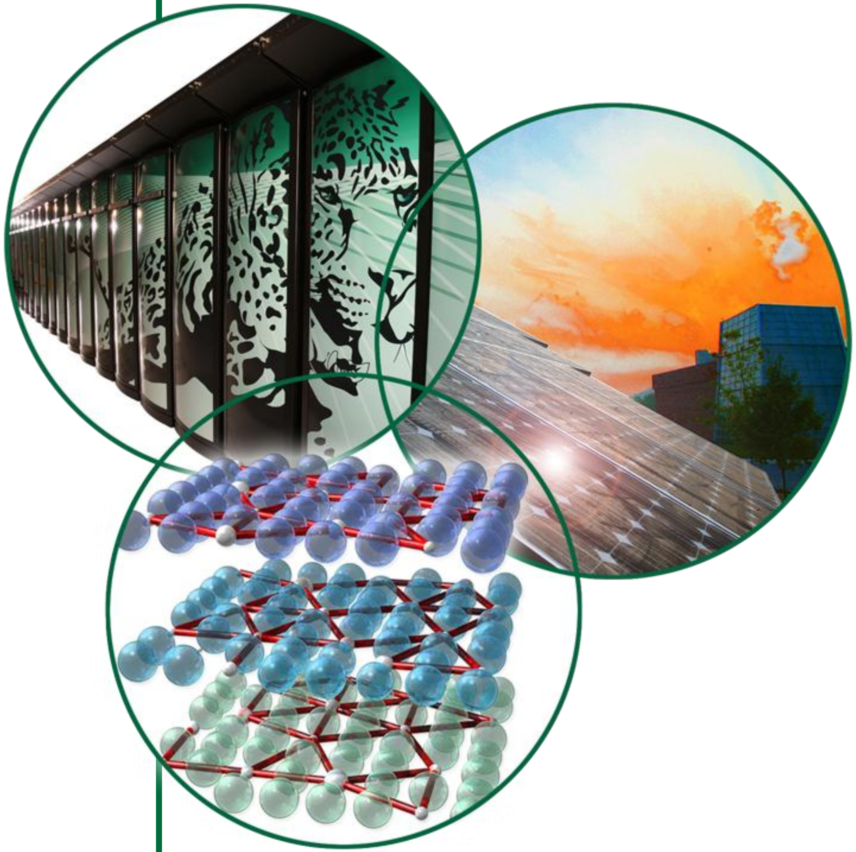
REVIEW OF RESULTS FOR THE OECD/NEA PHASE VII BENCHMARK:
STUDY OF SPENT FUEL COMPOSITIONS FOR LONG-TERM DISPOSAL



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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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Outline

- Overview of the benchmark specifications
- Participating organizations, computer codes, and nuclear data
- Results
  - Decay calculations for selected isotopes relevant to burnup-credit criticality safety analyses and for radiological dose assessments
  - Criticality calculations for actinide-only compositions and for actinide and fission product (FP) nuclide compositions
- Conclusions

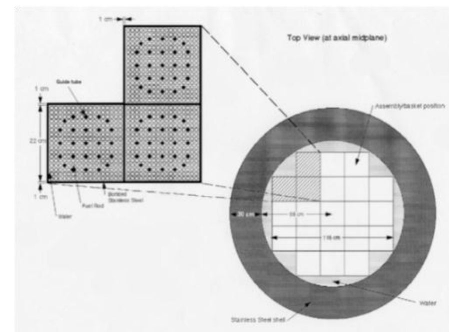
Overview of the Benchmark Specifications (1/3)

- Purpose
  - *Study the ability of relevant computer codes and associated nuclear data to predict spent fuel isotopic compositions and corresponding effective neutron multiplication factor (k_{eff})values in a cask configuration over the time duration relevant to spent nuclear fuel (SNF) long-term storage and disposal*

- Objective
  - *Improve understanding and confidence in our ability to predict k_{eff} and source terms for timeframes relevant to extended long-term storage and disposal of SNF*

Overview of the Benchmark Specifications (2/3)

- Specification (issued Nov 2008)
  - http://www.oecd-nea.org/science/wpncs/buc/specifications/
  - PWR UO_2 discharged fuel compositions for decay calculations
    - 4.5-wt% ^{235}U initial enrichment and 50 GWd/MTU burnup
    - Nuclides relevant to burnup credit and radiological dose as well as their precursors (113 total nuclides)
  - Representative cask model for k_{eff} calculations
    - Borrowed from previous benchmark specifications



- Requested results
  - Predicted isotopic concentrations for 30 time steps (0 – $1x10^6$ years)
  - Predicted k_{eff} values for each time step
    - Actinide-only (11 total isotopes) fuel compositions
    - Actinide and fission product (30 total isotopes) fuel compositions

Overview of the Benchmark Specifications (3/3)

Nuclides selected for benchmark calculations based on relevance to radiological dose and burnup-credit criticality safety analyses

Nuclides relevant to radiological dose assessments (44 total)
^{14}C, ^{36}Cl, ^{41}Ca, ^{59}Ni, ^{79}Se, ^{93}Zr, ^{90}Sr, ^{93m}Nb, ^{94}Nb, ^{93}Mo, ^{99}Tc, ^{107}Pd, ^{126}Sn, ^{126}Sb, ^{126m}Sb, ^{129}I, ^{135}Cs, ^{137}Cs, ^{151}Sm, ^{210}Pb, ^{226}Ra, ^{228}Ra, ^{227}Ac, ^{229}Th, ^{230}Th, ^{232}Th, ^{231}Pa, ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{245}Cm, ^{246}Cm
Nuclides relevant to actinide-only burnup-credit criticality safety analyses (11 total)
^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am
Nuclides relevant to actinide and fission product burnup-credit criticality safety analyses (30 total)
^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{143}Nd, ^{145}Nd, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{151}Eu, ^{153}Eu, ^{155}Gd
Note: 16 nuclides are relevant to both burnup credit criticality and radiological dose analyses.

