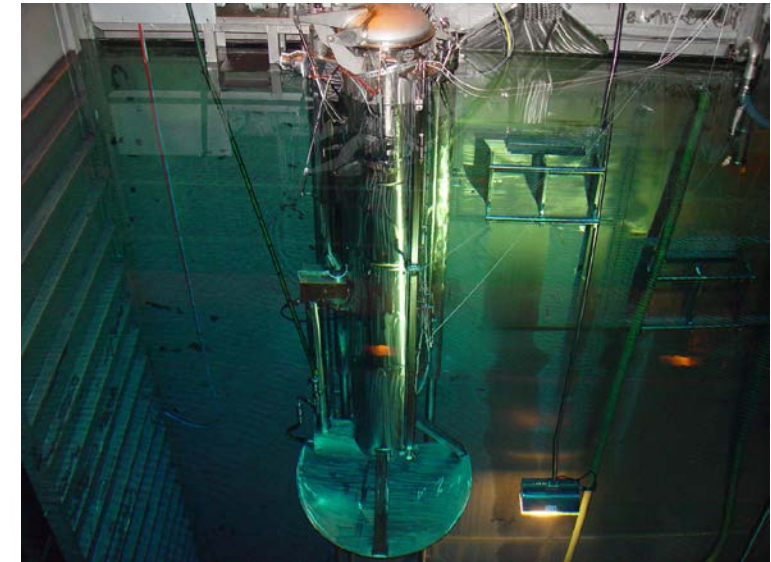
# Methodology for Decay Heat Validation

## Step 2 –ORIGEN simulations



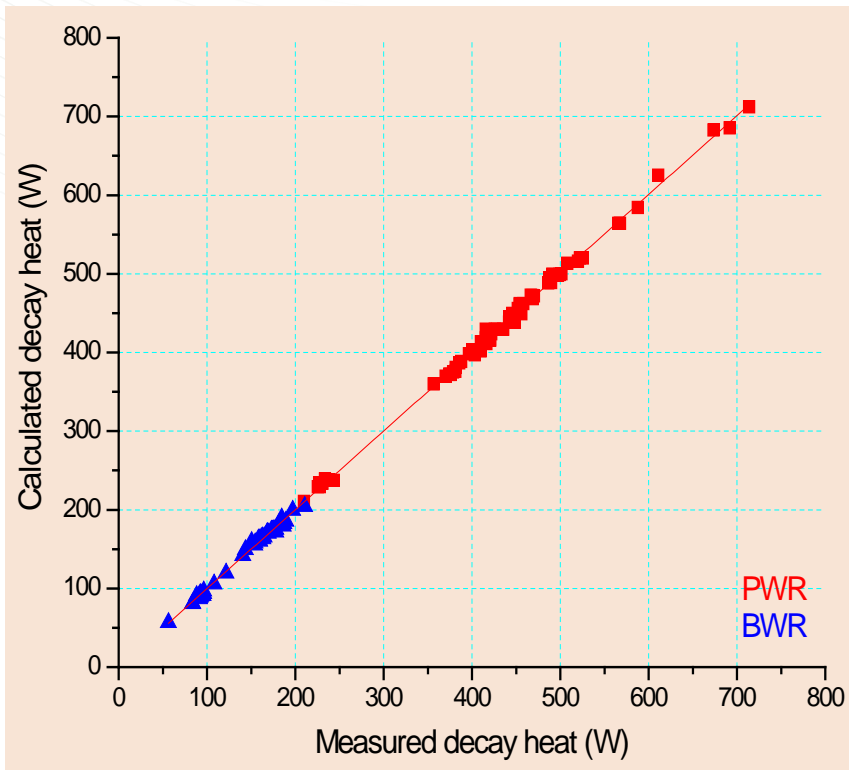
# Decay Heat Validation Data (Clab Measurements)

| Reactor type | Assembly design | Reactor name | Enrichment (wt % <sup>235</sup> U) | No. of assemblies measured | No. of meas. | Max. burnup (GWd/MTU) |
|--------------|-----------------|--------------|------------------------------------|----------------------------|--------------|-----------------------|
| BWR          | 8 x 8           | Ringhals 1   | 2.258 - 2.911                      | 17                         | 45           | 44.9                  |
|              | 8 x 8           | Oskarshamn 2 | 2.201                              | 5                          | 5            | 24.3                  |
| PWR          | 15 x 15         | Ringhals 2   | 3.095 – 3.252                      | 18                         | 33           | 51.0                  |
|              | 17 x 17         | Ringhals 3   | 2.100 – 3.404                      | 16                         | 38           | 47.3                  |



