Application of TSUNAMI and TSURFER for Validation of Burnup Credit in the Criticality Safety Analysis of a Transport Cask

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Introduction

- Burnup credit in criticality analyses
  - – Transport casks, storage pools, waste disposals
- Validation of codes
  - – especially for applications with fission products
- "International Handbook of evaluated Criticality Safety Benchmark Experiments" (ICSBEP)
- Problem:
  - No experiments meet all conditions of a transport cask or waste disposal including fission products
  - Method to calculate a bias?
  - Partial bias of fission products?
  - Estimate uncertainties?

Source of uncertainties

- Method
  - Statistical uncertainties
  - Resonance treatment
  - Algorithm , approximations

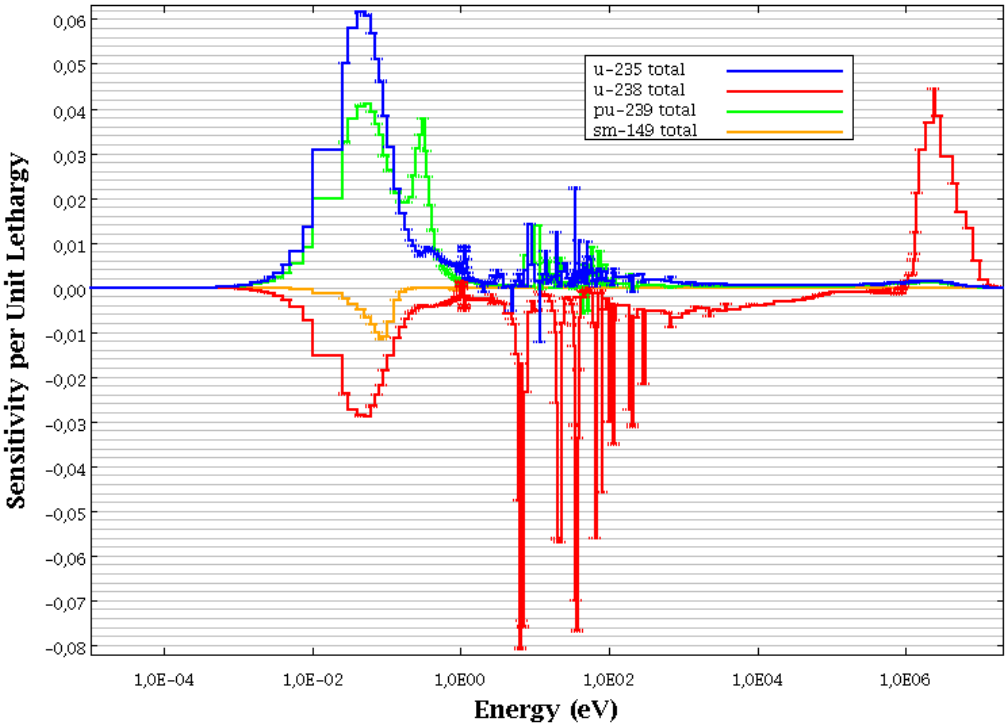
- Modeling
  - Uncertainties in geometry or materials
  - Neglecting of details
  - homogenization of materials
  - Benchmark experiments $\rightarrow$ bias + experimental uncertainties
  - Correlations

- Uncertainties in nuclear data $\rightarrow$ TSUNAMI + TSURFER
  - Assumption of TSURFER: uncertainty of nuclear data is the main uncertainty

TSUNAMI

Typical situation:

- Application case, e.g. transport cask
- Calculation of sensitivity data with TSUNAMI
- Choosing suitable experiments → modeling + calculation → k_{eff}, sensitivity data



$$S = \frac{\partial k}{\partial \alpha} \frac{\alpha}{k}$$

Sensitivity profile of a generic transport cask (U-235 total, U-238 total, Pu-239 total, Sm-149 total)

TSURFER

- adjusting nuclear data to meet $k_i^{calc}(\alpha') = k_i^{exp}$ for all experiments simultaneously (Generalized linear least squares method)
- Recalculation of $k(\alpha') \rightarrow$ bias = $k(\alpha) - k(\alpha')$
- Uncertainty of the bias = uncertainty of $k(\alpha')$
- Assumption: bias is mainly caused by uncertainties of nuclear data

