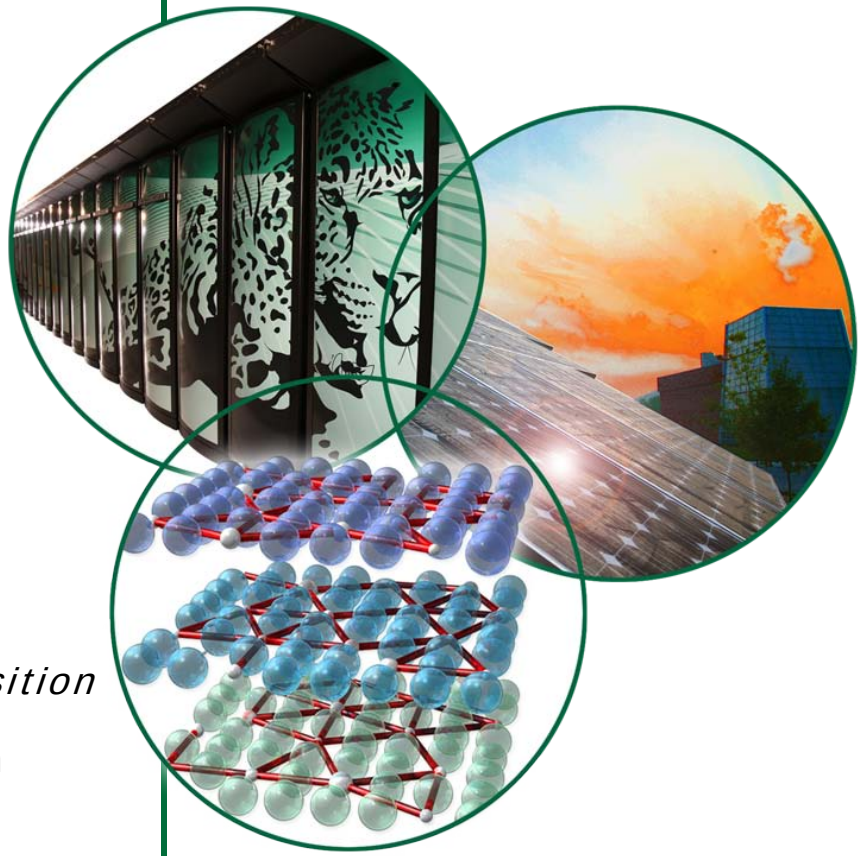
REVIEW OF RESULTS FOR THE OECD/NEA PHASE VII BENCHMARK: STUDY OF SPENT FUEL COMPOSITIONS FOR LONG-TERM DISPOSAL



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International Workshop on Advances in Applications of Burnup Credit for Spent Fuel Storage, Transport, Reprocessing, and Disposition

Organized by: Nuclear Safety Council of Spain (CSN) and the International Atomic Energy Agency (IAEA)

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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

- Overview of the benchmark specification
- Participating organizations, computer codes, and nuclear data
- Results
  - Decay calculations for selected isotopes
  - Criticality calculations
    - Sensitivity calculations
- Summary Remarks / Observations

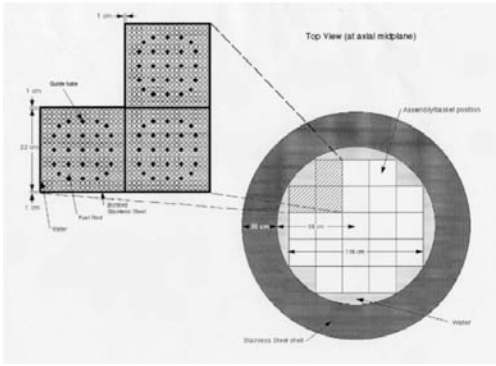
Overview of the benchmark specification (1/2)

- Purpose
  - *Study the ability of relevant computer codes and associated nuclear data to predict spent fuel isotopic compositions and corresponding k_{eff} values in a cask configuration over the time duration relevant to SNF disposal*

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

Overview of the benchmark specification (1/2)

- Specification (issued Nov 2008)
  - http://www.nea.fr/html/science/wpncs/buc/specifications/phase-VII/Phase-VII_BenchmarkSpecification_REV01.pdf
  - PWR UO_2 discharge fuel compositions for decay calculations
    - 4.5-wt% ^{235}U initial enrichment and 50 GWd/MTU burnup
    - Isotopes relevant to burnup credit and public dose as well as their precursors (113 total isotopes)
  - Representative cask model for k_{eff} calculations
    - Borrowed from previous benchmark specifications



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

Excerpts from benchmark specification

Table 1. Discharge fuel composition (4.5 initial wt% ^{235}U, 50-GWd/MTU) for calculating time-dependent spent fuel compositions

Isotope	Atom density (atom/barn·cm)	Benchmark nuclide[a]	Area of applicability		
			Actinide-only burnup credit	Actinide + FP burnup credit	Public dose
^{14}C	1.8462E-09	X			X
^{16}O[b]	4.7923E-02		X	X	
^{36}Cl[c]	1.0000E-06	X			X
^{41}Ca[c]	1.0000E-06	X			X
^{59}Ni[c]	1.0000E-06	X			X
^{79}Se	5.0582E-07	X			X
^{93}Zr	6.3637E-05	X			X
^{93}Rb	1.6072E-12				
^{90}Sr	4.8584E-05	X			X
^{93}Sr	2.3719E-10				
^{93}Y	1.9886E-08				
^{95}Y	3.8958E-10				
^{93m}Nb	6.6305E-11	X			X
^{94}Nb	6.2143E-11	X			X
^{95}Nb	1.9348E-06				
^{93}Mo	1.1478E-14	X			X
^{95}Mo	6.0803E-05	X		X	

Excerpts from benchmark specification

Table 2: Times for calculating and reporting isotopic compositions

Time case number	Time (y)	Time case number	Time (y)
1	0	16	1000
2	1	17	2000
3	2	18	5000
4	5	19	8000
5	10	20	10,000
6	20	21	15,000
7	40	22	20,000
8	60	23	25,000
9	80	24	30,000
10	100	25	40,000
11	120	26	45,000
12	150	27	50,000
13	200	28	100,000
14	300	29	500,000
15	500	30	1,000,000

Excerpts from benchmark specification

Table 3: Nuclide sets to be used in k_{eff} calculations

Set 1: Actinide-only burnup-credit nuclides (11 total)
^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, and ^{241}Am
Set 2: Actinide + fission product burnup-credit nuclides (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, and ^{155}Gd

Participating Organizations and Computer Codes/Data Used

Country	Organization	Decay Code	Decay Data Library	Criticality Code	Cross-section Data Library
Slovakia	VUJE [a]	SCALE 5.1/ ORIGEN-S	ENDF/B-VI and V	SCALE 5.1/ KENO VI	ENDF/B-V, 44 energy groups (EGs)
USA	ORNL [b]	SCALE 6/ ORIGEN-S (CCC-750)	ENDF/B-VI and V	SCALE 6/ KENO V.a	ENDF/B-VII.0, continuous energy (CE)
Japan	JAEA [c]	ORIGEN2.2UPJ (NEA-1642)	ORLIB33 [d]	MCNP-4C2	JENDL3.3, CE
Sweden	E Mennerdahl Systems	SCALE6/ ORIGEN-S	ENDF/B-VI and V	SCALE 6/ KENO V.a	ENDF/B-VII.0, CE
Spain	DENIM/CSN/ SEA Ingenieria [e]	ACAB V2008 (NEA-1839)	JEFF-3.1	MCNPX-2.5	JEFF-3.1.1, CE
				MCNPX-2.4.0	ENDF/B-VI, CE
		ACAB V2008	From ORIGEN-S	MCNPX-2.5	JEFF-3.1.1, CE
France	AREVA-TN	DARWIN 2.1	JEF-2.2	CRISTAL V1.0	JEF-2.2, 172 EGs

[a] Nuclear Power Plant Research Institute Trnava Inc, VUJE
[b] Oak Ridge National Laboratory
[c] Japan Atomic Energy Agency
[d] JNDC FP nuclear data library and JENDL3.3
[e] Additional criticality calculations and analyses were provided by these organizations to be included as an Annex to the final report.

Participating Organizations and Computer Codes/Data Used

Country	Organization	Decay Code	Decay Data Library	Criticality Code	Cross-section Data Library
France	IRSN [a]	DARWIN 2.0	JEF-2	MORET 5 [b]	JEFF-3.1, CE
		PHOENIX 1.0.0a [b]	DECAY.LIB (ORGEN2.2)	N/A	N/A
Germany	GRS [c]	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/ ORIGEN-S	ENDF/B-VI and V	SCALE 6/ KENO V.a	ENDF/B-VII.0, 238 EGs
				SCALE 6/ KENO V.a	ENDF/B-VII.0, CE
Finland	VTT [d]	SCALE 6/ ORIGEN-S	ENDF/B-VI and V	MCNP5, version 1.40	ENDF/B-VI, CE
Hungary	KFKI [e]	SCALE 6/ ORIGEN-S	ENDF/B-VI and V	MCNP5	ENDF/B-VI.2 and V, CE
		TIBSO (NEA-1592)	JEF-2.2	MCNP5	ENDF/B-VI.2 and V, CE

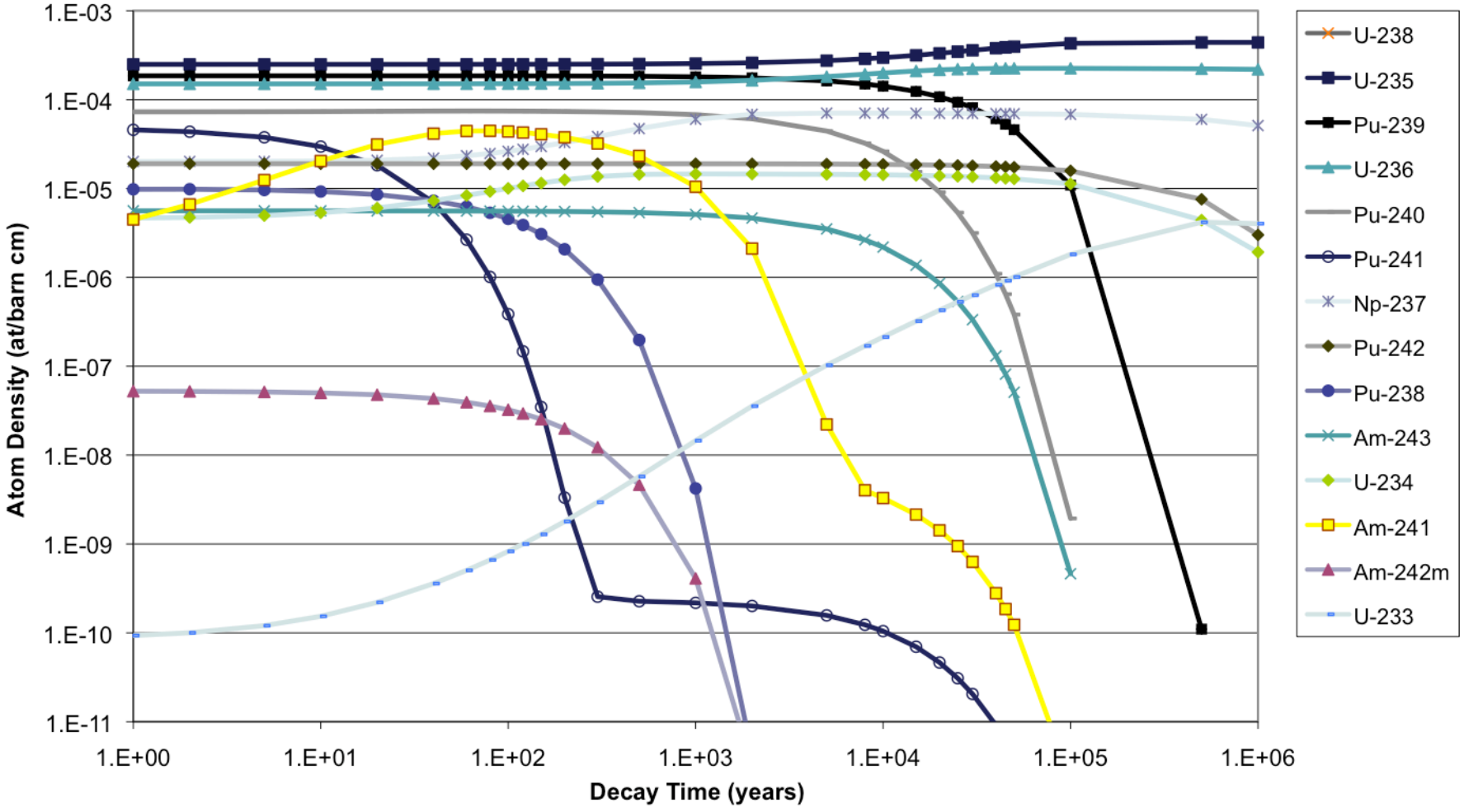
[a] Institut de Radioprotection et de Sûreté Nucléaire
[b] Under development
[c] Gesellschaft für Anlagen-und Reaktorsicherheit mbH
[d] VTT Technical Research Centre of Finland
[e] KFKI Atomic Energy Research Institute