# Decay Heat Validation Results (SCALE 6.1.3 / ENDF/B-VII.0)

## Calculated vs. measured decay heat



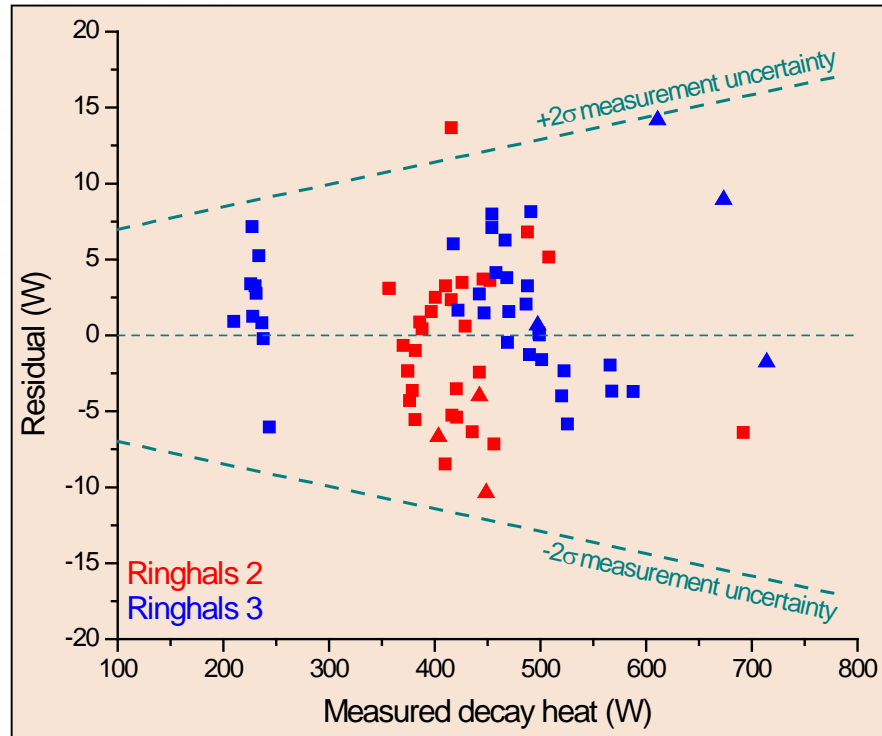
## Summary of results

| Data set | No. of measurements | C/E   |          | Residual (W) |          |
|----------|---------------------|-------|----------|--------------|----------|
|          |                     | mean  | $\sigma$ | mean         | $\sigma$ |
| PWR      | 71                  | 1.002 | 0.012    | 0.57         | 4.91     |
| BWR      | 50                  | 0.997 | 0.024    | -0.25        | 3.36     |
| PWR+BWR  | 121                 | 1.000 | 0.017    | 0.23         | 4.34     |

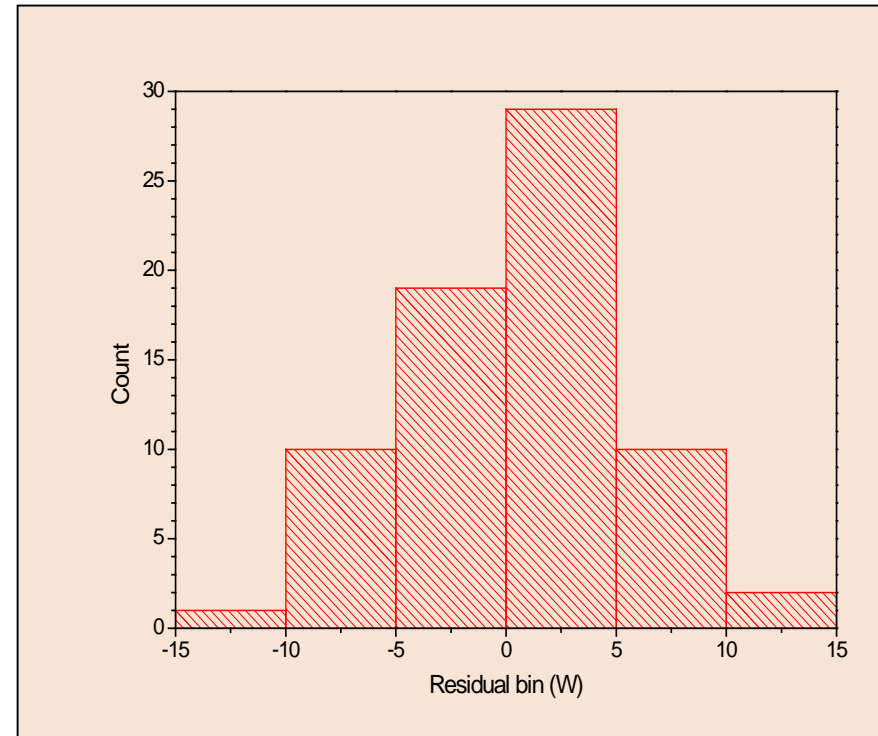


# Decay Heat Validation - PWR Results

## Decay heat residual (calculated – measured)



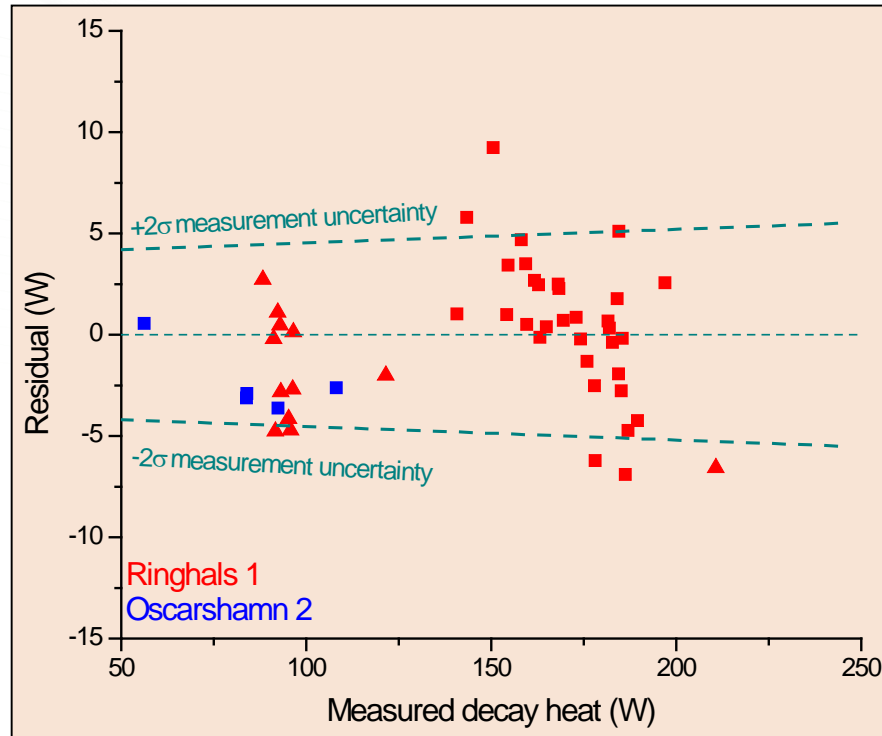
## Histogram plot of decay heat residual