Participating Organizations and Computer Codes/Data [1/2]

Country	Organization	Decay Code	Decay Data Library	Criticality Code	Cross-Section Data Library
Slovakia	Nuclear Power Plant Research Institute Trnava Inc, (VUJE)	SCALE 5.1/ ORIGEN-S	ENDF/B-VI	SCALE 5.1/ KENO VI	ENDF/B-V, 44 EGs
USA	Oak Ridge National Laboratory	SCALE 6.1/ ORIGEN-S (beta)	ENDF/B-VII	SCALE 6.0/ KENO V.a	ENDF/B-VII.0, CE
Japan	Japan Atomic Energy Agency	ORIGEN2.2-UPJ	ORLIBJ33	MCNP-4C2	JENDL3.3, CE
Sweden	E Mennerdahl Systems	SCALE 6.0/ ORIGEN-S	ENDF/B-VI	SCALE 6/ KENO V.a	ENDF/B-VII.0, CE
Spain	DENIM/CSN/ SEA Ingenieria	ACAB-2008	JEFF-3.1	MCNPX-2.5	JEFF-3.1.1, CE
				MCNPX-2.4.0	ENDF/B-VI, CE
		ACAB-2008	ENDF/B-VI	MCNPX-2.5	JEFF-3.1.1, CE
France	Institut de Radioprotection et de Sûreté Nucléaire (IRSN)	DARWIN 2.0	JEF-2	MORET 5	JEFF-3.1, CE
		PHOENIX 1.0.0a (beta)	ORGEN2.2 DECAY.LIB	N/A	N/A

EGs = energy groups
CE = continuous energy

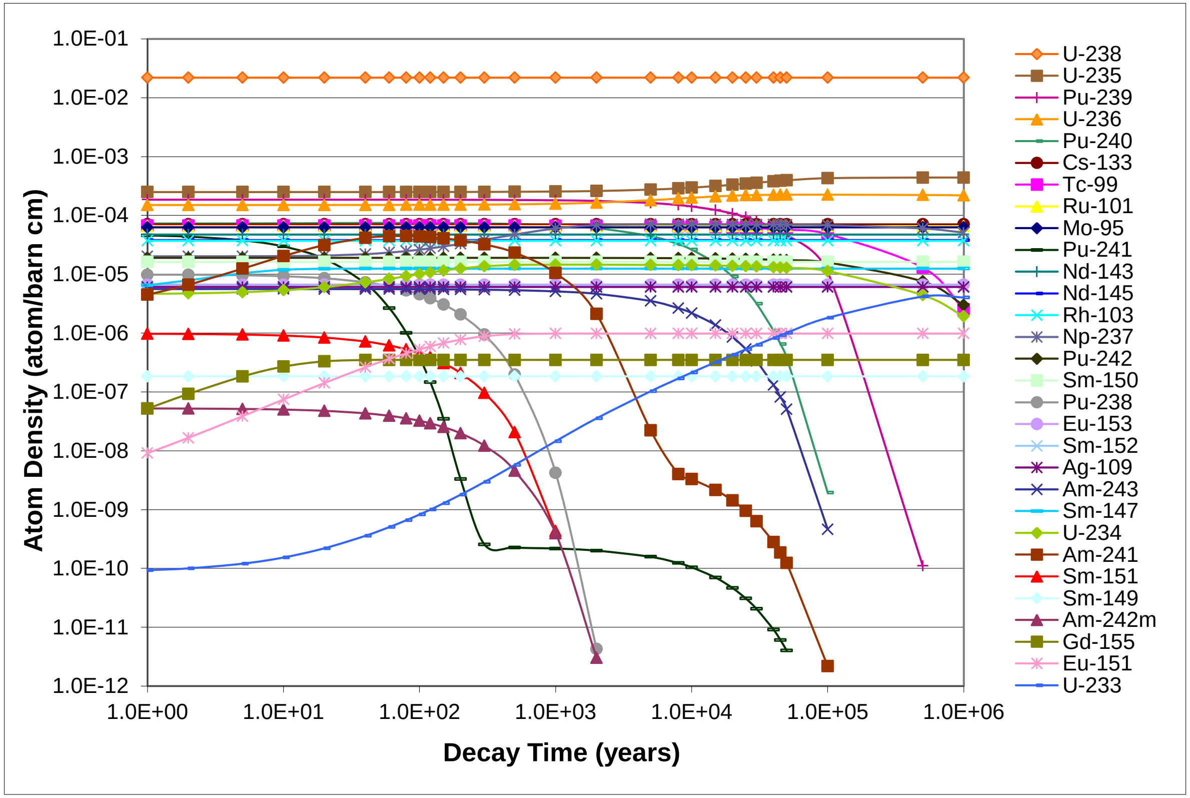
Participating Organizations and Computer Codes/Data [2/2]