Summary: Participation

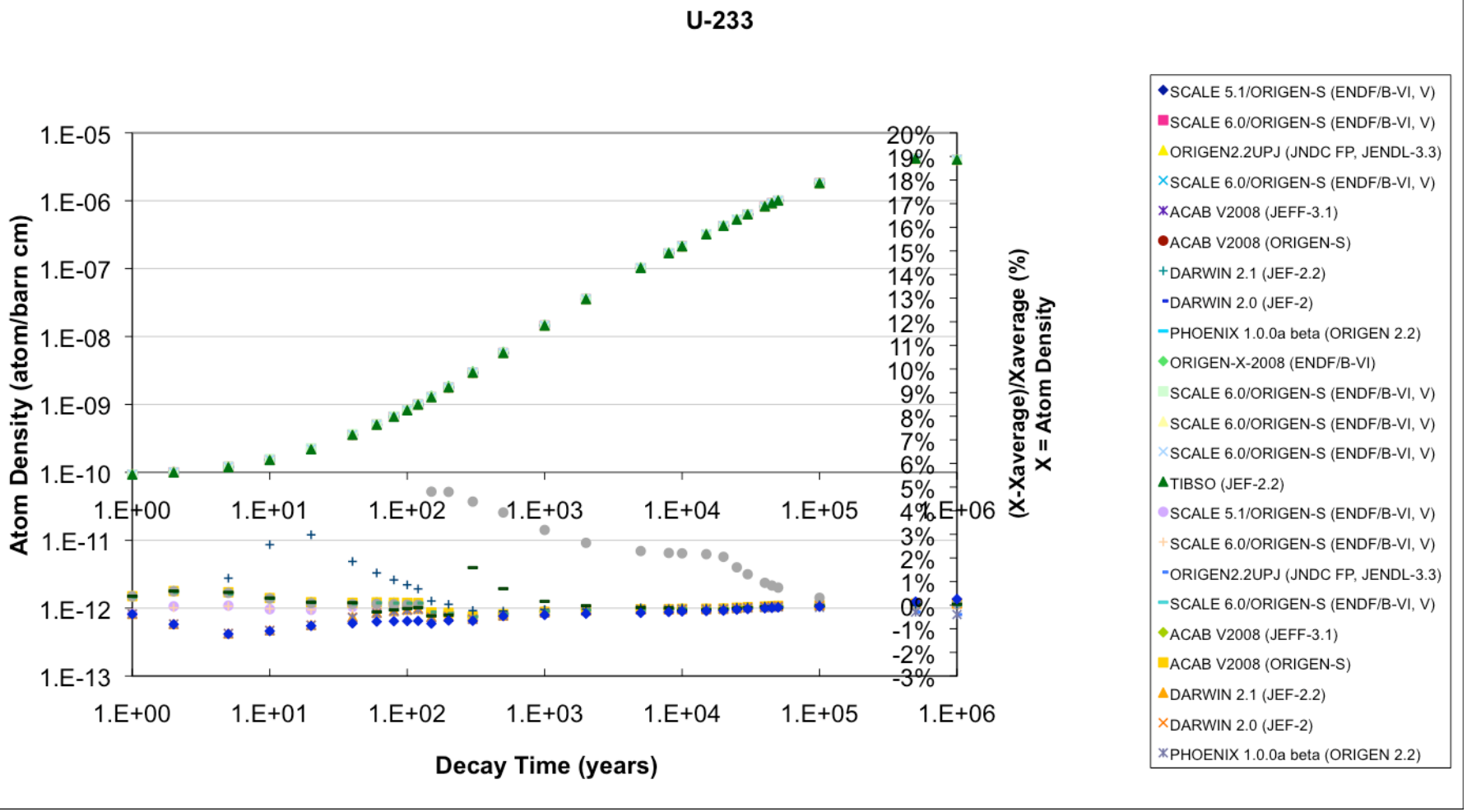
- 11 countries, 13 organizations, 14 decay calculations, 15 criticality calculations
- ORIGEN, ORIGEN-based, DARWIN, PHOENIX decay calculation codes
  - Numerical and analytical methods for solving decay chain equations
    - Matrix exponential method (ORIGEN, PHOENIX)
    - Analytical method and 4th order Runge Kutta numerical method (DARWIN, PHOENIX)
  - Decay data libraries
    - ENDF/B-V, VI
    - JENDL3.3
    - JEFF-3.1
    - JEF-2.2
- SCALE, MCNP, MORET Monte Carlo criticality codes
  - Neutron cross-section data libraries
    - ENDF/B-V, 44 energy groups
    - ENDF/B-VI continuous energy
    - ENDF/B-VII.0 continuous energy
    - ENDF/B-VII.0 238 energy groups
    - JEF-2.2, 172 energy groups
    - JENDL3.3 continuous energy
    - JEFF-3.1 continuous energy
    - JEFF-3.1.1 continuous energy