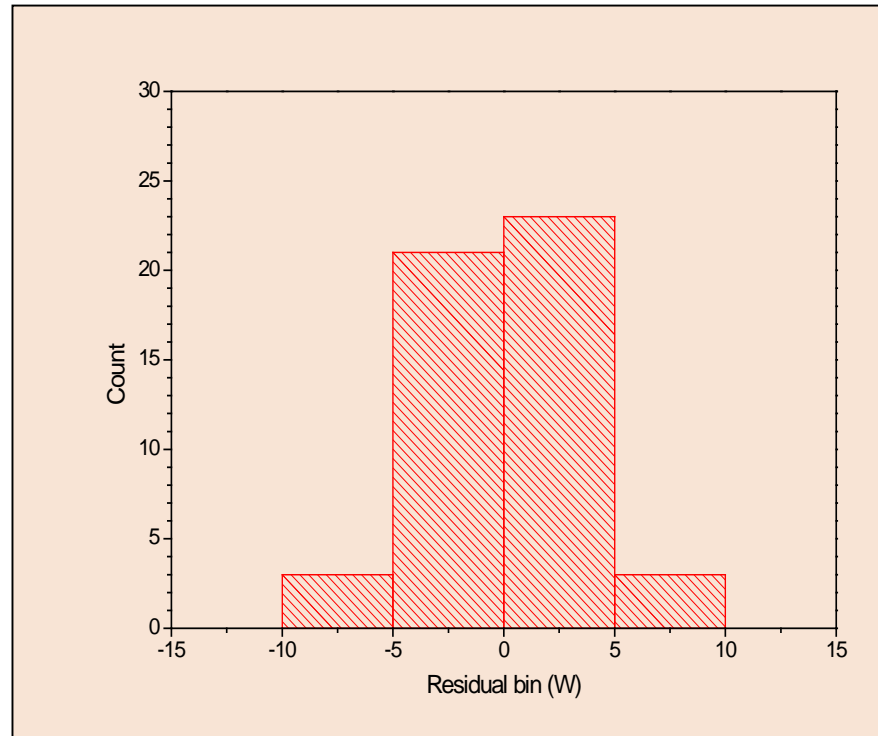
$2\sigma_{\text{exp}}$  [SKB Report R-05-62, 2006]  
 $\pm 9.2 \text{ W (3.7\%)} \text{ at } 250 \text{ W}$   
 $\pm 18.8 \text{ W (2.1\%)} \text{ at } 900 \text{ W}$

# Decay Heat Validation - BWR Results

## Decay heat residual (calculated – measured)



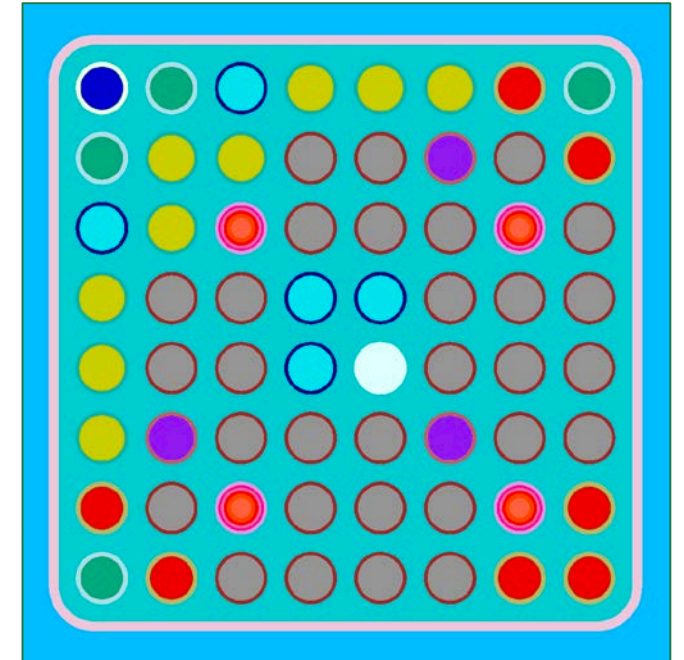
## Histogram plot of decay heat residual



$2\sigma_{\text{exp}}$  [SKB Report R-05-62, 2006]  
 $\pm 4.2 \text{ W (8.4\%)} \text{ at } 50 \text{ W}$   
 $\pm 6.2 \text{ W (1.8\%)} \text{ at } 350 \text{ W}$

# Decay Heat Uncertainty Estimation

- Perform decay heat simulations for a measured assembly to estimate
  - Effect of nuclear data uncertainties
  - Effect of selected manufacturing and operating parameters uncertainties
- Compare calculated and measurement data and uncertainties
- Selected assembly has multiple measurements



Burnup at discharge 36.9 GWd/MTU  
Average enrichment 2.9 wt% <sup>235</sup>U  
63 fuel rods (4 gadolinia) and 1 water rod  
Corner rods with smaller diameter

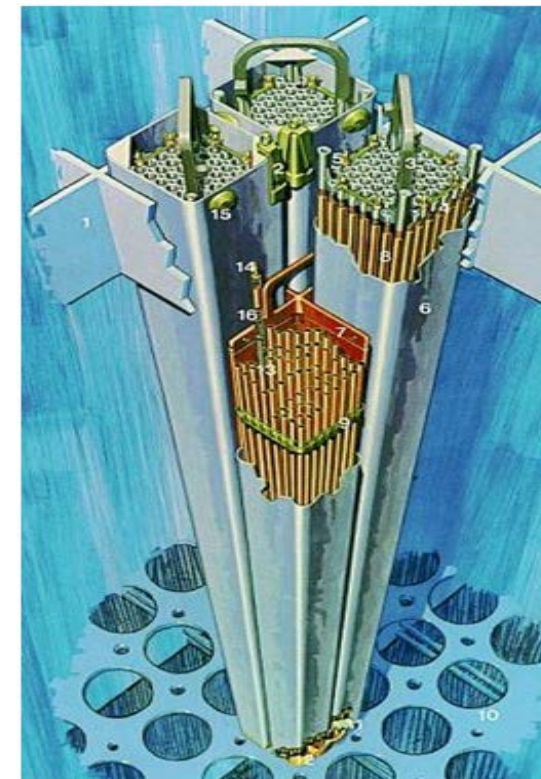
# Perturbed Modeling Data

- Nuclear data (cross sections and fission yields)
- Modeling parameters
  - Fuel design data