Country	Organization	Decay Code	Decay Data Library	Criticality Code	Cross-section Data Library
France	AREVA-TN	DARWIN 2.1	JEF-2.2	CRISTAL V1.0	JEF-2.2, 172 EGs
Germany	Gesellschaft für Anlagen-und Reaktorsicherheit mbH (GRS)	ORIGEN-X-2008	ENDF/B-VI	SCALE 6/ KENO V.a	ENDF/B-VII.0, 238 EGs
Czech Republic	Nuclear Research Institute at Rez	SCALE 6.0/ ORIGEN-S	ENDF/B-VI	SCALE 6.0/ KENO V.a	ENDF/B-VII.0, 238 EGs
				SCALE 6.0/ KENO V.a	ENDF/B-VII.0, CE
Finland	VTT Technical Research Centre of Finland	SCALE 6.0/ ORIGEN-S	ENDF/B-VI	MCNP5 1.40	ENDF/B-VI, CE
Hungary	KFKI Atomic Energy Research Institute	SCALE 6.0/ ORIGEN-S	ENDF/B-VI	MCNP5	ENDF/B-VI.2 and V, CE
		TIBSO	JEF-2.2	MCNP5	ENDF/B-VI.2 and V, CE
USA	Los Alamos National Laboratory	CINDER 90	ENDF/B-VI	N/A	

ISOTOPIC RESULTS

Time-Dependent Nuclide Concentrations [1/2]

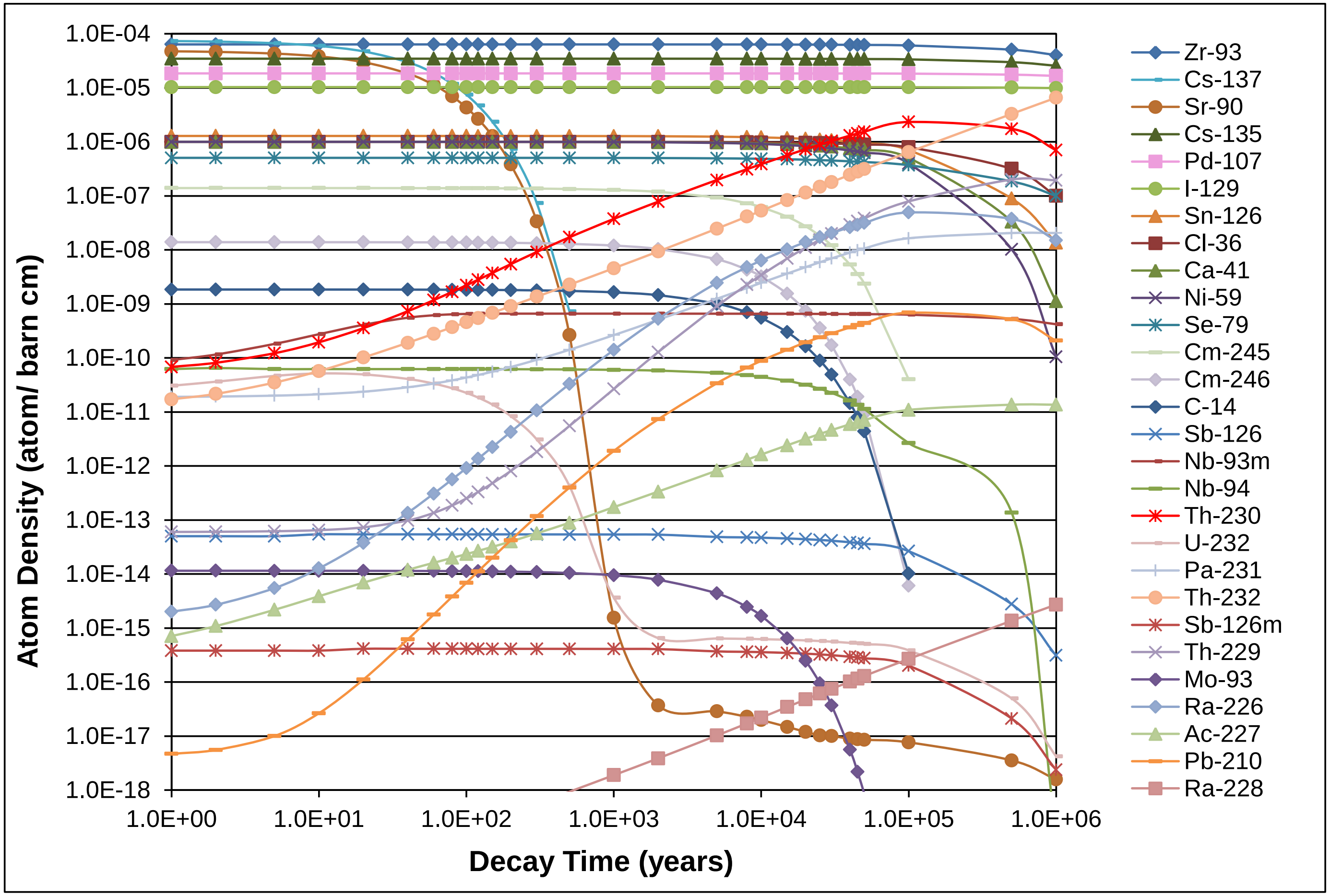
Showing actinides and fission product nuclides relevant to burnup credit



- Note: Nuclides ^{99}Tc, ^{151}Sm, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, and ^{243}Am are also relevant to radiological dose assessments.