ISOTOPIC RESULTS

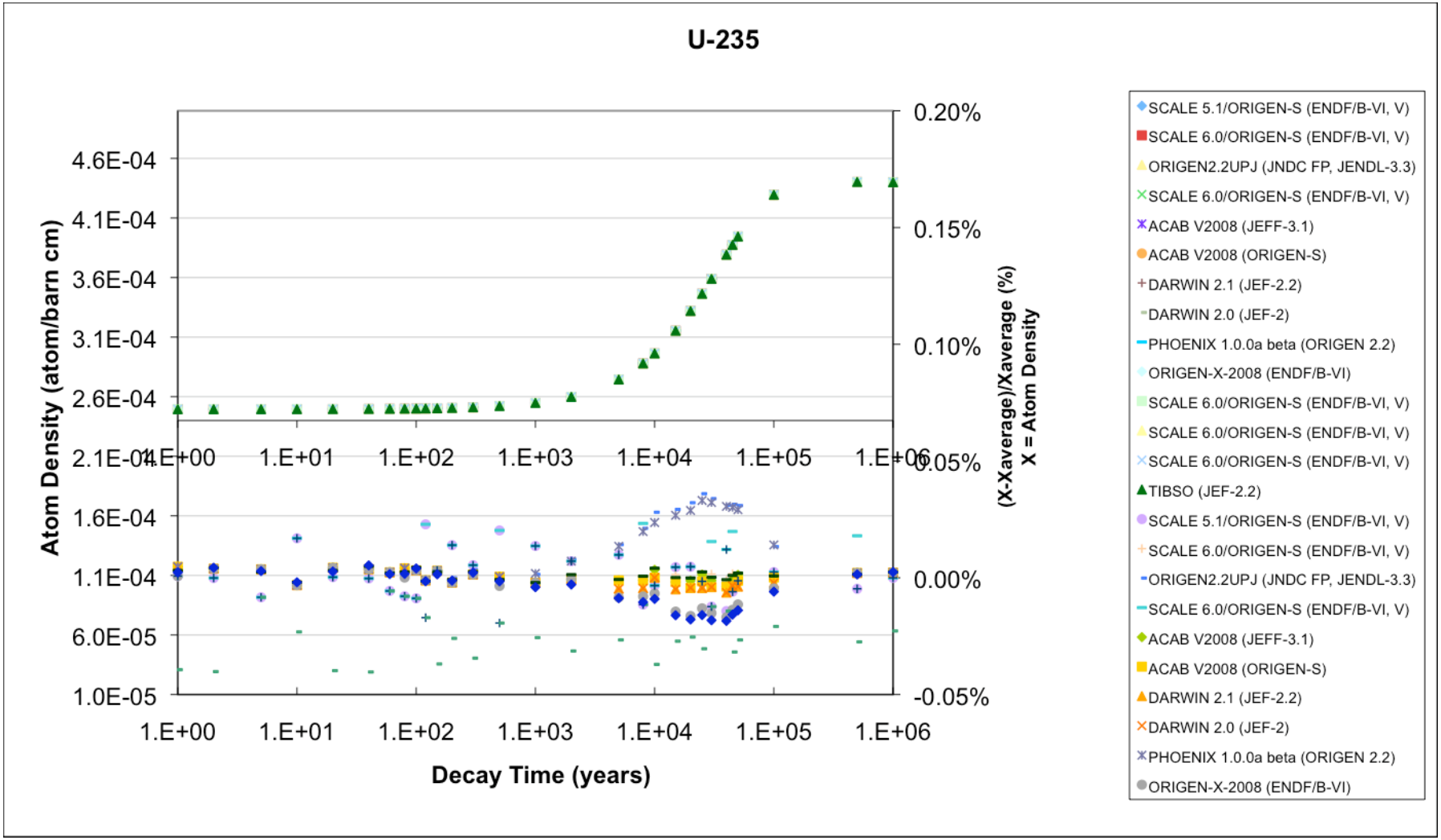
Time-dependent Actinide Concentrations



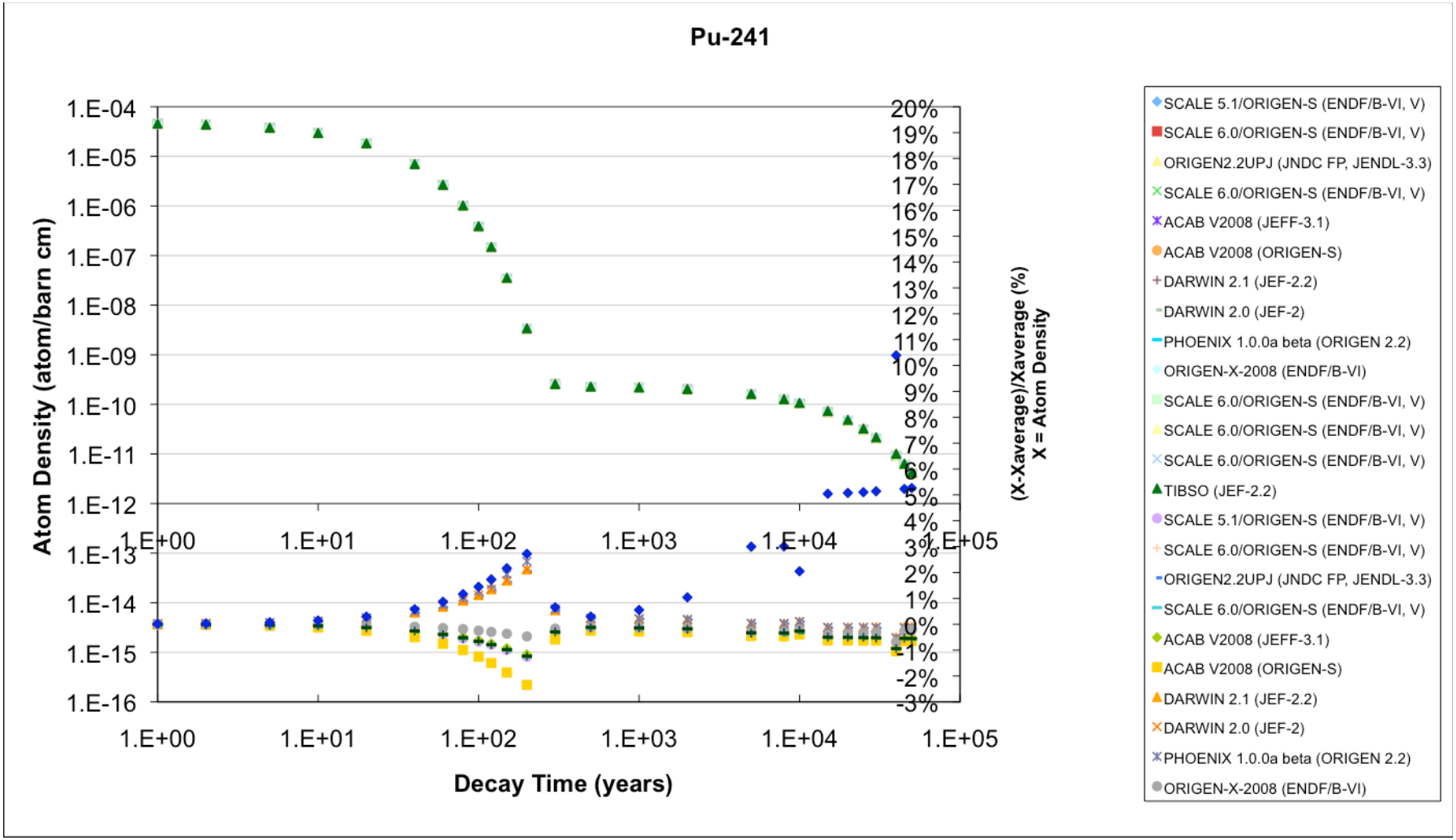
Comparison of Decay Calculation Results for U-233



Comparison of Decay Calculation Results for U-235



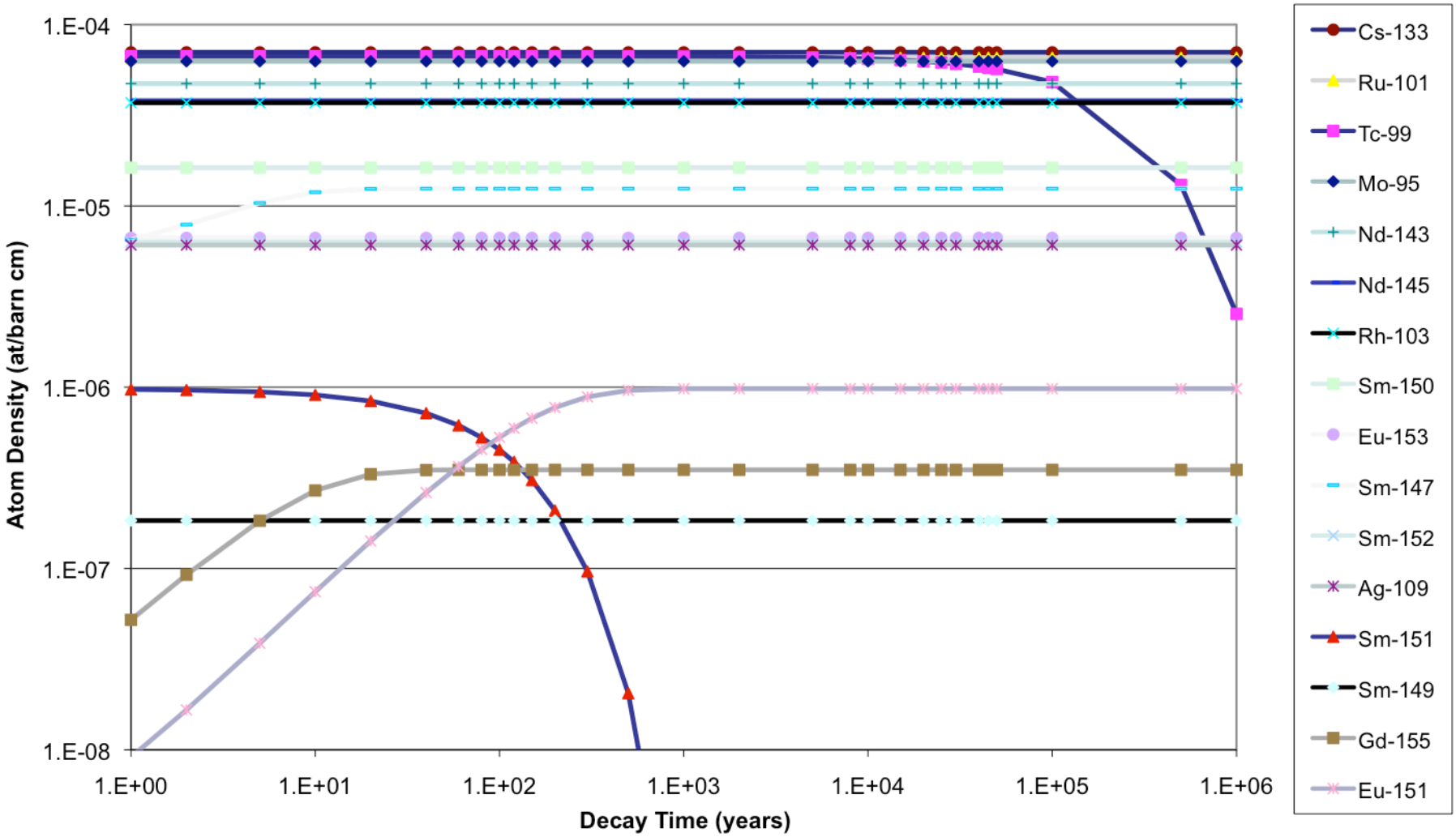
Comparison of Decay Calculation Results for Pu-241



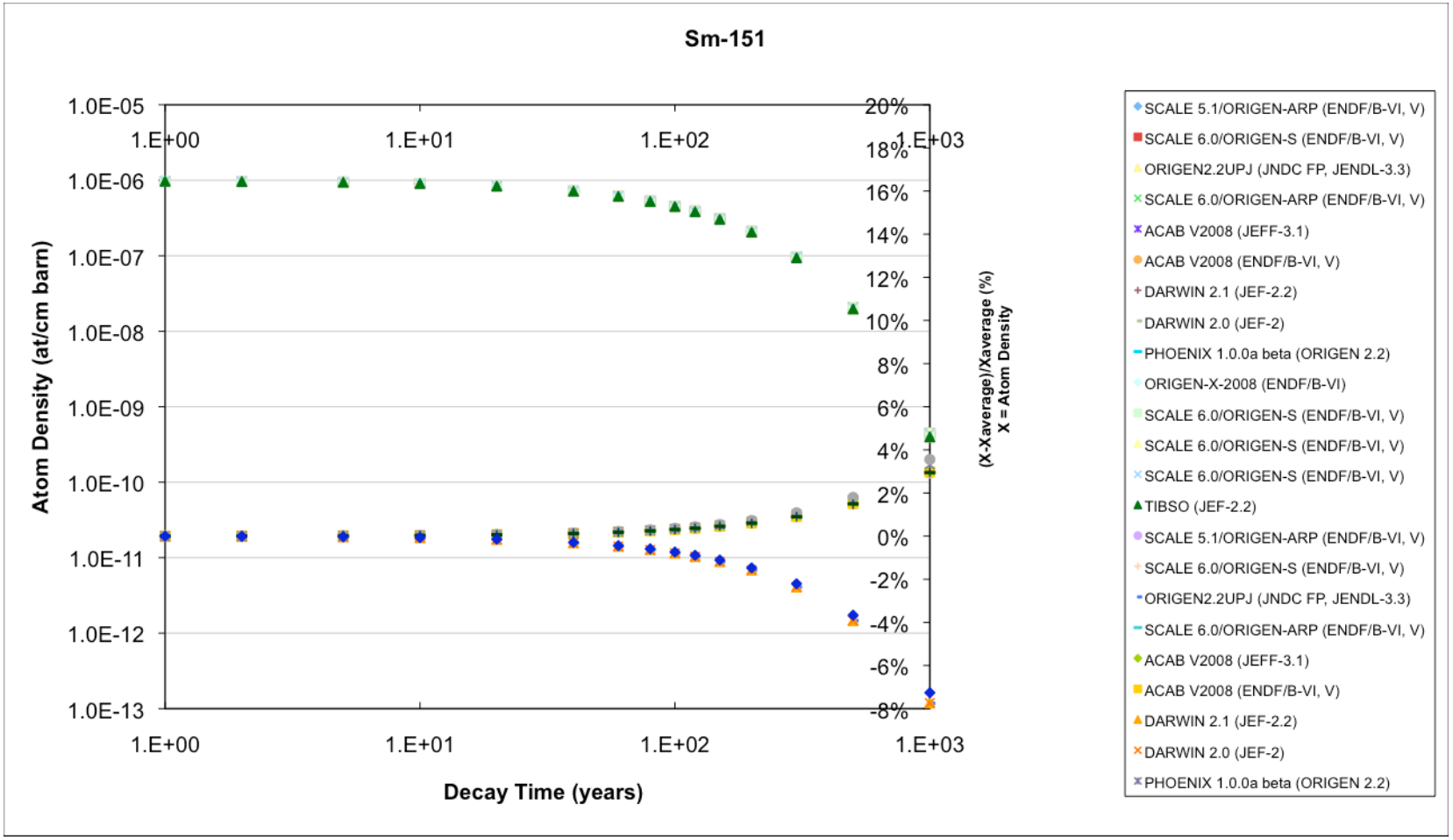
^{241}Pu (14.4y) → ^{241}Am (432.7y)

^{241}Pu result variability for the first 200 years after fuel discharge indicates differences in ^{241}Pu half-life values.

