Nuclear Data Uncertainty Quantification for Applications in Energy, Security, and Isotope Production

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Workshop on Nuclear Data Needs and Capabilities for Applications
Berkeley | 27-29 May 2015
Outline

• Data needs in nuclear energy, with cross cutting applications to safeguards and isotope production
• Spent fuel safeguards nuclear data roadmap project
• Quantitative approaches to data evaluation
• Tools for uncertainty analysis
• Covariance data
• Experimental benchmarks
• Examples of data needs
Applications and Data

Applications
• Nuclear energy (safety)
• Safeguards and security
• Isotope production
• Non proliferation
• Nuclear forensics

Nuclear Data
• Cross sections
• Nuclear decay data
• Fission product yields
• Neutron emission
• Gamma emission
• Multiplication and multiplicity
• Covariance information

Nuclear data are common to all applications – importance dependents on the end use
We are becoming data limited

- R&D focus has been more on transport methods
- Advanced 3-D geometries and continuous energy methods enable very detailed analysis
- Accuracy is increasingly limited by data

HFIR central target region and surrounding core (L), and detailed HFIR core model (R).

Watts Bar reactor modeling performed under the CASL project.
Example – $^{239}$Np capture cross section

$^{239}$Np$(n,\gamma)$

Cross Section (b)

Incident Neutron Energy (eV)
From qualitative to quantitative analysis

Experience-based needs assessments

- Expert opinions
- More subjective
- Aging experts
- We rely increasingly on analysis tools

Quantitative data UQ framework for decision making

- Sponsor needs
- Applications
- Costs
- Measurement facilities
- Prioritized needs
- UQ tools
- Benchmarks
- Covariance data

Experience-based needs assessments

Quantitative data UQ framework for decision making
Towards systematic data uncertainty analysis

The Three Stages and Six Steps of Quantitative Analysis

1. Problem recognition
2. Review of previous findings
3. Modeling
4. Data collection
5. Data analysis
6. Result presentation and action

Nuclear energy applications – Defining the problem

- Conventional reactors
- Advanced reactors
- Spent nuclear fuel data
  - Decay heat (reactor, pool storage, dry storage, repositories)
  - Nuclear criticality safety (spent fuel burnup credit for transportation, interim pool and dry storage, and repositories)
  - Safety analysis – releases and off-site dose consequence
  - Repository safety analysis
  - Dose assessment
  - Spent fuel verification for safeguards (neutron and gamma sources for NDA, multiplication)
Spent Nuclear Fuel Data UQ Project* (Roadmap of priority data needs)

- ORNL/LLNL/LANL collaboration
- Methods and data development
- Benchmarks - Advanced instruments being tested in Sweden
- Methods: PG, PN, DDA, DDSI
- Nuclear data
  - Fuel compositions
  - Gamma emission
  - Neutron emission
  - Neutron multiplication
  - Detector models

*U.S. Department of Energy, Office of Defense Nuclear Nonproliferation R&D
Nuclear data reviews

- OECD/NEA WPEC Subgroup 25 on decay heat data needs*
- OECD/NEA WPEC Nuclear Data High Priority Request List (HPRL)
- IAEA Intermediate-term Nuclear Data Needs for Medical Applications INDC(NDS)-0596
- A Survey of Nuclear Data Deficiencies Affecting Nuclear Non-Proliferation, LA-UR-14-26531
Spent Fuel Assay Data Benchmarks

- SFCOMPO 2.0 database developed through the international OECD/NEA Expert Group on Assay Data now contains >600 fuel samples with destructive analysis measurements
- Experimental uncertainties are included
- SFCOMPO expanded for world reactor data
  - Commercial PWR and BWR designs
  - VVER-440 and VVER-1000
  - Russian RBMK graphite
  - AGR and MAGNOX graphite
  - CANDU heavy water
  - Recent data from Hanford B production reactors, Magnox and CANDU fuel
Isotopic validation
(ENDF/B-V and ENDF/B-VII.0)

Actinides

Fission products

(C/E)_{avg}-1 (%)
Benchmarks – calorimeter measurements

Comparison calculation – experiment *

- Cooling times 12 – 30 years
- BWR assemblies
  - number of measurements = 45
  - average C/E = 1.003 ± 0.025
  - average residual = -0.2 ± 3.4 W
- PWR assemblies
  - number of measurements = 38
  - average C/E = 1.011 ± 0.012
  - average residual = 4.7 ± 5.0 W

Spent fuel assembly calorimeter at the SKB CLAB facility Sweden

Benchmarks – decay heat at short times after fission ($^{235}\text{U}$)

# Modeling Methods for Nuclear Data UQ

## Total Monte Carlo Method

**Stochastic Sampling**

- **Covariances of input data sampled; statistical analysis of output distribution gives uncertainties**

- **Pros**
  - Can be used with existing codes
  - Obtains uncertainties for all responses at once

- **Cons**
  - Cannot quantify individual contributors to uncertainty
  - Requires many calculations

## Sensitivity Analysis

**Adjoint method**

- **Sensitivities are computed; combined with covariances to obtain uncertainties**

- **Pros**
  - Quantifies individual uncertainty contributors
  - Obtains sensitivities for all data and single response at once

- **Cons**
  - Requires implementation of adjoint solution
  - Adjoint calculation for each response.
Sources of covariance data

- **Cross section covariances**
  ENDF-VII.1 supplemented by other sources (SCALE cov library) – 423 nuclides, 190 with cov data
- **Fission product yield**
  No covariance data. Retroactive generation by combining independent and cumulative yield uncertainties
- **Decay data**
  ENDF-VII.1 modified to include branching correlations
- **Gamma emissions**
  ENDF-VII.1, no covariance data
- **Neutron emissions**
  ENDF-VII.1, except $^{252}$Cf, no covariance data
Fission yield covariance data

- Retroactive covariance data generated using a Bayesian approach by Lack of covariance data –
- Strong negative correlations exist within chains
- Relative strong positive correlations (delayed-neutrons)

Decay scheme

ENDF/B-VII.1
ENDF/B-V

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Fission yield data

- Fission yield and decay data in ENDF/B-VII.1 are inconsistent
- Yields are largely from England and Rider (1994)
- Decay data revised in ENDF/B-VII.1 (2011)
- Direct and cumulative yields are highly correlated
- Krypton noble gases have 5-8% error

\[ C_i(I) = I_i + \sum_{j \in K^i} C_j(I) b_{i,j} \]

- Decay data and fission yields should not be developed independently

Neutron source covariance data

- SOURCES code used for spontaneous fission and \((\alpha,n)\) has no uncertainties
- ENDF/B-VII.1 only contains SF covariance data for \(^{252}\text{Cf}\)
- A retroactive covariance data generation performed using the SAMMY code with R-Matrix evaluation for alpha cross sections

![Graphs and contour plots showing covariance data](images)
Summary/Recommendations

• Sponsors need unbiased information on data needs and priorities

• Require a structured quantitative process to evaluate uncertainties – cannot rely entirely on judgement
  – Rigorous sensitivity/uncertainty analysis tools
  – More complete covariance information for all nuclear data
  – Better covariance data
  – Experimental benchmarks for diverse applications
  – A prioritized data roadmap with acquisition paths and costs
  – A coordinated and clear message to funding organizations and measurement institutes

• Tools and data for the Safeguards UQ project will be applicable to many different applications