Time-dependent Nuclide Concentrations [2/2]

Showing nuclides relevant to radiological dose assessments



Nuclides Important to Burnup Credit Criticality Safety Analyses

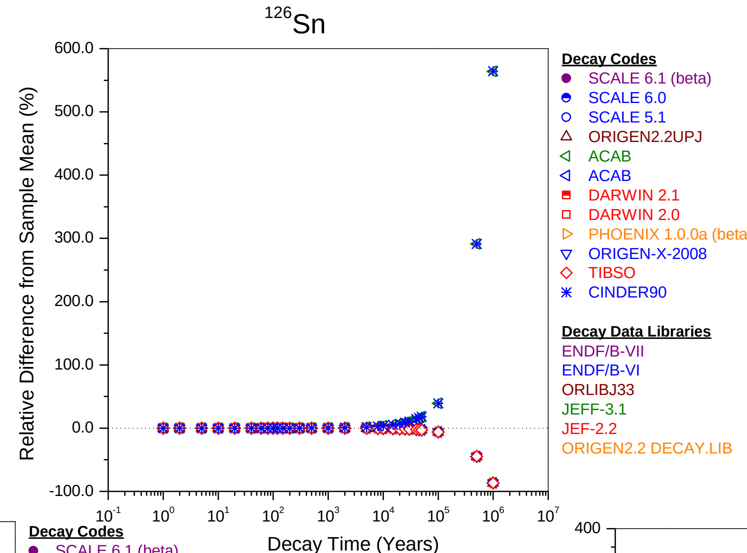
- Negligible dispersions (RSD < 0.1%) of the calculated time-dependent concentrations for major actinide nuclides ^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, and ^{242}Pu

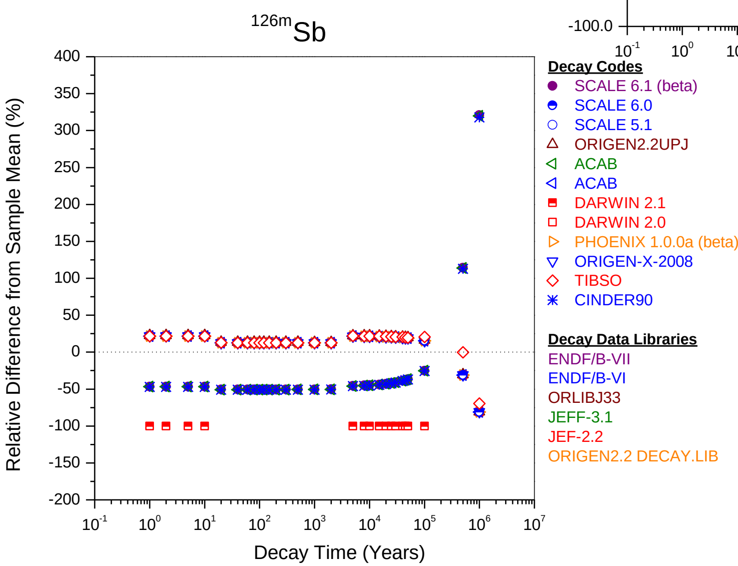
- Insignificant dispersions of the calculated atom densities for stable fission product nuclides ^{95}Mo, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{143}Nd, ^{147}Sm, and ^{149}Sm whose concentrations slightly increase due to the decay of their shot-lived precursors

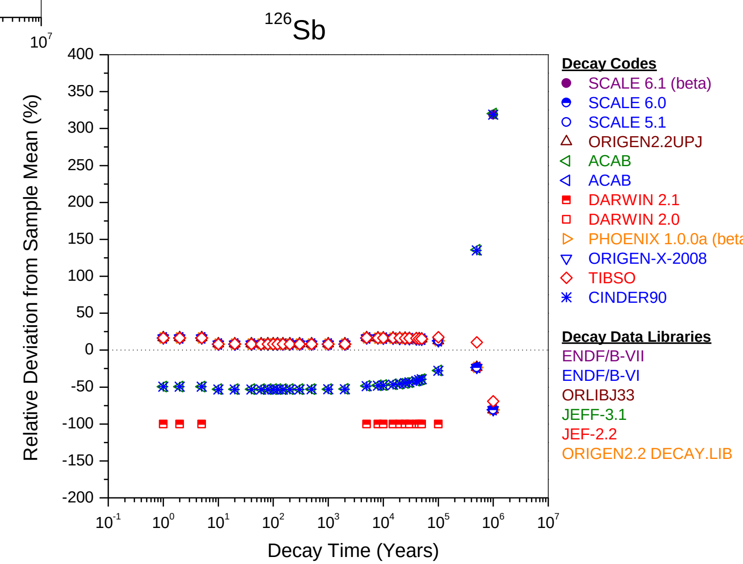
- Dispersion of the decay calculation results (1% < RSD < 5%) observed for ^{99}Tc, ^{151}Sm, ^{155}Gd, ^{233}U, ^{234}U, ^{237}Np, ^{241}Pu, and ^{241}Am

Comparison of Decay Calculation Results [1/3]

Showing the relative difference from sample mean for ^{126}Sn, ^{126m}Sb, and ^{126}Sb