Time-dependent FP Concentrations

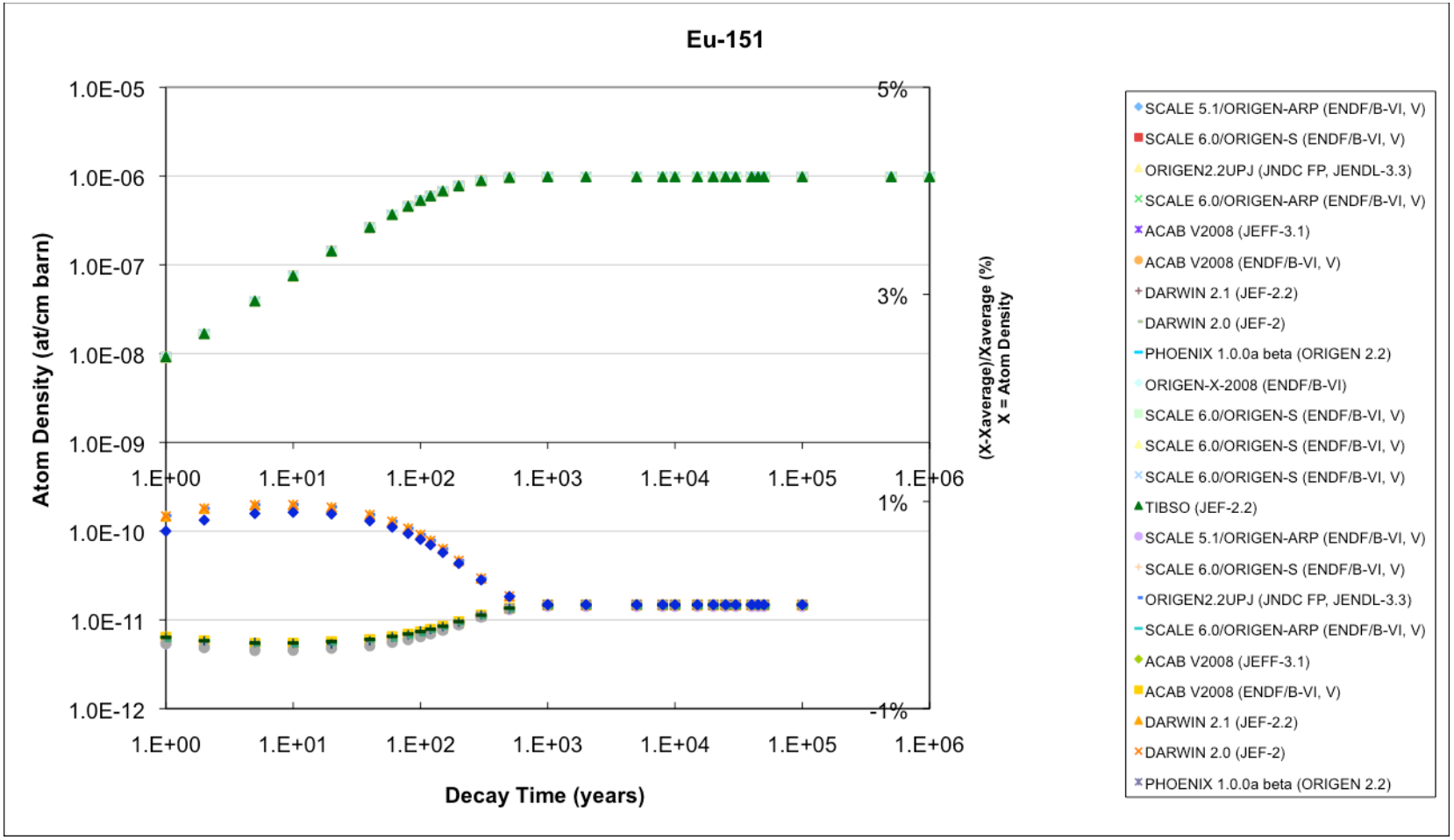


Comparison of Decay Calculation Results for Sm-151



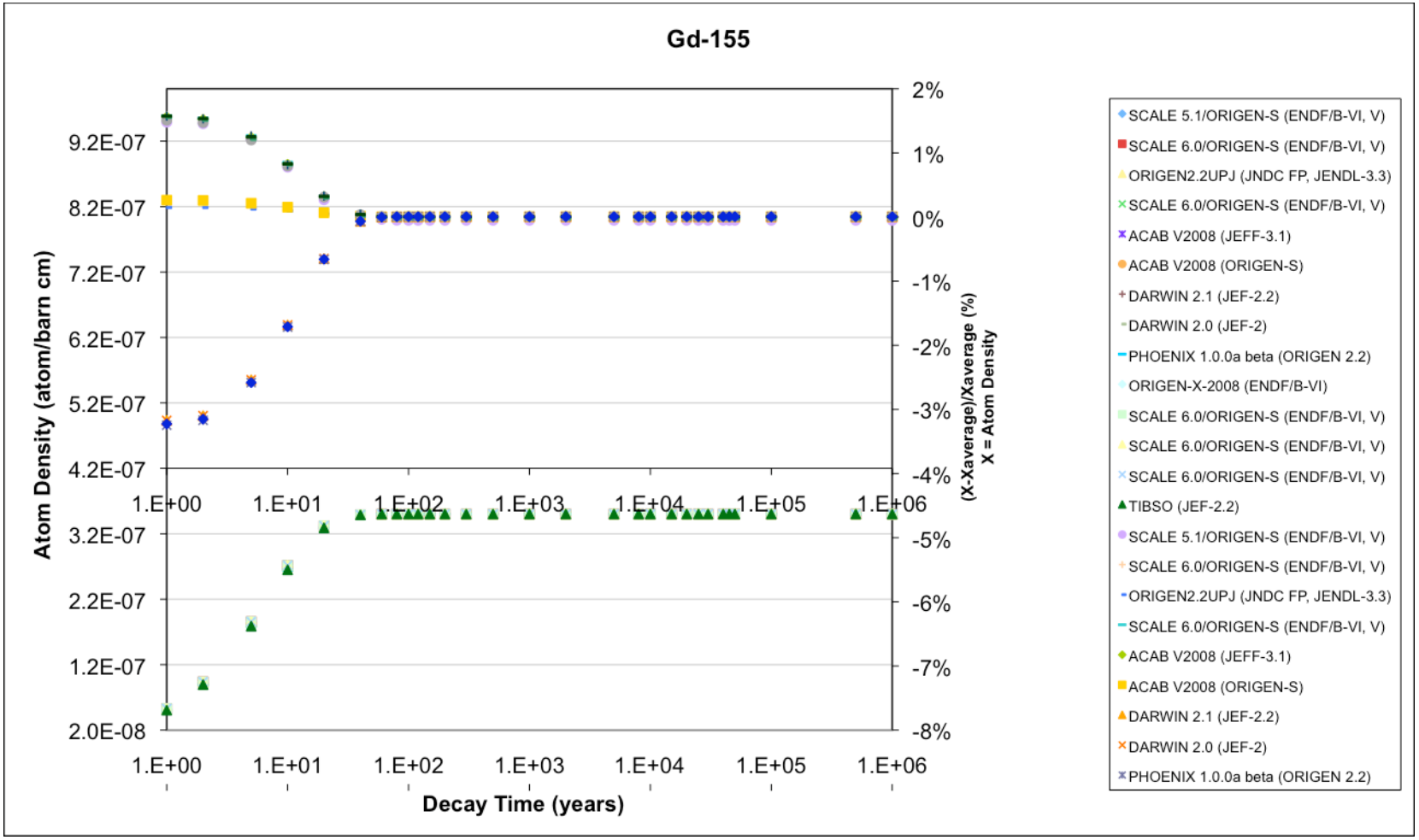
Note: Different trends between the results obtained with JEF and JENDL decay libraries (DARWIN, TIBSO, and ORIGEN2.2UPJ) and the other results.

Comparison of Decay Calculation Results for Eu-151



Note: Different trends between the results obtained with JEF and JENDL decay libraries (DARWIN, TIBSO, and ORIGEN2.2UPJ) and the other results. ^{151}Sm (90y) → ^{151}Eu.

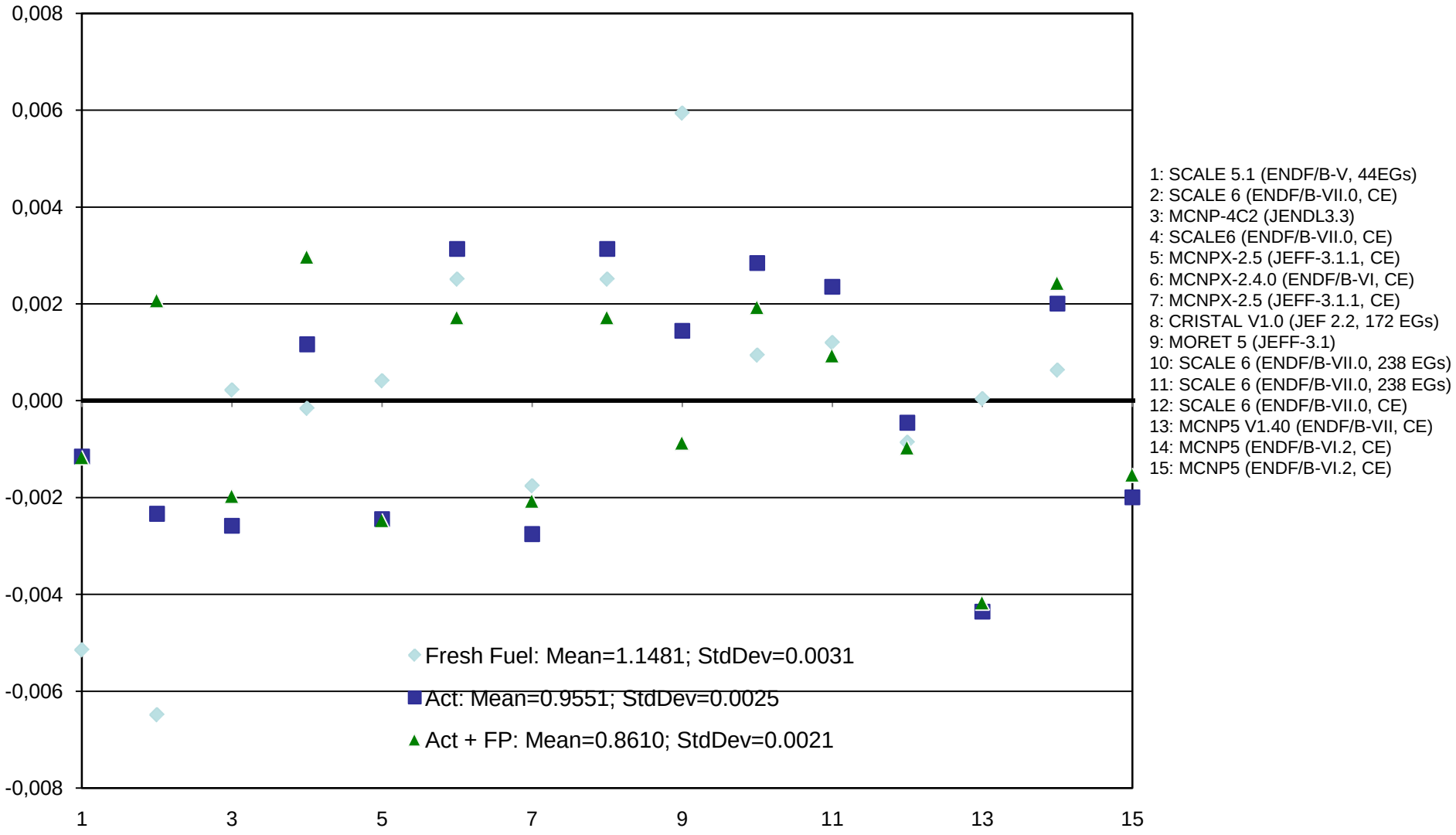
Comparison of Decay Calculation Results for Gd-155