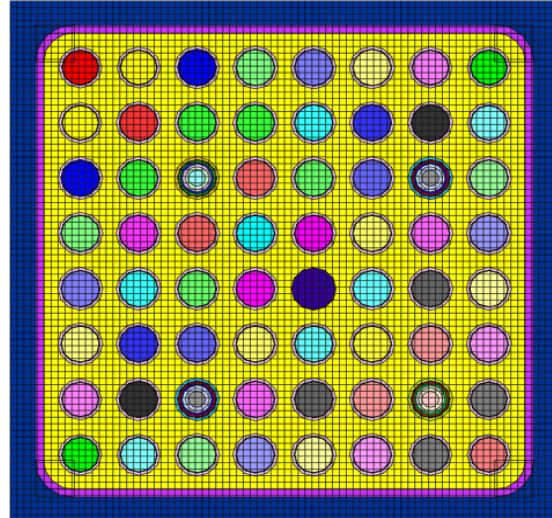
| Parameter                              | 1 $\sigma$ | Units                              |
|----------------------------------------|------------|------------------------------------|
| Enrichment                             | 0.0167     | wt% $^{235}\text{U}$               |
| UO <sub>2</sub> density                | 0.0417     | g/cm <sup>3</sup>                  |
| Gd <sub>2</sub> O <sub>3</sub> content | 0.0333     | wt% Gd <sub>2</sub> O <sub>3</sub> |
| Pellet radius                          | 0.025      | mm                                 |
| Clad outer radius                      | 0.083      | mm                                 |

- Operating data

| Parameter                  | 1 $\sigma$ (%) |
|----------------------------|----------------|
| Specific power (or burnup) | 1.67           |
| Coolant density            | 3.33           |
| Fuel temperature           | 3.33           |



# Computational Model and Tools



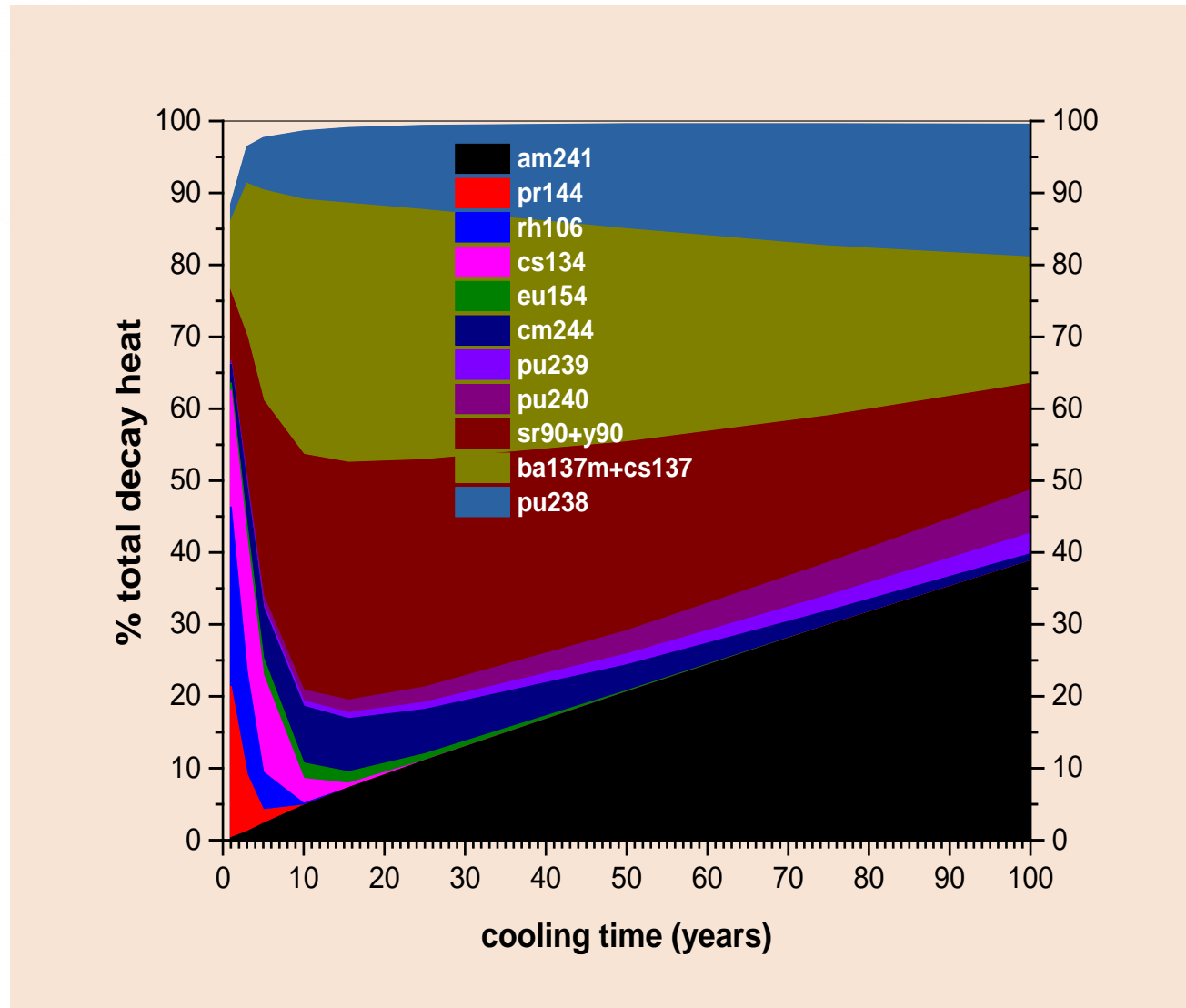
SAMPLER – TRITON depletion  
500 samples for each perturbed set