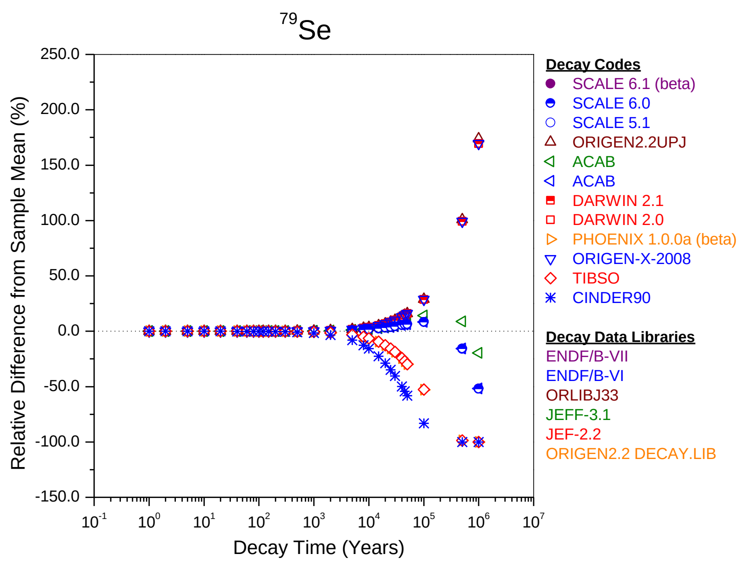


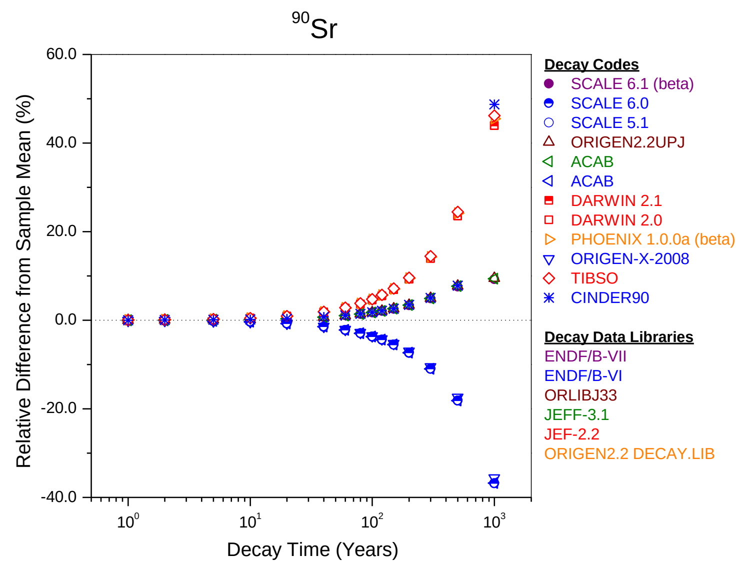


Library	ENDF/B-VII.0	ENDF/B-VI.8	JEFF-3.1	JEF-2.2	ORIGEN2.2-UPJ ORLIBJ33	ORIGEN 2.2 DECAY.LIB
^{126}Sn half-life (s)	7.25824E+12	3.15569E+12	7.25809E+12	3.15569E+12	3.15600E+12	3.15600E+12

Comparison of Decay Calculation Results [2/3]

Showing the relative difference from sample mean for ^{79}Se and ^{90}Sr

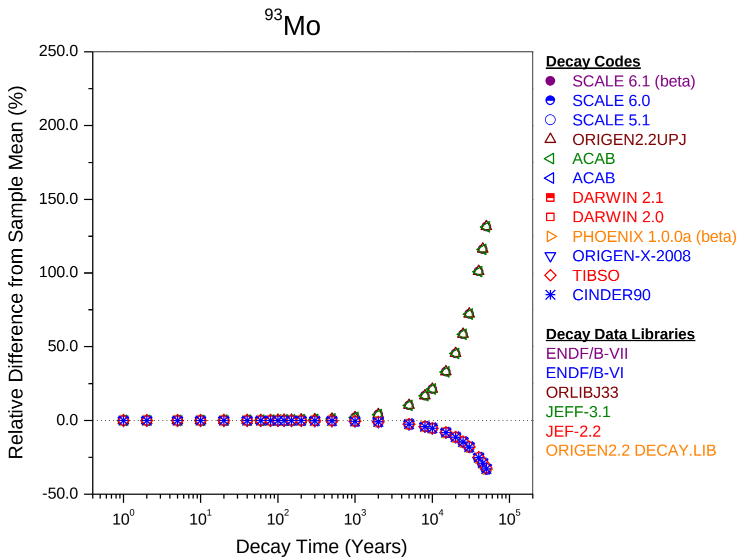


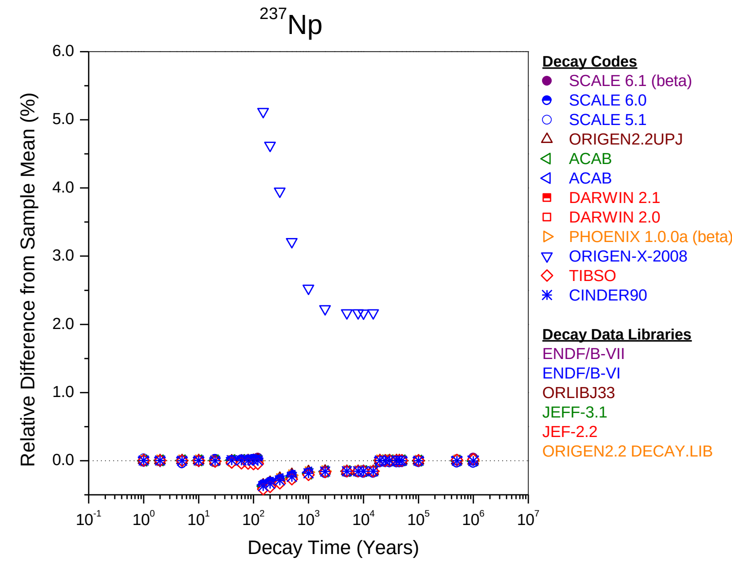


Library	ENDF/B-VII.0	ENDF/B-VI.8	JEFF-3.1	JEF-2.2	ORIGEN2.2-UPJ ORLIBJ33	ORIGEN 2.2 DECAY.LIB
^{79}Se Half-life (s)	9.30949E+12	1.04138E+12	1.18970E+13	2.05120E+12	2.05124E+12	2.05000E+12
^{90}Sr Half-life (s)	9.08543E+08	8.88327E+08	9.08524E+08	9.18938E+08	9.08226E+08	9.19000E+08

Comparison of Decay Calculation Results [3/3]

Showing the relative difference from sample mean for ^{93}Mo and ^{237}Np





Note: Small deviations might occur in the ORIGEN-X-2008 calculated concentrations for times beyond 150 years due to a splitting of the calculation and due to the choice of large time steps.

