Predicting the Bias of SNF Depletion Calculations: Application of Polaris, Sampler, and Machine Learning

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Background

- Nagra, the WMO in Switzerland, plans for nuclear waste disposal in deep geological repository

- General licence application is in preparation, to be submitted around 2024

- SNF is high-level waste, ~13k FA by the end-of-life of the Swiss NPPs

- SNF characteristics, e.g., decay heat, are calculated using codes (e.g., Polaris) and data (e.g., fuel irradiation data)
Background

**Downstream Applications**
Requiring accuracy and precision of the bias

**Economics**
Reducing DH uncertainty could lead to reduction in the no. of disposal canisters

**Safety**
Ensure subcriticality, e.g., burnup credit CSA penalizes $k_{eff}$ with bias and uncertainty (e.g., nuclide concentrations (Gauld and Mertyurek, 2019))

$\sum DH \leq 1500 W$
Main topics

Validation of Depletion Calculations → Propagation of Uncertainties → Machine Learning (ML) for Bias Prediction → Assessment of the Validation Sufficiency

**SCALE-6.2.3/Polaris** → **SCALE-6.2.3/Sampler** → **R Language** → **R Language**

$$Bias \rightarrow B = C - E$$

- Few measurements, with limited range of properties
- ~ hundreds of PIE, SFCOMPO (F. Michel-Sendis et al., 2017)
- ~ 133 DH FA at Clab < 51 GWd/tU (SKB, 2006) & < 55 GWd/tU (EPRI, 2020)
Topic 1: Validation of the depletion calculations

Calculations using SCALE-6.2.3 Polaris and ORIGEN applied on the 152 DH measurements at Clab (SKB, 2006)

- On average, calc. DH are within 5% of the measured ones
- Large variances (potential improvements)
**Topic 2: Uncertainty propagation of ND and DO uncertainties (also SA)**

Calculations using **SCALE-6.2.3 Sampler/Polaris** applied on the 152 DH measurements at Clab (SKB, 2006)

Bias informative features (Spectral index $SI_i = \frac{\varphi_{Fast}}{\varphi_{Total}}$, $SI = \frac{\sum_{i}^N (BU_i \times SI_i)}{\sum_{i}^N (BU_i)}$, Calc. value $C$, Correlation coeff. $\rho_{ij} = \frac{1}{N-1} \sum_{k=1}^{N} \frac{(c^i_k - \bar{c}^i)(c^j_k - \bar{c}^j)}{\sigma_i \sigma_j}$)

$\rho$ between calc. DH, ordered by BU (top to bottom, left to right)
**Topic 3:** Application of Machine Learning (ML) for the bias prediction

\[ C - \epsilon = f(X) + \epsilon \]

- \( f(X) \): predictable part (systematic bias)
- \( \epsilon \): unpredictable part (random bias)

- \( f \): model (e.g., similar benchmarks)
- \( X \): bias informative features,
- assumptions: correlations \( \rho \)
- many features/selection (RFE): \( SI, C, \rho \)

**Weighted k-Nearest Neighbors (KNN):**
\[ B_{(\rho=1)} = \sum_{k=1}^{K} w_k \ B_k, \quad w_k \propto f(\Delta\rho) \]

**Random Forest (RF):**
\[ B_{(\rho=1)} \approx \frac{1}{N} \sum_{n=1}^{N} w_n \ B_n, \quad I_{\rho > co} \]
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**Application in ML algorithm**

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<tr>
<th>Application in ML algorithm</th>
<th>Method</th>
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<td>Resampling technique</td>
<td>LOOCV</td>
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<td>Test metrics</td>
<td>( R^2 ), KS-test, Regression</td>
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<td>Treatment of outliers</td>
<td>Z-score, Cook’s distance (3( \sigma ) and distance, apply AND)</td>
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<td>Multiple measurements (same FA)</td>
<td>Random sampling</td>
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**Topic 3: Application of Machine Learning (ML) for the bias prediction**

RF model predicted bias of the DH benchmarks of Clab-2006, using **LOOCV**:
- 149 measurements on 83 FA
- 3 outliers (of multiple measurements on C20 and 5F2 FA), 2% of the data

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**Topic 3:** Application of Machine Learning (ML) for the bias prediction

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\[ C - E = f(X) + \epsilon \]

\[ \bar{B} \pm \sigma \rightarrow f(\rho, C, SI) \pm \epsilon \]

**Diagram:**
- **Polaris Bias**
- **ML Predicted Bias** $f(x)$
- **Outliers**

**Statistics:**
- RMSE = 3.36 W
- KS p-value = 0.84
- $R^2 = 0.451$
**Topic 4: Assessment of the sufficiency of the measurements**

Sufficiency of the measurements/experimental gaps, range of applicability?

83 FA DH measurements at Clab: <51 GWd/tU 11-27 yrs of cooling (SKB, 2006)

1. No MOX
2. No high burnup

\[ C - E = f(X) + \epsilon \]

\( f(X), \epsilon \) predictable/unpredictable

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**Clab-2006 (random sampling)**

\( RF \ R_{\text{ref}}^2 = 0.38, \quad KKNN \ R_{\text{ref}}^2 = 0.40 \)

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1. 3 pin-cells having the same $H/X$ ratio as the full lattice: W15x15 UO$_2$ and MOX, GE14 UO$_2$
2. Sampler perturbations (625 ND and 625 DO)
3. ML on the application side

![Clab – 2006: Validation Data](image)
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**Application**

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Summary

SCALE in our organization

- Support SNF characterization and downstream applications
- Polaris & ORIGEN calculate fuel assembly wise decay heat and nuclide inventory (large-scale verification)
- Sampler is used for uncertainty propagation

+ Machine Learning
  - Bias prediction in applications (e.g., potentially for decay heat and nuclide inventory for burnup credit)
  - Assessment of the validation data, highlight the parameters of potential future measurements

+ Participation in international projects using SCALE (Polaris, ORIGEN, KENO, Sampler)
  - EJP-EURAD (decay heat and PIE analysis, activated cladding samples)
  - NEA WPNCS subgroups (decay heat and PIE analysis)
thank you for your attention
References