ORIGEN – decay only

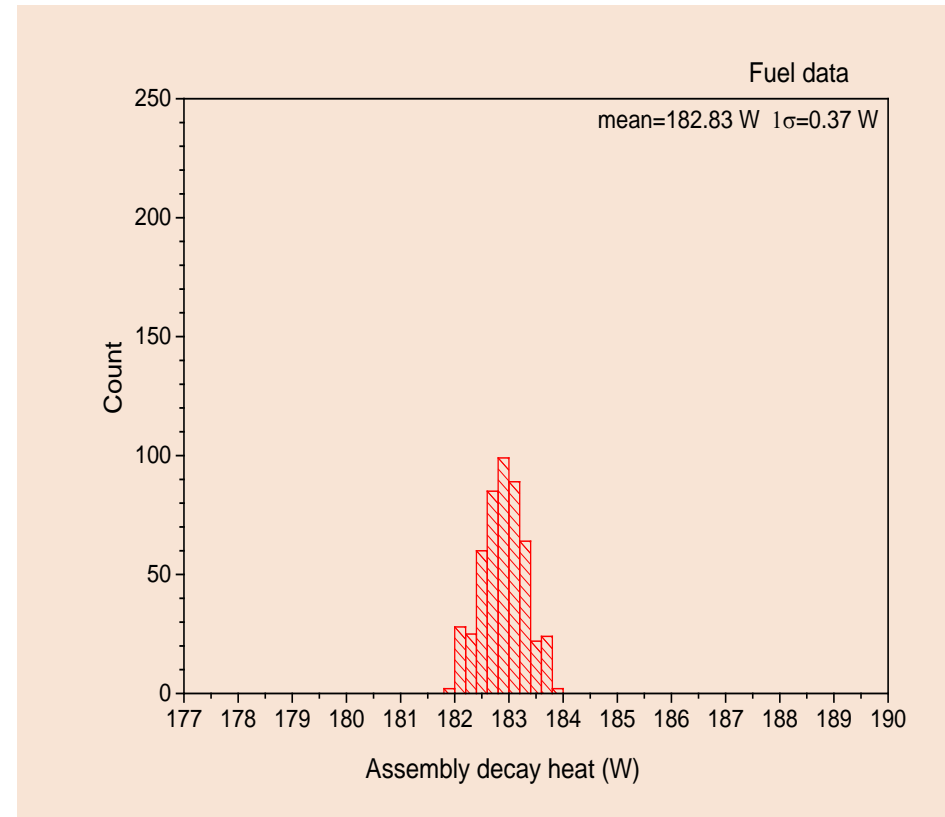
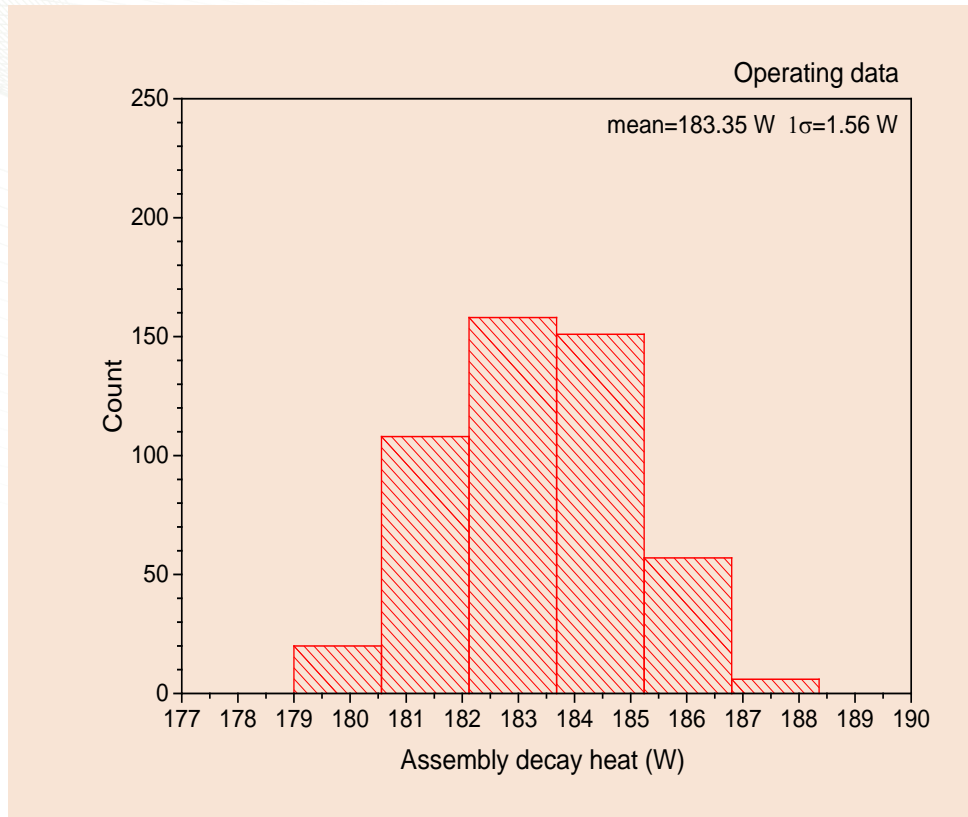
Post-processing, analysis