Library	ENDF/B-VII.0	ENDF/B-VI.8	JEFF-3.1	JEF-2.2	ORIGEN2.2-UPJ ORLIBJ33	ORIGEN 2.2 DECAY.LIB
^{93}Mo half-life (s)	1.26230E+11	1.10449E+11	1.26228E+11	1.10449E+11	1.26230E+11	1.10400E+11
^{237}Np half-life (s)	6.76594E+13	6.75318E+13	6.75318E+13	6.75318E+13	6.75318E+13	6.75300E+13

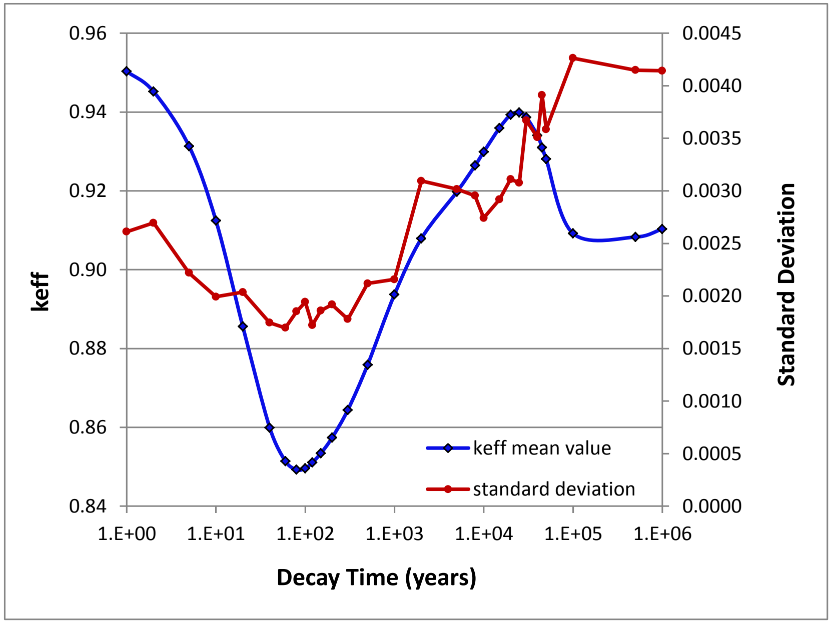
Factors Affecting the Accuracy of Decay Calculation Results

- Different half-life values among the ENDF/B-VII.0, JEFF-3.1, ENDF/B-VI.8, and JEF-2 evaluations:
  - ^{14}C, ^{41}Ca, ^{59}Ni, ^{79}Se, ^{90}Sr, ^{94}Nb, ^{93}Mo, ^{99}Tc, ^{126}Sn, ^{151}Sm, ^{155}Eu, ^{229}Th, ^{232}U, ^{236}Np, ^{236}Pu, and ^{246}Cm
- Outdated half-life values in ORIGEN2.2 DECAY.LIB (based on ENDF/B-IV):
  - ^{41}Ca, ^{59}Ni, ^{93m}Nb, ^{228}Ra, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, and ^{242m}Am
- Different branching ratio values for ^{93}Zr beta decay (0.95, 0.975, 1)
- Approximations related to the number of time steps allowed by a decay code, which affected contributions from short-lived precursor nuclides
- Neglected contributions from relevant precursor decay chains
  - ^{210}Pb and ^{228}Ra time-dependent atom densities most impacted
- Numerical approximations made by the participants

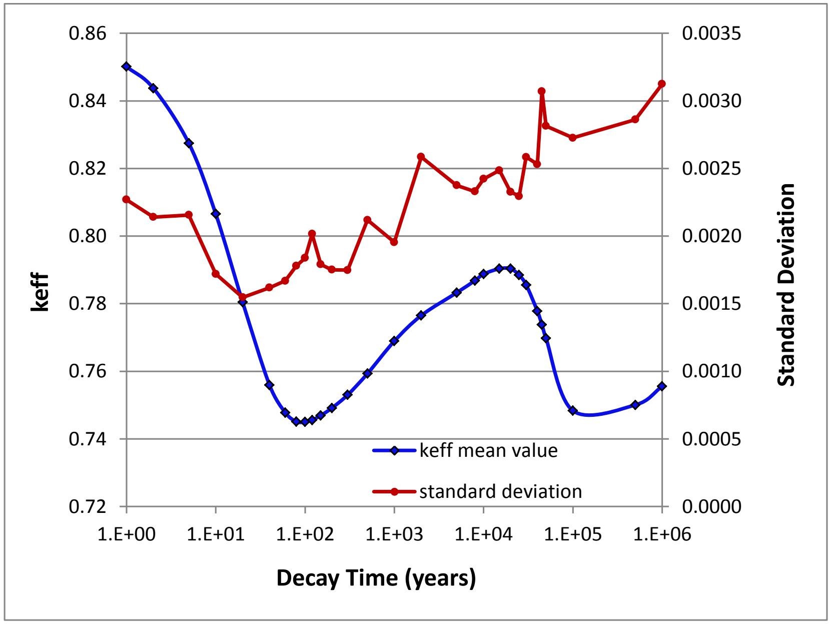
CRITICALITY CALCULATION RESULTS

k_{eff} Values – Mean and Standard Deviation as a Function of Decay Time

	$\overline{k_{eff}}$	Standard Deviation
Fresh fuel	1.1485	0.0026
Discharged actinide-only compositions	0.9548	0.0027
Discharged actinide + FP compositions	0.8604	0.0021