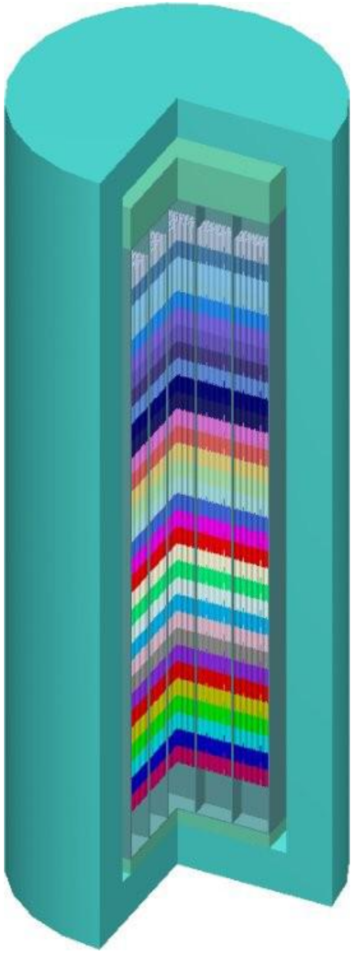
$$\alpha \rightarrow \alpha'$$

  - $k(\alpha)$ neutron multiplication factor of application (depending on nuclear data α)
  - k_i^{exp} measured neutron multiplication factor of experiment i
  - $k_i^{calc}(\alpha)$ calculated neutron multiplication factor of experiment i

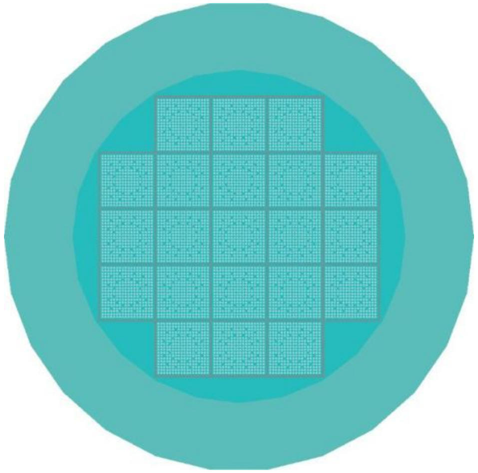
- Input:
  - Sensitivity data
  - Covariance data
  - Uncertainties + correlations of experiments

Application case

- Transport cask (OECD/NEA WPNCS phase II-C burnup credit criticality benchmark), 21 PWR fuel assemblies, 40GWd/t_{HM}



- **Actinides**: U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-243
- **Fission products**: Ag-109, Cs-133, Eu-151, Eu-153, Gd-155, Mo-95, Nd-143, Nd-145, Rh-103, Ru-101, Sm-147, Sm-149, Sm-150, Sm-151, Sm-152, Tc-99