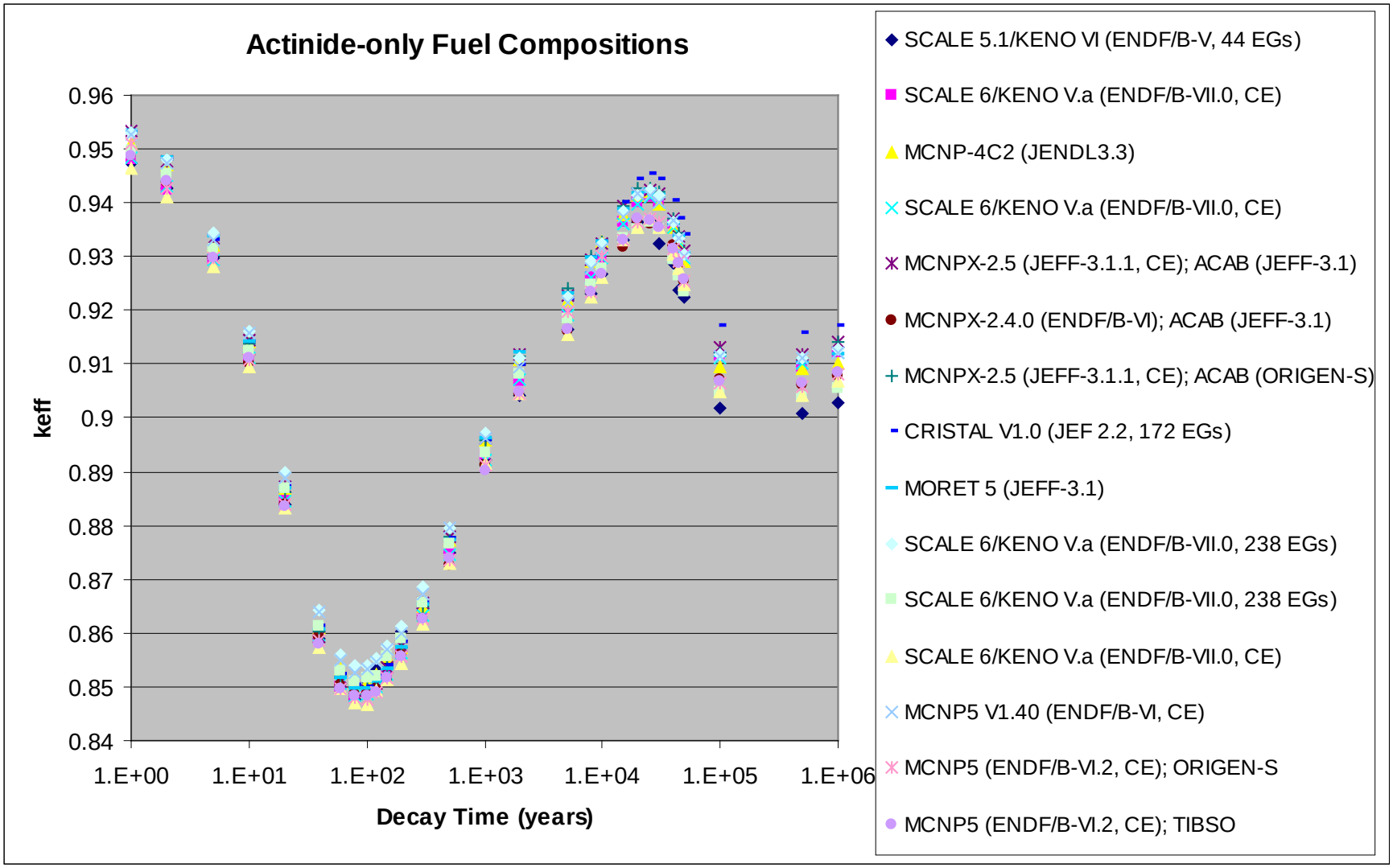
Note: DARWIN, TIBSO, and PHONIX 1.0.0a beta results are lower than the results of the other calculations for short decay times. ^{155}Eu (4.75 y) $\rightarrow$ ^{155}Gd.

