SCALE Uncertainty Quantification Methodology for Criticality Safety Analysis of Used Nuclear Fuel

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Criticality Analysis of Used Nuclear Fuel (UNF) is Required in Several Areas

- Spent fuel storage pools
- UNF cask design and evaluation
- UNF transportation accident scenarios
- Burnup credit

• Uncertainties and biases in computed $k_{\text{eff}}$ impact safety margins and economics
Flowchart of UNF Criticality Analysis

- Fresh fuel assembly models
- Fission product yield data
- Decay data
- Assembly Burnup Calculation
- Resonance-shielding data (Bondarenko factors; PW cross sections)
- MG cross section data
- UNF assembly models
- Model for UNF storage environment
- Critically Calculation for storage environment
Uncertainty in $k_{\text{eff}}$ for UNF Systems Depends on ...

- Uncertainties in the criticality calculation, due to
  - Reaction cross sections
- Uncertainties in the depletion calculation for computed burned fuel composition, due to
  - Reaction cross sections
  - Fission product yield data
  - Half-lives
  - Decay branching ratios
SCALE-TSUNAMI Sequences Provide Uncertainty in Criticality Calculations--

- Uses perturbation theory to compute sensitivity coefficients of $k_{\text{eff}}$ to nuclear data
- Sensitivity coefficients are folded with nuclear data covariances to obtain $k_{\text{eff}}$ uncertainty

--- BUT, TSUNAMI Can Not Determine Uncertainty in Depletion Calculation of UNF Composition

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SCALE-6.2 Includes Two Approaches for Sensitivity/Uncertainty Analysis

- Perturbation Approach with TSUNAMI Modules
  - Current capability based on multigroup transport codes: TSUNAMI-3D, TSUNAMI-2D, TSUNAMI-1D
  - Also, new methodology based on continuous energy Monte Carlo is being developed for SCALE-6.2

- NEW! Statistical Sampling with Sampler Module
  - SCALE-6.2 includes new module **Sampler** for statistical uncertainty analysis of any SCALE sequence
  - Makes random perturbations in input data; response uncertainty computed by statistical analysis of output response distribution
Features of Sampler Module

• A “super-sequence” that executes any Scale sequence using perturbed data parameters

• Performs perturbations in
  • multigroup XS’s, self-shielding data (Bondarenko factors, pointwise XS’s)
  • Fission yields, decay data
  • Model parameters: initial concentrations, dimensions, temperatures, etc.

• Automated statistical analysis for selected responses

• Parallel computations using MPI or OpenMP
Features of Sampler Module, continued

- Uses pre-generated libraries of perturbation factors computed by code such as XSUSA
  - XS perturbations sampled from SCALE Cov library
  - Decay perturbations from ENDF/B-VII uncertainties
  - Yield perturbations sampled from yield covariances developed by ORNL

U238 yield correlation matrix with chain-yield constraints (*)

(*) from Pigni et al
Overview of Sampler Calculations
Generation of Perturbed Data Libraries

XS covariances

yield covariances

decay covariances

XSUSA/Medusa covariance sampling tool

Pre-generated MG perturbation factors from XSUSA

Pre-generated yield perturbation factors from XSUSA

Pre-generated decay perturbation factors from XSUSA

ClaroI_Plus

Crawdad_Plus

YieldSampler

DecaySampler

$\delta f, \delta \sigma_g$

$\delta \sigma(E)$

$\delta Y$

$\delta \lambda$

perturbed MG library for transport solve

perturbed CE library for self-shielding

perturbed yield library for ORIGEN

perturbed decay library for ORIGEN
Typical Sampler Input for Assembly Burnup:

```plaintext
=sample
read parameters
    n_samples=200  perturb_XS=yes
    perturb_yield=yes
    library=”v7-252”
end parameters
read case
    sequence=t-depl
        (SCALE input for t-depl sequence)
end sequence
end case
read responses[nucs]
    type=origen_nuclides
    nuclides = u-235 pu-239 sm-149  end
end responses
read responses[homxs]
    type=triton
    data= kinf sigma_fission
    sigma_absorption end
end responses
end
```