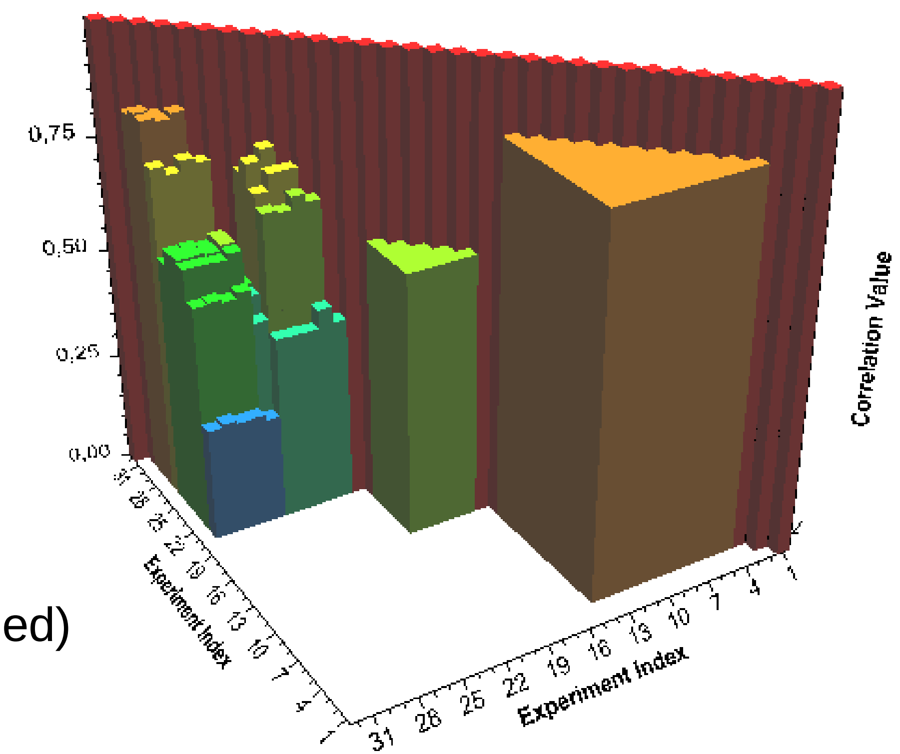
Experiments

	#	c_k	E	G(TS)
LCT003-3	1	0.44	0.77	0.91
LCT050-9	1	0.37	0.76	0.92
LMT005	12	0.38-0.39	0.76-0.77	0.91-0.92
LCT052	6	0.41-0.42	0.71-0.75	0.88-0.93
MCT007	5	0.86-0.88	0.73-0.82	0.91-0.94
MCT008	6	0.87-0.91	0.71-0.78	0.92-0.96

- No experiments with both, fission products and plutonium
- Experiments contain only parts of the nuclides of interest

Correlation matrix:

- Not given in ICSBEP (will be included)
- Has to be defined by the user !



TSURFER: χ^2 test

- TSURFER checks consistency and excludes experiments with large impact on χ^2

$$\chi^2 = \Delta\alpha^T C_{\alpha\alpha}^{-1} \Delta\alpha + \Delta m^T C_{mm}^{-1} \Delta m$$

- In our example six experiments are excluded by χ^2 test:
  - LCT003 / 3
  - LCT050 / 9
  - LMT005 / 1 + 9
  - LCT052 / 1 + 3
- Ok from mathematical point of view
- Inconsistencies could be due to:
  - Underestimated experimental uncertainty
  - Oversimplification of the computational model
  - Wrong correlations
  - Underestimated uncertainties of nuclear data
  - Always correlated with a large impact on χ^2?
- Omission of experiments should be based on physical reasons

Consistency check

- Use one experiment as application:

Experiment	k_{eff}, calc	k_{eff}, exp	Bias, exp. (Δk)	K_{eff}, TSURFER	Bias TSURFER (Δk)
LCT003 / 3	0.9882(2)	1.0000±0.0039	-0.0118±0.0039	0.9881±0.0010	+0.0001±0.0010
LCT050 / 9	0.9966(2)	1.0000±0.0010	-0.0034±0.0007	0.9946±0.0013	+0.0020±0.0013
LMT005 / 1	1.0022(2)	1.0000±0.0007	+0.0022±0.0007	0.9997±0.0007	+0.0025±0.0007
LMT005 / 11	1.0027(2)	0.9998±0.0007	+0.0029±0.0007	1.0004±0.0006	+0.0023±0.0006
MCT008 / 1	0.9975(1)	0.9997±0.0031	-0.0022±0.0031	1.0005±0.0026	-0.0030±0.0026

  - LCT003 / 3, LCT050 / 9: incompatible biases, experiments are omitted
  - LMT005 / 1: compatible biases, but omitted by TSURFER!