Actinide-only nuclides



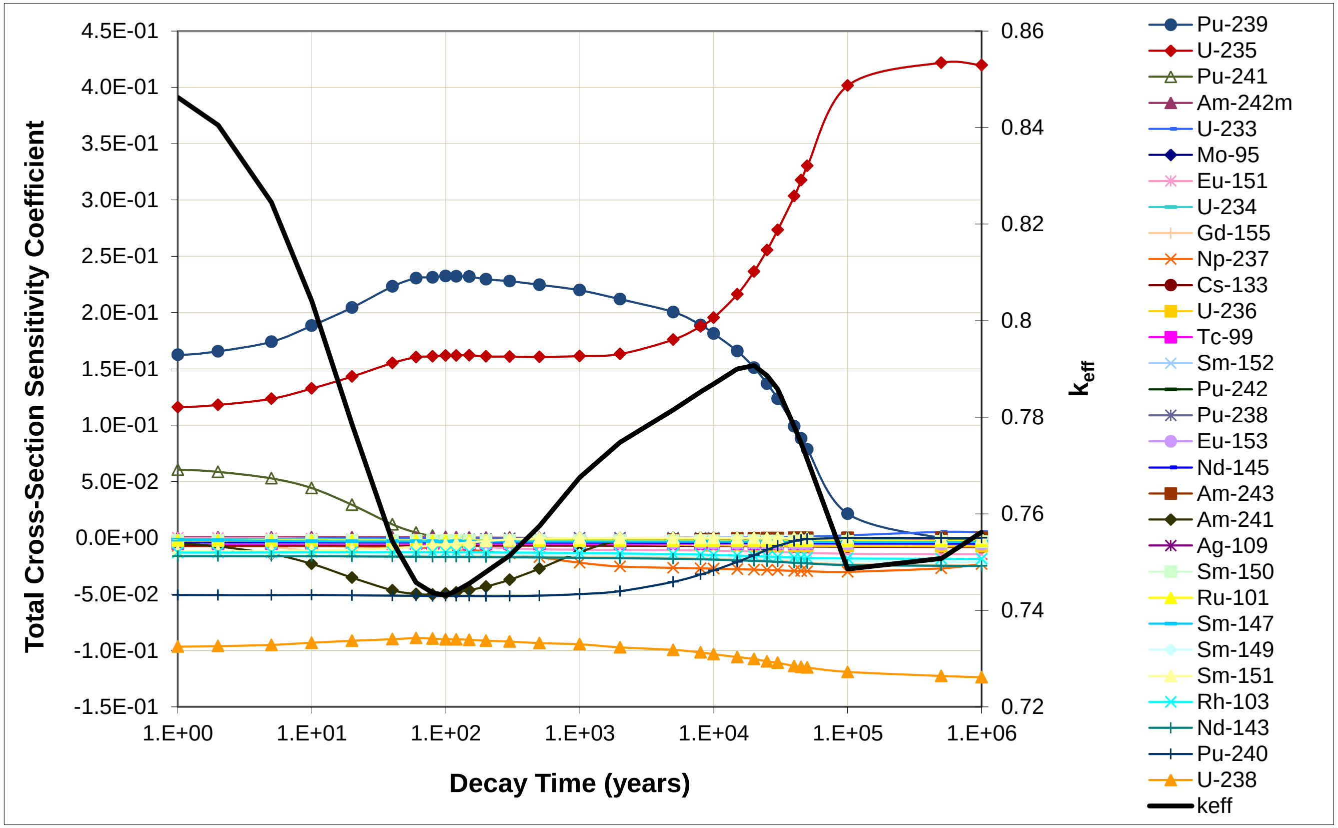
Actinides and FP nuclides

Analysis of Criticality Calculation Results

- Factors that may cause the variability of the criticality calculation results
  - Differences among nuclear cross-section data
  - Dispersion of decay calculation results for nuclides important to burnup credit (^{99}Tc, ^{151}Sm, ^{155}Gd, ^{233}U, ^{234}U, ^{237}Np, ^{241}Pu, and ^{241}Am)
  - Modeling and numerical approximations made by participants

- Cross-section sensitivity and uncertainty analysis performed using the TSUNAMI tools in SCALE to understand what may have caused the small dispersion of the criticality calculation results
  - Determined k_{eff} sensitivity to the total cross section of individual nuclides
    - Sensitivity coefficient: $$S_{k,\Sigma_x^n} = \frac{\delta k_{eff} / k_{eff}}{\delta \Sigma_x^n / \Sigma_x^n}$$
    - 238-group cross-section library based on ENDF/B-VII evaluations
  - Determined k_{eff} uncertainty (1 sigma confidence level) due to cross-section uncertainties
    - 44-group covariance data developed from ENDF/B-VII, ENDF/B-VI, and JENDL3.3 evaluations