CRITICALITY RESULTS

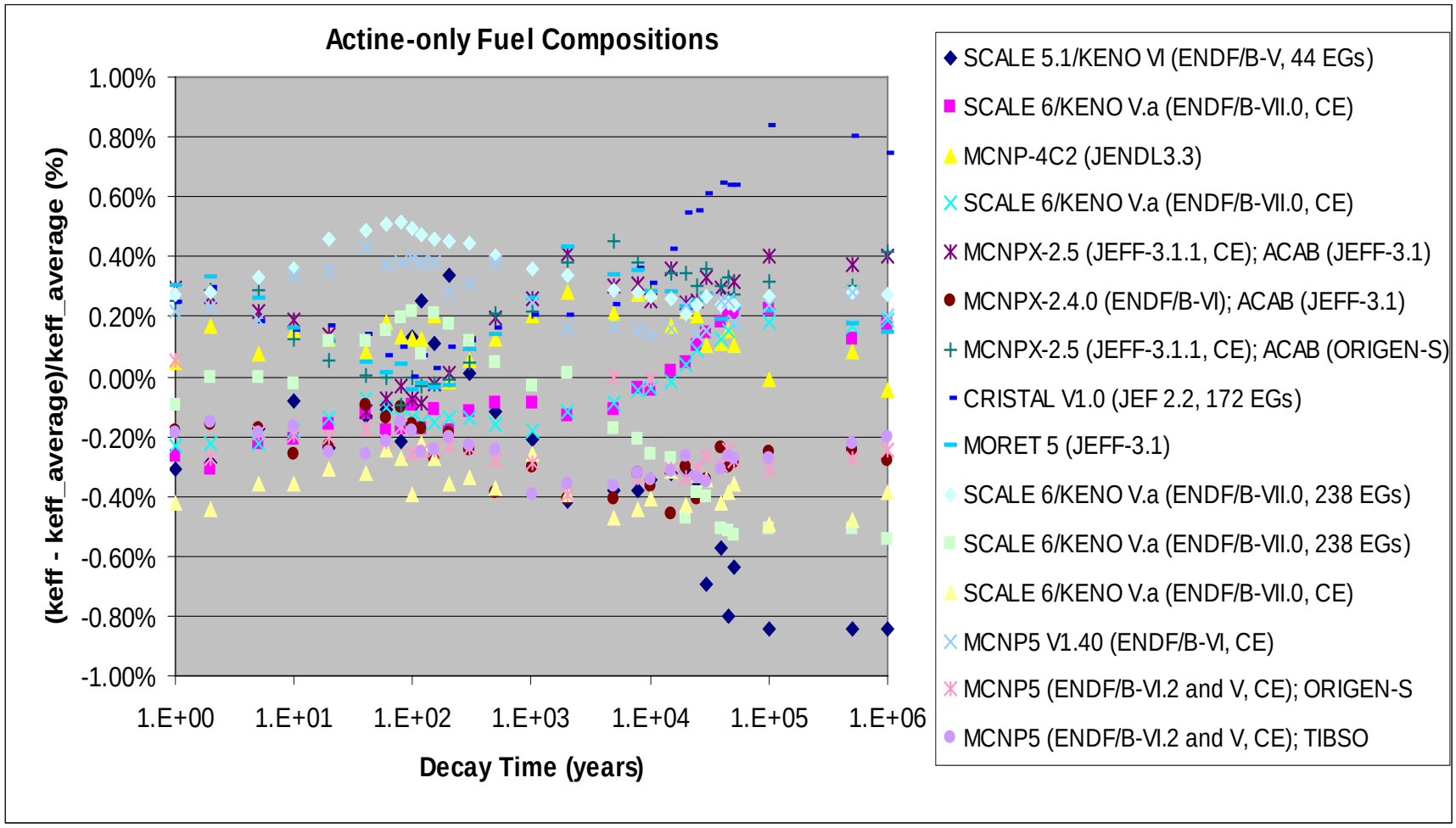
k_{eff} Values – difference from mean



k_{eff} as a Function of Decay Time for Actinide-only Fuel Compositions

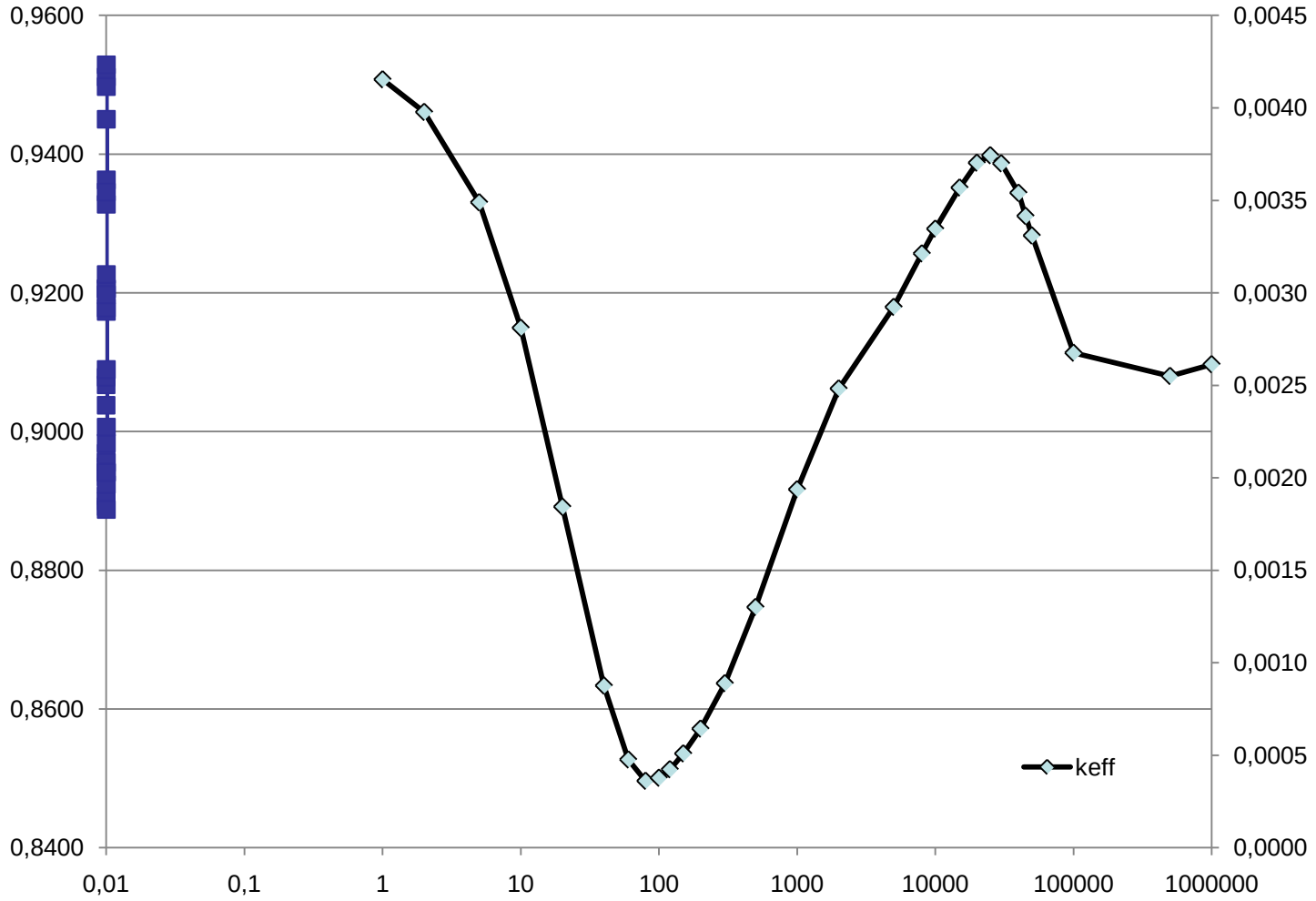


k_{eff} Result Variability as a Function of Decay Time

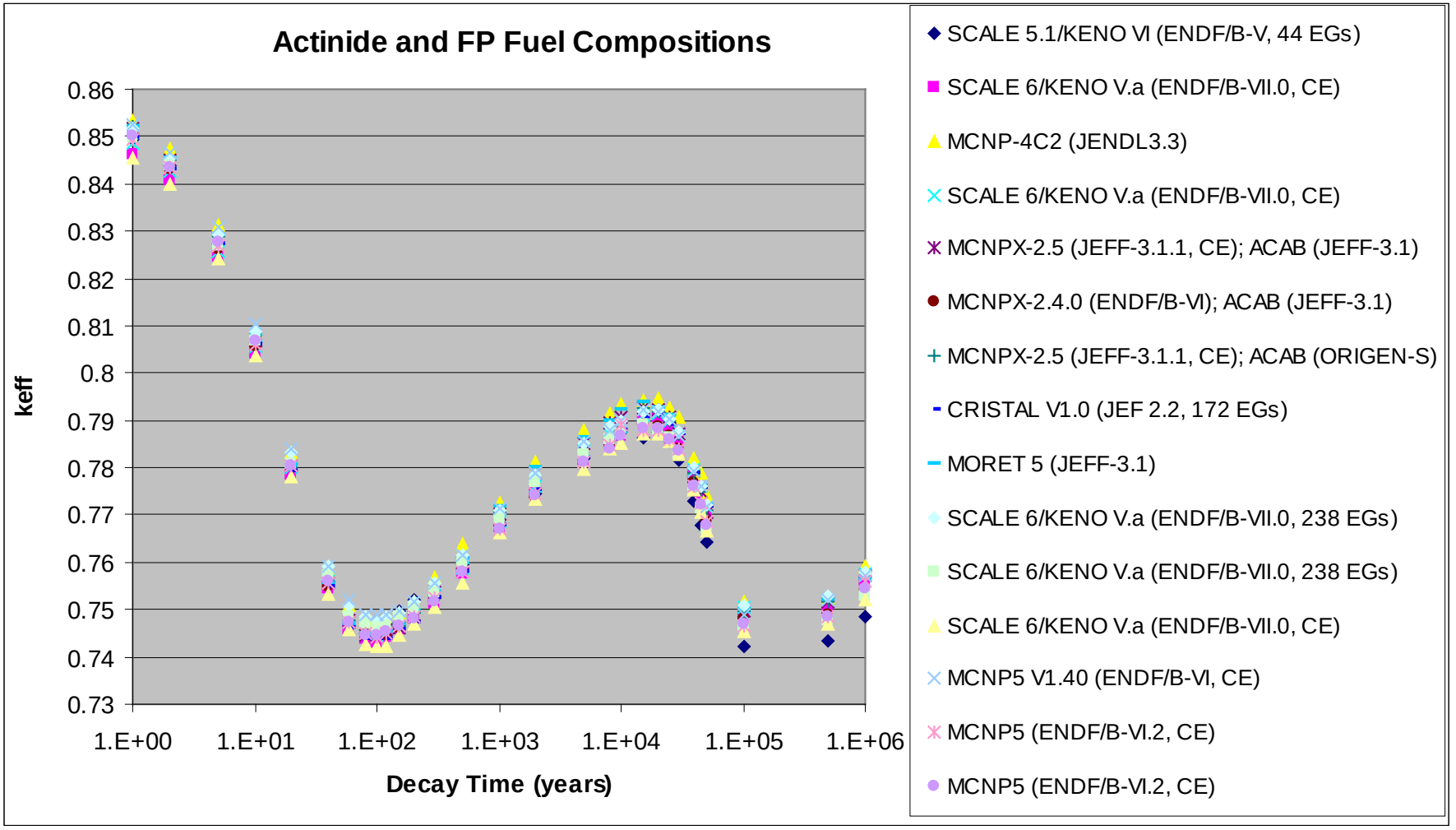


$\Delta k_{eff\text{-}min}$ = 0.0062 (150 years)
$\Delta k_{eff\text{-}max}$ = 0.0153 (1,000,000 years)

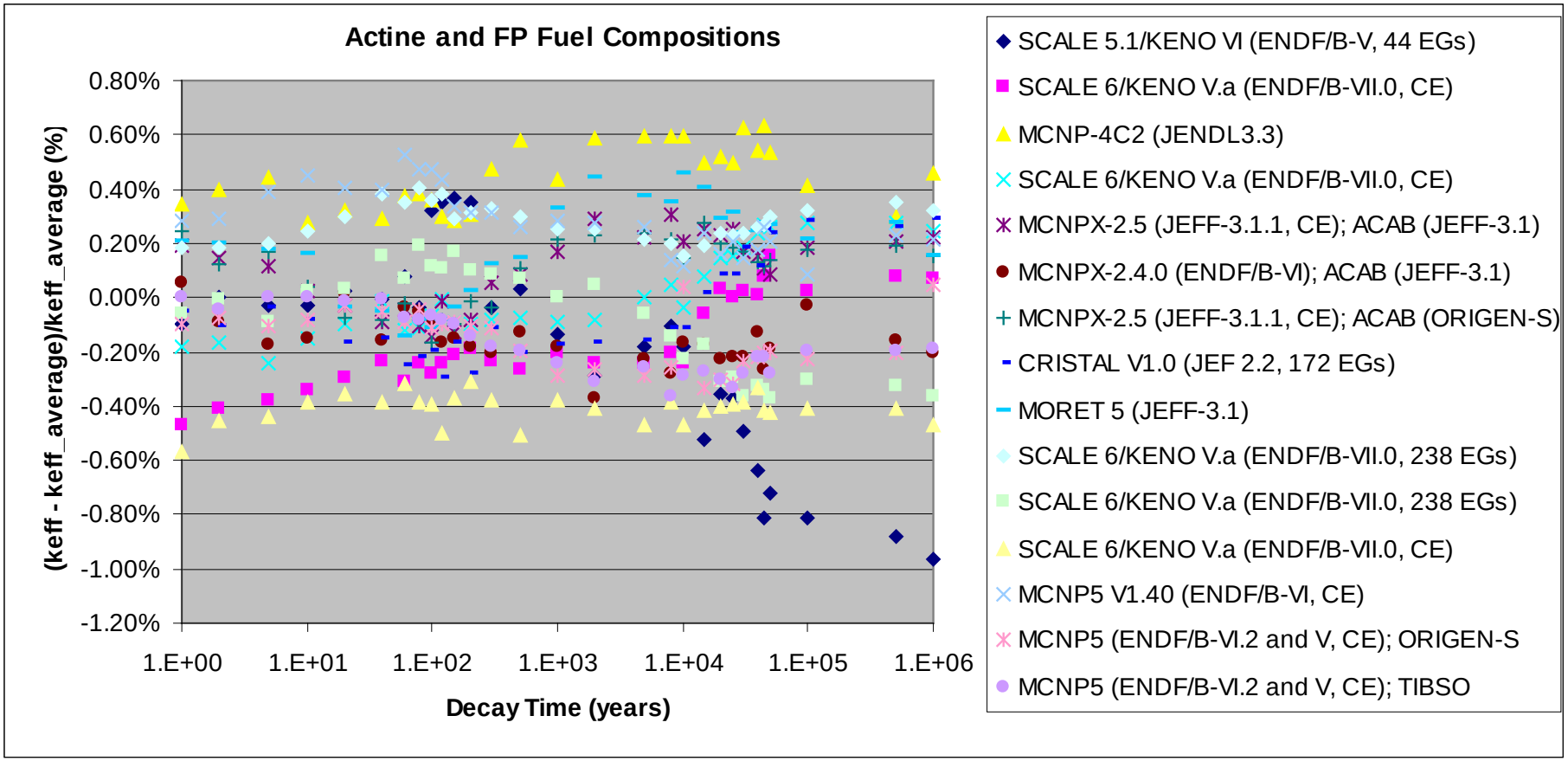
Actinide-only k_{eff} Values – Mean and Standard Deviation as a Function of Decay Time



k_{eff} as a Function of Decay Time for Actinide and FP Fuel Compositions



k_{eff} Result Variability as a Function of Decay Time



$\Delta k_{eff\text{-}min}$ = 0.0059 (20 and 40 years)
$\Delta k_{eff\text{-}max}$ = 0.0112 (45,000 years)