# Assembly Decay Heat

Nuclide contribution to assembly decay heat vs. cooling time

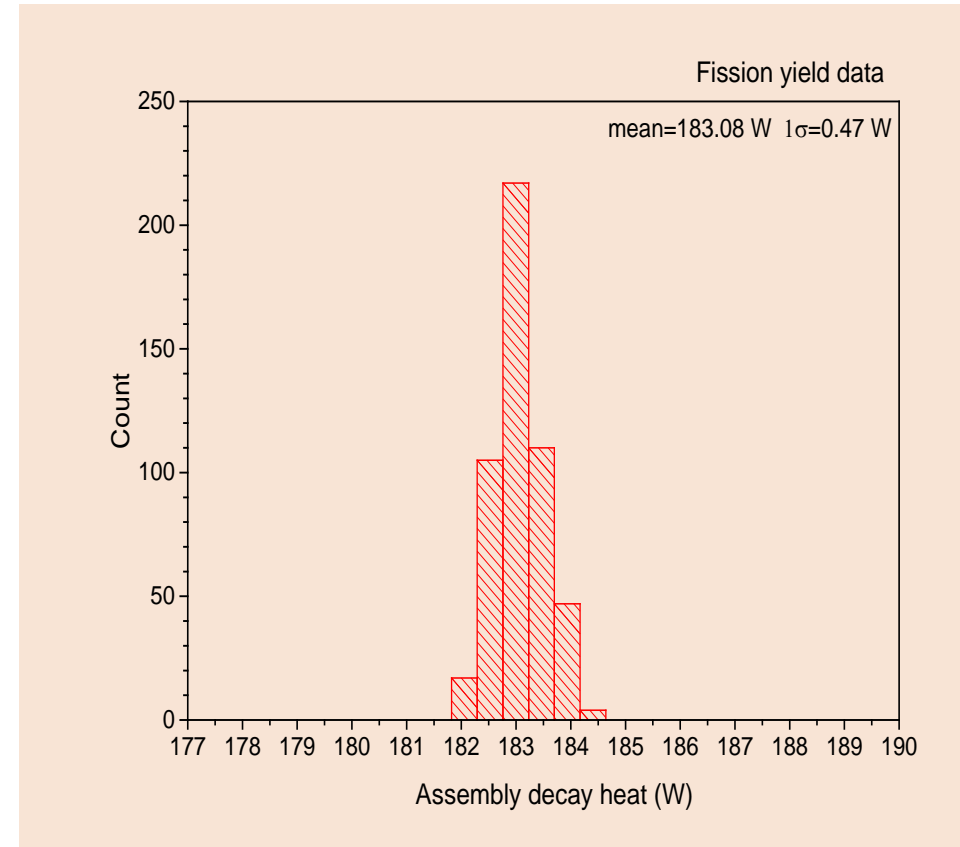
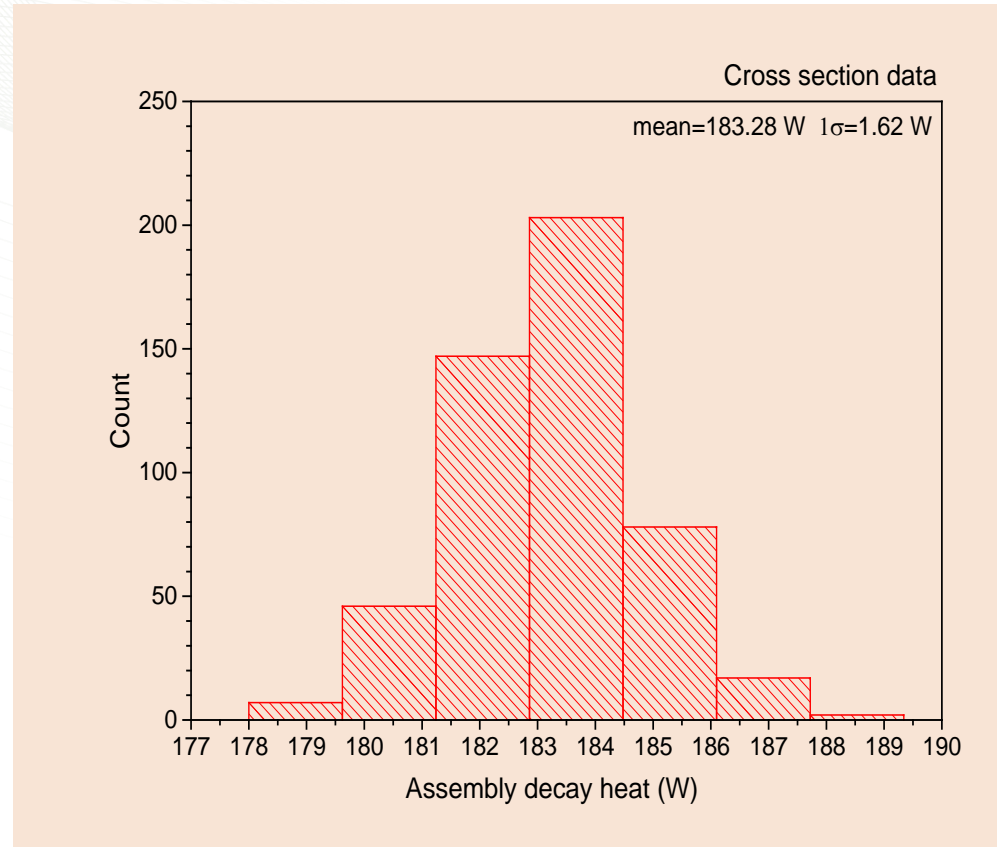


# Effect of Uncertainty in Fuel Design and Operating Data



**Histogram of calculated decay heat variation at time of measurement**

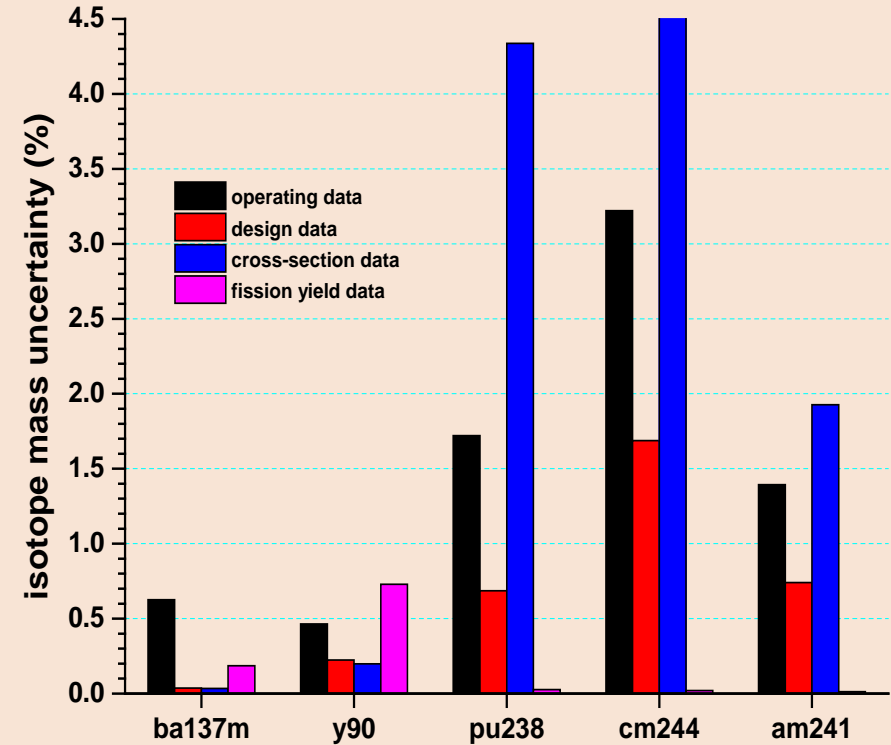
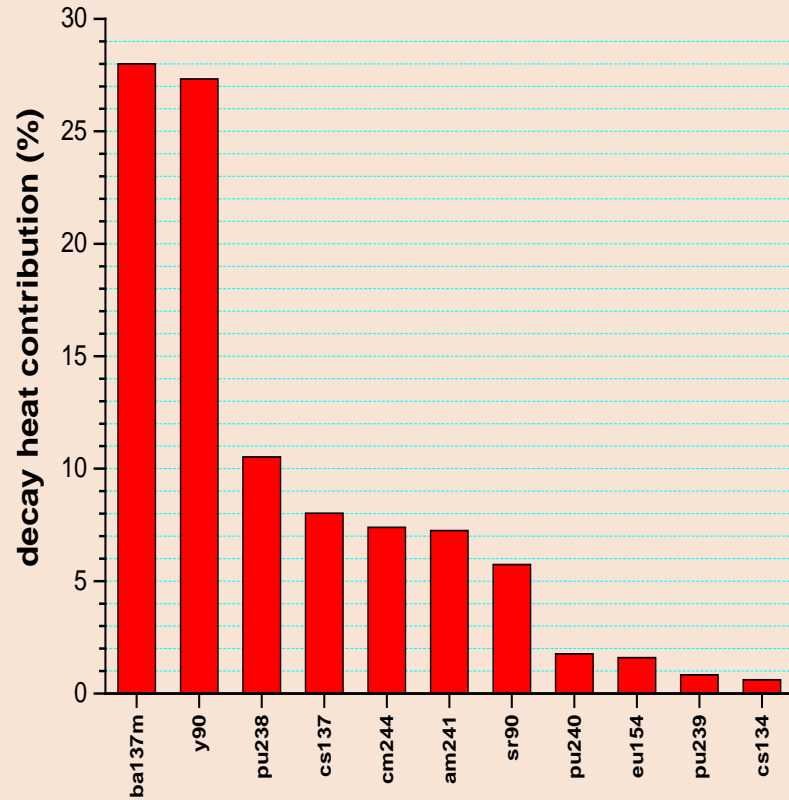
# Effect of Uncertainty in Nuclear Data