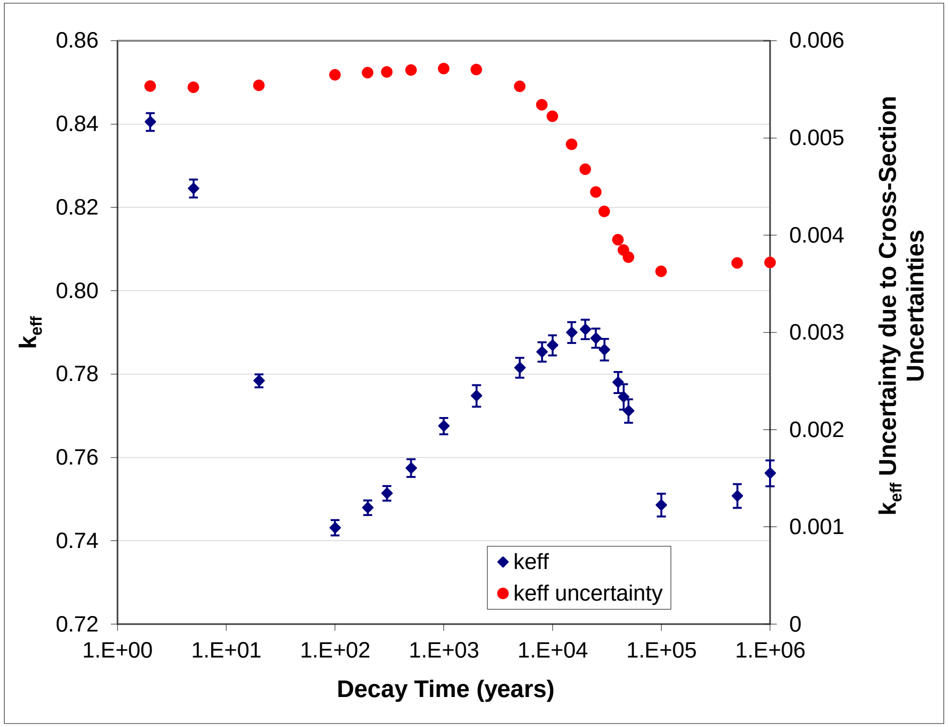
k_{eff} Sensitivity to ENDF/B-VII Total Cross-Section Data for Actinides and Fission Product Nuclides

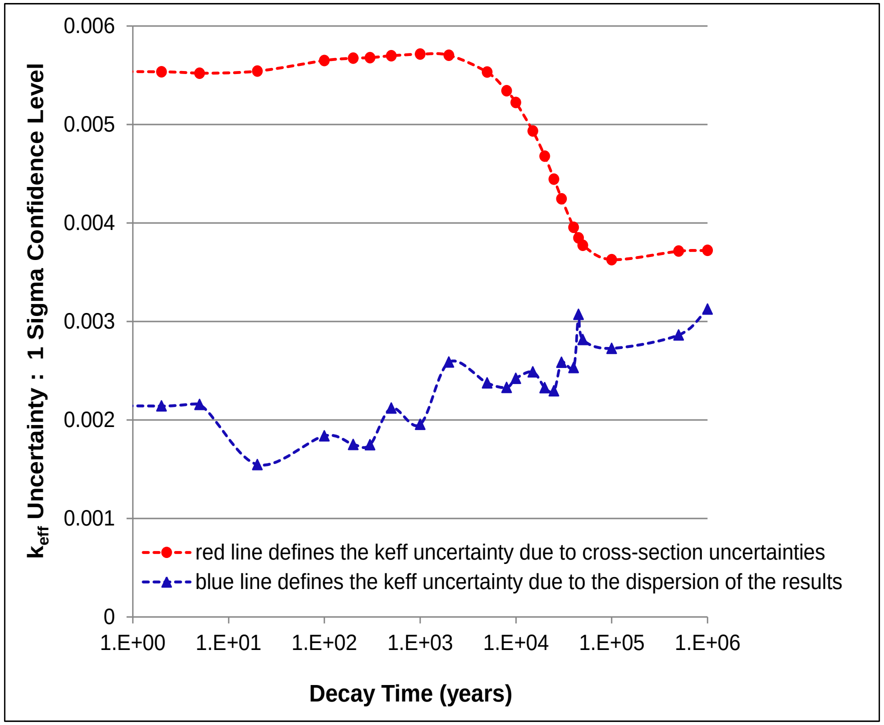


- k_{eff} has large sensitivities to perturbations in ^{239}Pu, ^{235}U, and ^{238}U cross-section data
- k_{eff} has negligible sensitivities to perturbations in the cross-section data of the nuclides for which slightly different atom densities were calculated (^{99}Tc, ^{151}Sm, ^{155}Gd, ^{233}U, ^{234}U, ^{237}Np, ^{241}Pu, and ^{241}Am)

k_{eff} Uncertainty Due to Cross-Section Uncertainties

Showing the results for Actinide and Fission Product Fuel Compositions





Note: Error bars show the uncertainty in k_{eff} due to uncertainties associated with cross-section data.

- Variability of the benchmark k_{eff} results
  - Bounded by the uncertainty in k_{eff} due to cross-section covariance data
  - May be predominantly attributed to the criticality calculation methods and cross-section data

Conclusions of the OECD/NEA Phase VII Benchmark Results

- 15 organizations in 10 countries contributed
  - 15 decay calculations using 12 different decay codes/data libraries
  - 15 criticality calculations using 13 different criticality codes/nuclear cross-section data libraries
- Time-dependent concentrations for major burnup credit actinides and fission product nuclides were very similar
- Small dispersions (RSD < 5%) of the decay calculation results for some of the nuclides important to burnup credit
- Significant variability of the decay calculation results for ^{79}Se, ^{90}Sr, ^{126}Sn, ^{126m}Sb, and ^{126}Sb (nuclides important to radiation dose assessments)
- Small variability of the benchmark criticality results (RSD < 0.5%)
- Variability of the decay calculation results may be attributed to:
  - Different half-life and branching ratio values among the evaluated libraries
  - Approximations related to the number of time steps allowed by a decay code
  - Neglected contributions from relevant precursor decay chains (e.g., ^{210}Pb and ^{228}Ra)
- Variability of the k_{eff} results may be predominantly attributed to differences among the evaluated criticality calculation methods and cross-section data

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