TSUNAMI / TSURFER results

- Transport cask, TSUNAMI / KENO V (ENDF-B VII) k_{eff} = 0.84743 ± 0.00021
- TSURFER:

	Bias (Δk)
Best guess	-0.00230±0.00231
No correlations	-0.00153±0.00200
Increased exp. uncertainties LCT050 : 0.0010 → 0.0015 LMT005: 0.0007 → 0.0015	-0.00184±0.00211

- Additional uncertainty in the order of |Δk| ≈ 0.001 due to “uncertain input parameters”

TSURFER (best guess):Transport cask		
Isotop	Prozess	Partial bias
^{239}Pu	nubar	- 0.00092
^{235}U	nubar	- 0.00062
^{238}U	n,gamma	- 0.00048
^{235}U	fission	- 0.00032
^{239}Pu	fission	- 0.00027
^{238}U	n,n'	0.00022

TSURFER (no corr.):Transport cask		
Isotop	Prozess	Partial bias
^{238}U	n,gamma	- 0.00178
^{238}U	n,n'	- 0.00029
^{238}U	nubar	- 0.00028
^{90}Zr	elastic	0.00026
^{235}U	chi	- 0.00015
^{1}H	elastic	0.00021

Partial bias of fission products

- Bias (best guess): $\Delta k = -0.00230 \pm 0.00231$
- Sensitivity and partial bias:

TSUNAMI: LMT005 / 11		
Isotop	Prozess	Sensitivität
^{235}U	nubar	9.6249E-01
^{1}H	scatter	3.6445E-01
^{235}U	fission	3.5183E-01
^{238}U	capture	-1.3939E-01
^{235}U	capture	-1.2180E-01
^{1}H	capture	-1.1414E-01
^{16}O	scatter	7.3828E-02
^{149}Sm	capture	-2.7304E-02
^{103}Rh	capture	-1.1529E-02
^{133}Cs	capture	-5.5395E-03

TSURFER (best guess):Transport cask		
Isotop	Prozess	Partial bias
^{239}Pu	nubar	- 0.00092
^{235}U	nubar	- 0.00062
^{238}U	n,gamma	- 0.00048
^{235}U	fission	- 0.00032
^{239}Pu	fission	- 0.00027
^{238}U	n,n'	0.00022
^{133}Cs	n,gamma	0.00019
….		
^{149}Sm	n,gamma	0.00013
^{103}Rh	n,gamma	- 0.00008

- fission products: only small contributions to bias → uncertainties?

Partial bias of fission products

- TSAR: difference of 2 experiments, one with and one without a fission product

  → calculating sensitivities

TSAR: Sensitivity			
		LMT005 / 3-5	LMT005 / 3-6
^{133}Cs	capture	-4.4320E+02	-6.5123E+02
^{16}O	scatter	-1.0032E+02	-1.2639E+02
^{14}N	capture	9.2127E+01	1.5413E+02
^{235}U	fission	-4.9874E+01	-6.5048E+01
^{238}U	capture	2.9342E+01	3.6751E+01
^{1}H	scatter	2.4561E+01	-4.5511E+01

- Calculating partial bias, e.g. J.A. Roberts, et al. NCSD 2009:

Experiment	Exp. partial bias ^{133}Cs	Sensitivity $S_{k,\alpha}$	$\hat{g}$	App. partial bias ^{133}Cs
LMT005 / 4	0.000001	-1.0735E-05	0.8041	0.000004
LMT005 / 5	0.000074	-3.0102E-05	0.8086	0.000115
LMT005 / 6	0.000200	-6.5338E-05	0.8130	0.000143

- fission products: only small contributions to bias → uncertainties?

Summary

- Validation of criticality calculations with fission products:
  - TSUNAMI / TSURFER powerful tool to calculate computational bias:
    - More experiments needed, especially with fission products
    - Correlations, high quality experimental data, experienced user are important
    - Provide partial biases $\rightarrow$ uncertainties?
    - All unconsidered uncertainties affect the adjustment of the nuclear data
- Analyzing the difference of 2 experiments to estimate partial bias: TSURFER + TSAR
  - Uncertainties?
- Criticality safety analysis:
  - Best estimate vs. conservative assumptions, bounding conditions: $\Delta k \approx 0.1$
  - Overall computational bias (95% confidence level): $\Delta k \approx 0.01 - 0.02$
  - Partial bias of fission products: $\Delta k \approx 0.0001 - 0.0002$
  - Is high-precision partial bias needed?