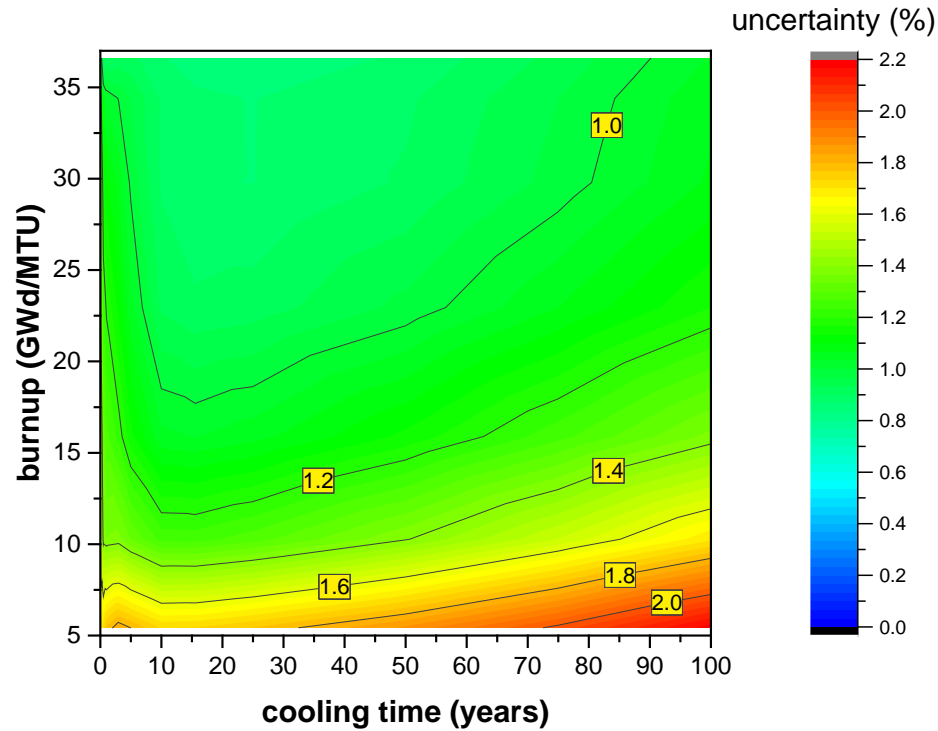
**Histogram of calculated decay heat variation at time of measurement**



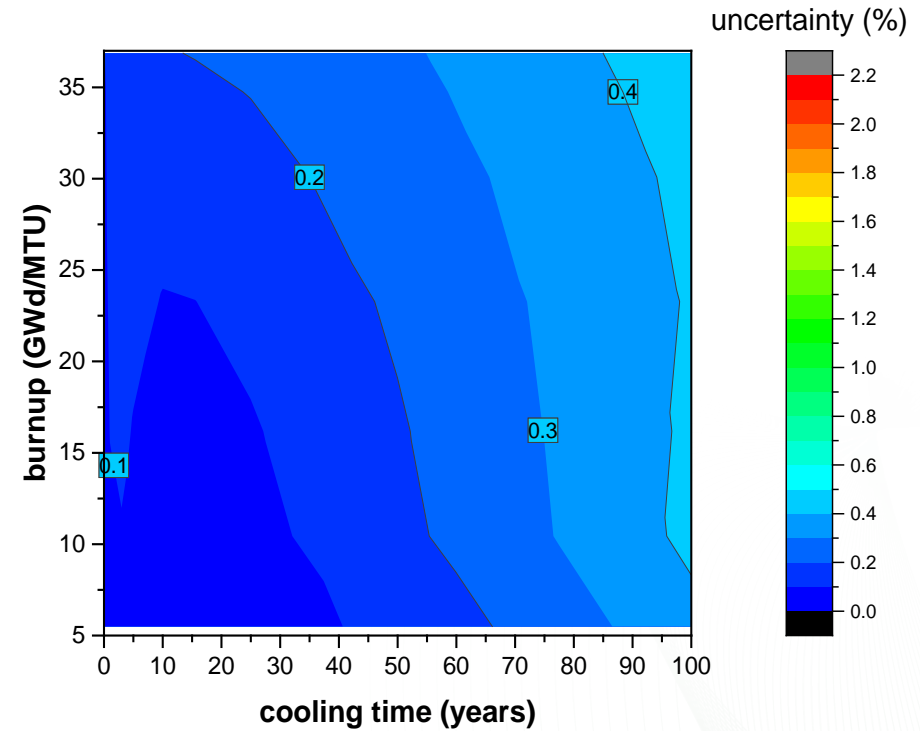
# Uncertainty in Major Contributors to Decay Heat at Measurement Time