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Sampler Output

- Sampling results for following types of responses
  - $K$ eigenvalue; (XSDRN, NEWT, KENO)
  - Microscopic reaction rates by nuclide (Newt/Opus)
  - Homogenized/collapsed macro cross sections (Newt)
  - Nuclide concentrations, activities (ORIGEN)
  - Decay heat, radiotoxicity, photon sources (ORIGEN)
  - Shield responses: doses, radiation damage, etc. (Mavric)

- Each response at every time-step includes:
  - Frequency distributions as histogram plot file
  - Mean values and standard deviations in CSV file
  - Results of chi-squared normality test for each response
  - Covariance and correlation coefficients between responses
TMI-1 PWR Assembly
Depletion for UAM Benchmark

- TMI PWR Assembly, 0-60 GWD/T burnup; 0-100 years cooling
  - Mean values, standard deviations, correlation coefficients computed for 10-GWD/T time steps; and decay times of 1, 3, 5, 10, 50, 100 years after shut down

- Responses considered
  - Time-dependent $K_{\text{inf}}$
  - U235, U238, Pu239, Pu40, Pu241 fission and capture rates
  - Collapsed/homogenized 2-group macro cross sections (XS), for $\Sigma_\alpha$, $\Sigma_f$, $\nu \Sigma_f$, $\Sigma_{1\rightarrow2}$, D
  - Time-dependent concentrations for 15 actinides and 36 fission products
Frequency Distributions of Representative Output Responses

$K_{inf}$ ; 0 GWD/T  

$K_{inf}$ ; 60 GWD/T

Group 1 nu-fission ; 30 GWD/T

Tc-99 concentration; 50 GWD/T
Chi Squared Normality Tests Are Done For Every Response

Example for time-dependent Cs-135 concentration

<table>
<thead>
<tr>
<th>time step</th>
<th>Normal?</th>
</tr>
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<tbody>
<tr>
<td>27</td>
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<tr>
<td>28</td>
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</tr>
<tr>
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<td>failed</td>
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<td>31</td>
<td>passed</td>
</tr>
<tr>
<td>32</td>
<td>passed</td>
</tr>
</tbody>
</table>
SUMMARY

- SCALE-6.2 will include new capabilities and data for uncertainty analysis
  - ENDF/B-VII.1 covariances for many nuclides
  - Fission yields and decay data covariances
  - Sampler statistical uncertainty analysis module
- Sampler is comprehensive super-sequence that greatly extends SCALE uncertainty analysis
Application of Sampler to Obtain Uncertainty in Burned Fuel Properties

- Sampler used 280 random samples for the “input data vector” = \{ multigroup XS’s, Bondarenko factors, pointwise XS’s, fission product yields \}
  - Perturbations obtained from sampling SCALE covariance libraries
- SCALE TRITON sequence calculation performed for each random sample of the input data vector
  - Newt 2D transport module with 252 group ENDF/B-VII.0
  - Bonami/CENTRM/PMC self-shielding
  - ORIGEN depletion with ~2000 isotopes
- Computations done in parallel with MPI on Linux cluster with 80 CPUs
Relative Standard Deviation in $k_{inf}$

% std. dev. vs. Burnup (GWD/T)
Relative Standard Deviations in Major Actinide Concentrations

% std. dev.

Burnup (GWD/T)
Relative Standard Deviations in Minor Actinide Concentrations

% std. dev.

Burnup (GWD/T)

Np237
Pu238
Am241
Am243
Cm244
Cm246
Relative Standard Deviations
in Sm Fission Product Concentrations

% std. dev.

Burnup (GWD/T)

Sm147
Sm148
Sm149
Sm150
Sm154