# Decay Heat Uncertainty vs Burnup and Cooling Time

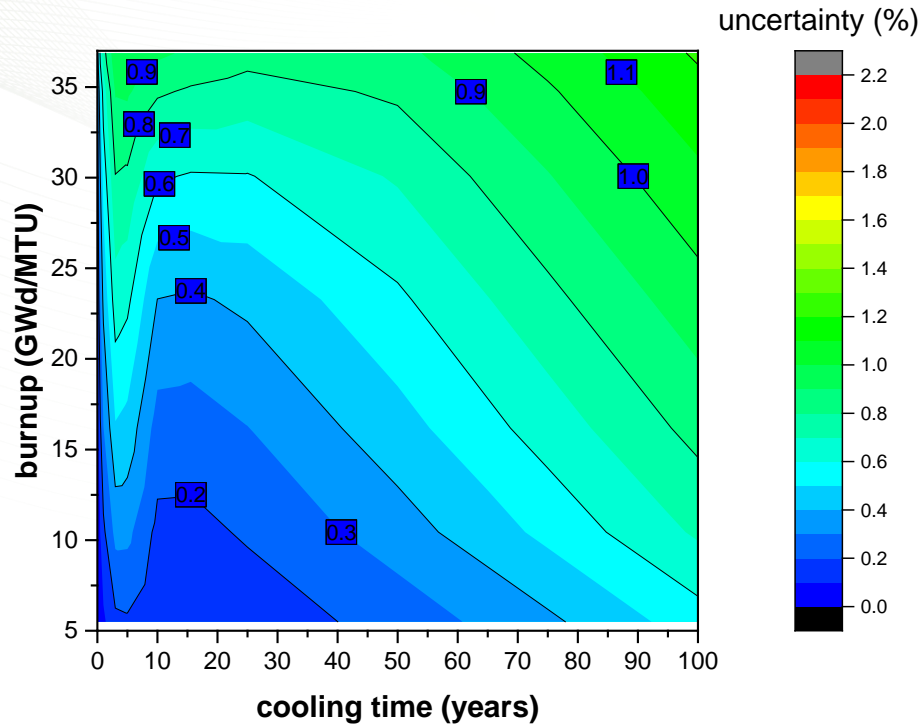


Operating data perturbation

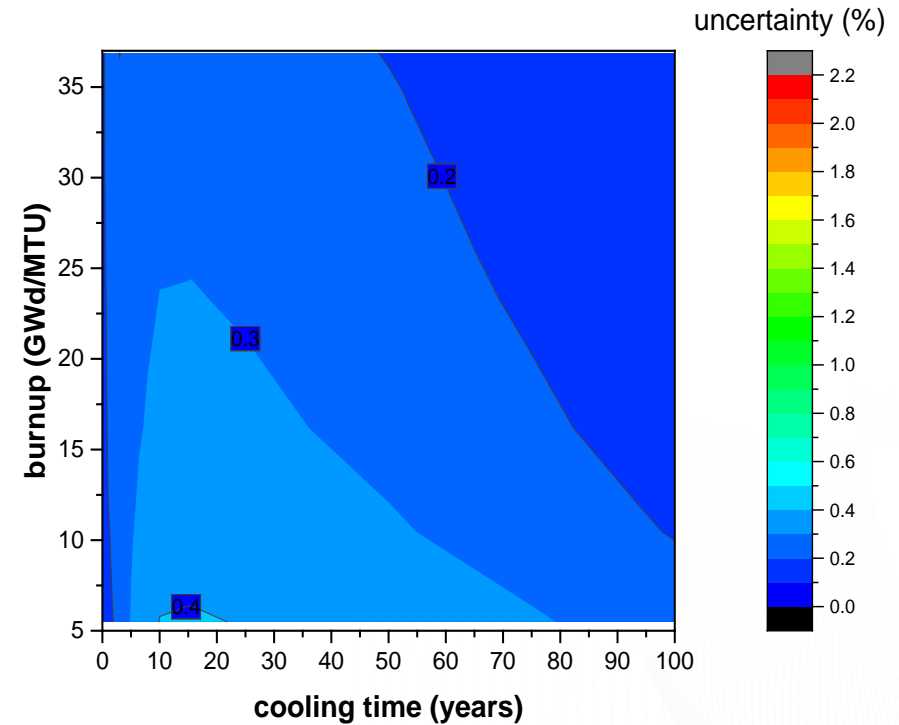


Fuel data perturbation

# Decay Heat Uncertainty vs Burnup and Cooling Time



Cross-section data perturbation



Fission yield data perturbation

# Conclusion

- SCALE/ORIGEN has well-established, well-validated capabilities for spent fuel M&S, including evaluation of uncertainties in calculated decay heat due to both modeling and nuclear data uncertainties
- Calculated decay heat agrees well with measurement data for PWR and BWR
  - average C/E is 1.002 ( $\sigma = 0.012$ ) for PWR and 0.997 ( $\sigma = 0.024$ ) for BWR
- Uncertainty in calculated decay heat
  - dominated by uncertainty in cross-section data ( $\sigma = 0.9\%$ ) and operating data ( $\sigma = 0.8\%$ )
  - small effect of uncertainty in fuel data ( $\sigma = 0.2\%$ ) and fission yield data ( $\sigma = 0.3\%$ )
- Decay heat uncertainty values are driven by uncertainty in isotopic masses of a handful of important decay heat contributors
- Uncertainty in calculated decay heat (separate effects) is comparable to measurement uncertainty ( $\sigma = 0.9\%$ ) for this assembly
- Quantifying uncertainty can provide useful information and inform decisions on design and operation of spent fuel storage facilities, particularly in regimes where measurement data are not available or are not practical to obtain.

# References

- G. Ilas and H. Liljenfeldt, "**Decay heat uncertainty for BWR used fuel due to modeling and nuclear data uncertainties**", Nuclear Engineering and Design, vol.319, p. 176-184 (2017) <https://doi.org/10.1016/j.nucengdes.2017.05.009>
- Williams, M., G. Ilas, M. A. Jessee, B. T. Rearden, D. Wiarda, W. Zwermann, L. Gallner, M. Klein, B. Krzykacz-Hausmann, and A. Pautz, 2013. **A statistical sampling method for uncertainty analysis with SCALE and XSUSA**, Nuclear Technology, vol.183, no.3, p 515-526 (2013). <http://dx.doi.org/10.13182/NT12-112>
- G. Ilas, I. C. Gauld, and H. Liljenfeldt, "**Validation of ORIGEN for LWR used fuel decay heat analysis with SCALE**", Nuclear Engineering and Design, vol.273, p. 58-67 (2014) <https://doi.org/10.1016/j.nucengdes.2014.02.026>

# Questions?