Cross-section Data Sensitivity and Uncertainty Analysis

ENDF/B-VII Neutron Cross-Section Data Actinide and Fission Product Compositions

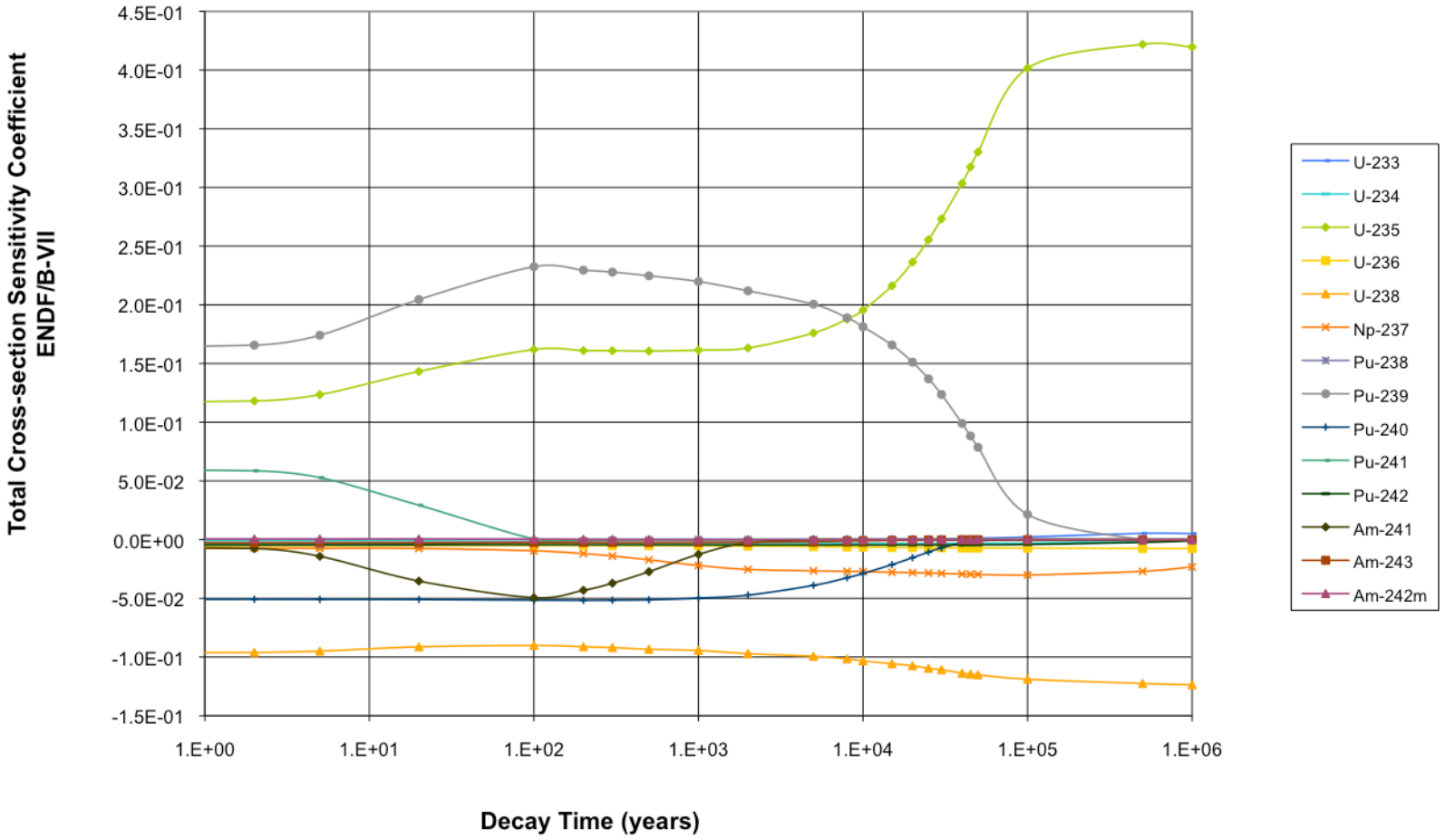
SCALE/TSUNAMI Cross-section Sensitivity and Uncertainty Analysis

- SCALE ENDF/B-VII 238 energy-group library
- Covariance data from ENDF/B-VII, ENDF/B-VI and JENDL3.3
- Energy and region integrated k_{eff} sensitivity to total and reaction-specific cross section (sensitivity coefficient)

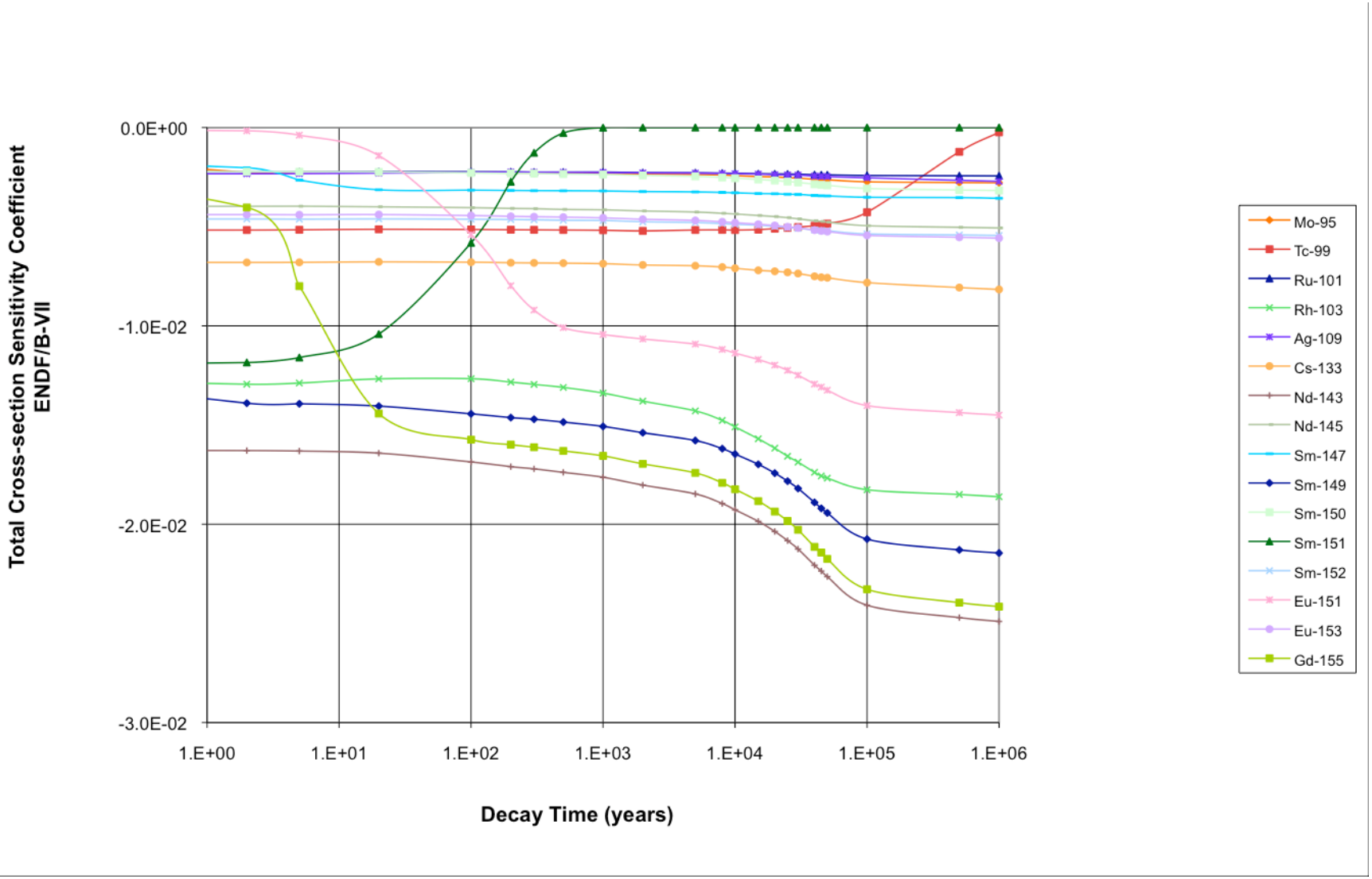
$$S_{k,\Sigma_x^n} = \frac{\delta k_{eff} / k_{eff}}{\delta \Sigma_x^n / \Sigma_x^n}$$

- k_{eff} uncertainty due to cross-section covariance data

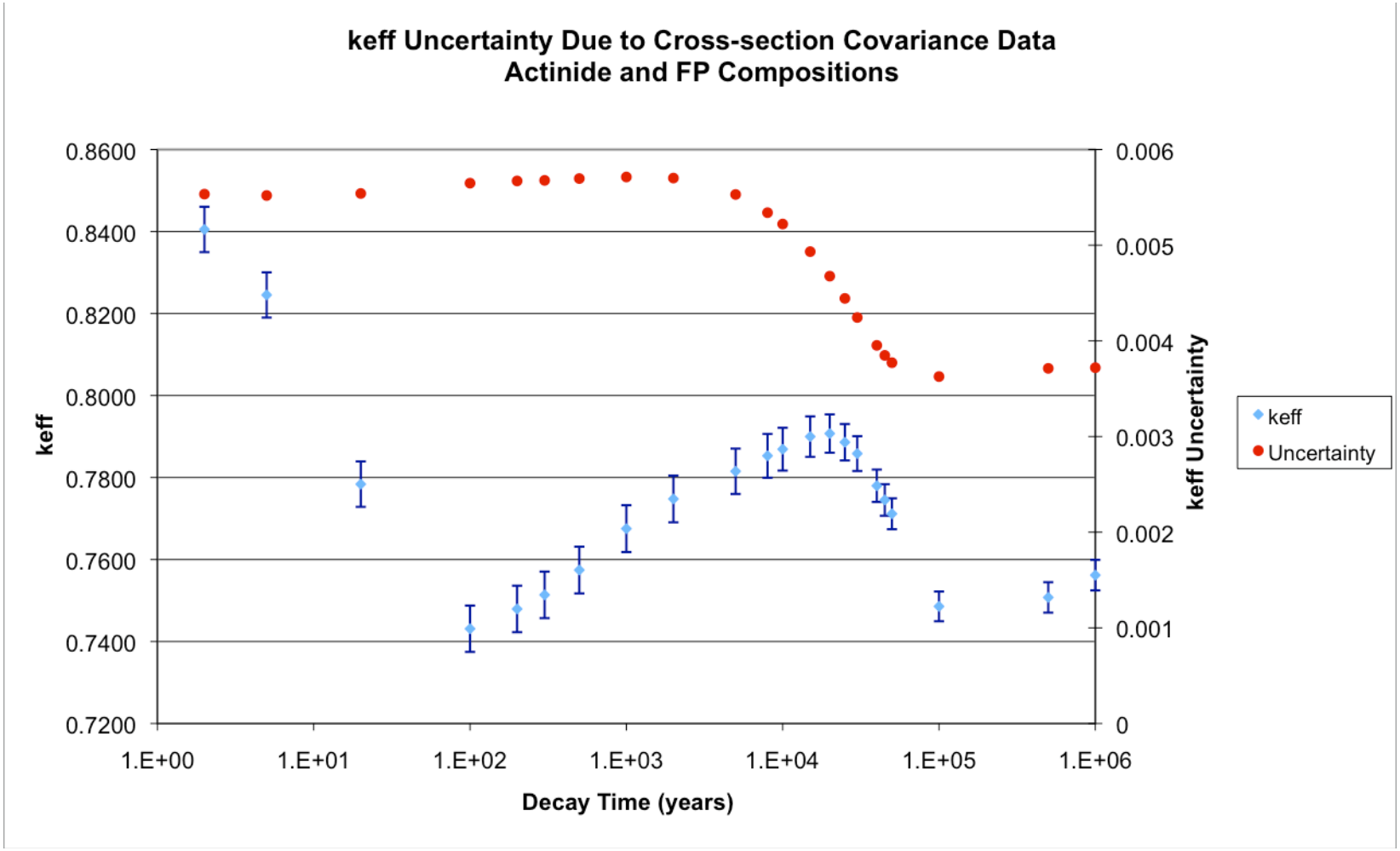
k_{eff} Sensitivity to ENDF/B-VII Cross-section Data for Actinides



k_{eff} Sensitivity to ENDF/B-VII Cross-section Data for FPs



k_{eff} Uncertainty Due to Cross-section Covariance Data



Main Contributions to k_{eff} Uncertainty: 5-Year Composition

Uncertainty Information

The relative standard deviation of k_{eff} (% Δk/k) due to cross-section covariance data is: 0.6694 +/- 0.0002 % Δk/k

contributions to uncertainty in k_{eff} (% Δk/k) by individual energy covariance matrices:

Covariance Matrix		Contributions to Uncertainty in k_{eff} (% Δk/k)
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{239}Pu nubar	^{239}Pu nubar	5.0778E-01 ± 9.0578E-06
^{239}Pu fission	^{239}Pu fission	2.2690E-01 ± 2.4978E-05
^{238}U n,gamma	^{238}U n,gamma	2.0611E-01 ± 2.2585E-05
^{239}Pu fission	^{239}Pu n,gamma	1.5414E-01 ± 8.8179E-06
^{239}Pu n,gamma	^{239}Pu n,gamma	1.2093E-01 ± 7.9528E-06
^{235}U nubar	^{235}U nubar	8.9091E-02 ± 4.4085E-07
^{238}U nubar	^{238}U nubar	8.3732E-02 ± 7.1339E-07
^{240}Pu n,gamma	^{240}Pu n,gamma	7.7584E-02 ± 5.1260E-06
^{239}Pu chi	^{239}Pu chi	6.4925E-02 ± 4.5365E-06
^{241}Pu fission	^{241}Pu fission	6.2628E-02 ± 2.3493E-06
^{143}Nd n,gamma	^{143}Nd n,gamma	5.6047E-02 ± 1.9577E-06
^{235}U fission	^{235}U fission	4.9051E-02 ± 1.6340E-06
^{242}Pu n,gamma	^{242}Pu n,gamma	4.4747E-02 ± 1.8145E-05
^{235}U n,gamma	^{235}U n,gamma	4.2852E-02 ± 1.0626E-06

Main Contributions to k_{eff} Uncertainty: 100-Year Composition

Uncertainty Information

The relative standard deviation of k_{eff} (% Δk/k) due to cross-section covariance data is: 0.7601 +/- 0.0002 % Δk/k

contributions to uncertainty in k_{eff} (% Δk/k) by individual energy covariance matrices:

Covariance Matrix		Contributions to Uncertainty in k_{eff} (% Δk/k)
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{239}Pu nubar	^{239}Pu nubar	5.7439E-01 ± 8.9982E-06
^{239}Pu fission	^{239}Pu fission	2.7783E-01 ± 2.7696E-05
^{238}U n,gamma	^{238}U n,gamma	2.0852E-01 ± 1.9370E-05
^{239}Pu fission	^{239}Pu n,gamma	1.7217E-01 ± 8.8669E-06
^{241}Am n,gamma	^{241}Am n,gamma	1.3039E-01 ± 1.1399E-05
^{239}Pu n,gamma	^{239}Pu n,gamma	1.2333E-01 ± 6.9922E-06
^{235}U nubar	^{235}U nubar	1.0226E-01 ± 4.5073E-07
^{238}U nubar	^{238}U nubar	9.3136E-02 ± 6.7540E-07
^{239}Pu chi	^{239}Pu chi	9.2804E-02 ± 5.4027E-06
^{240}Pu n,gamma	^{240}Pu n,gamma	7.9816E-02 ± 4.5176E-06
^{235}U fission	^{235}U fission	6.1910E-02 ± 1.8832E-06
^{143}Nd n,gamma	^{143}Nd n,gamma	5.7248E-02 ± 1.7462E-06
^{238}U n,n'	^{238}U n,n'	5.5646E-02 ± 1.8255E-04
^{235}U fission	^{235}U n,gamma	4.5423E-02 ± 7.6296E-07

Main Contributions to k_{eff} Uncertainty: 100,000-Year Composition

Uncertainty Information

The relative standard deviation of k_{eff} (% Δk/k) due to cross-section covariance data is: 0.4845 +/- 0.0003

contributions to uncertainty in k_{eff} (% Δk/k) by individual energy covariance matrices:

Covariance Matrix		Contributions to Uncertainty in k_{eff} (% Δk/k)
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U nubar	^{235}U nubar	2.5578E-01 ± 5.3053E-06
^{238}U n,gamma	^{238}U n,gamma	2.5539E-01 ± 3.7912E-05
^{235}U fission	^{235}U fission	1.5704E-01 ± 1.7943E-05
^{235}U fission	^{235}U n,gamma	1.1388E-01 ± 7.2070E-06
^{235}U n,gamma	^{235}U n,gamma	1.0610E-01 ± 9.0925E-06
^{235}U chi	^{235}U chi	9.1964E-02 ± 1.0218E-05
^{237}Np n,gamma	^{237}Np n,gamma	9.0969E-02 ± 9.0453E-06
^{238}U nubar	^{238}U nubar	9.0863E-02 ± 1.1547E-06
^{143}Nd n,gamma	^{143}Nd n,gamma	7.7838E-02 ± 4.7132E-06
^{239}Pu nubar	^{239}Pu nubar	5.0292E-02 ± 1.2969E-07
^{103}Rh n,gamma	^{103}Rh n,gamma	4.6700E-02 ± 1.0876E-05
^{1}H n,gamma	^{1}H n,gamma	4.2308E-02 ± 1.1226E-06
^{238}U n,n'	^{238}U n,n'	4.2102E-02 ± 2.2373E-04
^{242}Pu n,gamma	^{242}Pu n,gamma	4.1249E-02 ± 1.8701E-05

Summary Remarks / Observations

Summary: Participation

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    - JEFF-3.1 continuous energy
    - JEFF-3.1.1 continuous energy

Preliminary Observations: Decay Calculations

- Several different trends identified
  - Different trends between the results obtained with JENDL and ORIGEN2 DECAY.LIB data libraries (ORIGEN2.2UPJ and PHOENIX 1.0.0a) and the other results for
    - ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{242m}Am
  - Different trends among the results obtained with different libraries for
    - ^{241}Pu, ^{243}Am
  - Different trends between the results obtained with JEF and JENDL decay data libraries (DARWIN, TIBSO, and ORIGEN2.2UPJ) and the other results for
    - ^{151}Sm, ^{151}Eu
  - Different trends between the results obtained with JEF and ORIGEN2 DECAY.LIB data libraries (DARWIN, TIBSO, and PHOENIX 1.0.0a) and the other results for
    - ^{155}Gd (^{155}Eu)

Preliminary Observations: Criticality Calculations

- k_{eff} calculations were performed using a variety of criticality codes and cross-section data

- Results for specified compositions provide insights into variations due to criticality code and cross-section data
  - Fresh fuel composition
    - k_{eff} varied from 1.1429 ± 0.0008 (SCALE 5.1, ENDF/B-V 44 EGs) to 1.1540 ± 0.0003 (CRISTAL V1.0, JEF-2.2, 172 EGs)
  - Discharge actinide-only fuel composition
    - k_{eff} varied from 0.9507 ± 0.0004 (SCALE 6, ENDF/B-VII.0 CE) to 0.9582 ± 0.0003 (MCNPX-2.5, JEFF-3.1.1 CE)
  - Discharge actinide and FP fuel composition
    - k_{eff} varied from 0.8568 ± 0.0003 (SCALE 6, ENDF/B-VII.0 CE) to 0.8639 ± 0.0005 (MCNP-4C2, JENDL3.3 CE)

Preliminary Observations: Criticality Calculations

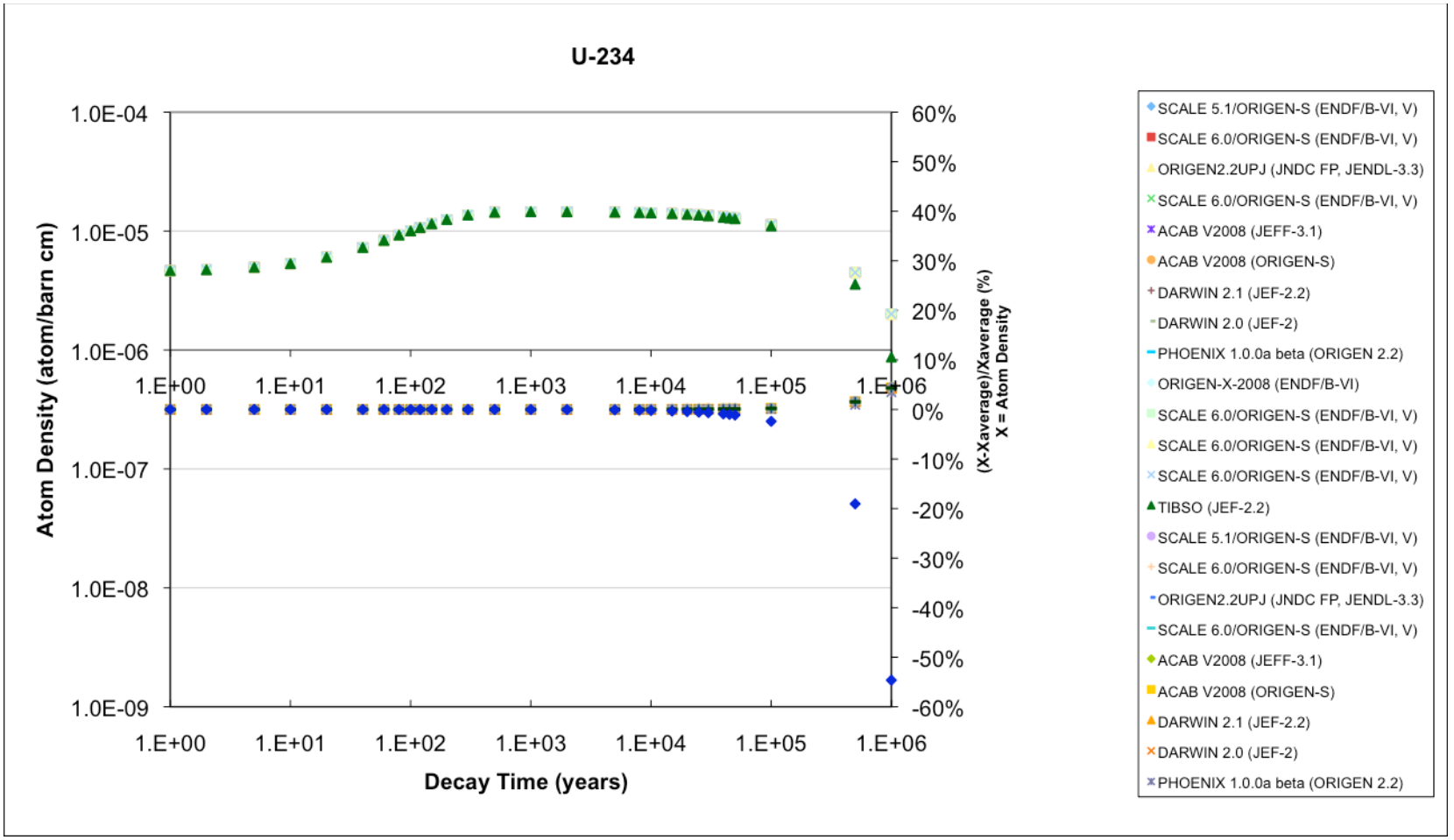
- k_{eff} results for time-dependent compositions show the impact of nuclear data, calculation method, and isotopic composition bias
- Computational method and cross-section data appear to have a larger impact on k_{eff} than differences in isotopic composition predictions
- k_{eff} results for time-dependent actinide-only compositions
  - $\Delta k_{eff\text{-}min}$ = 0.0062 (150 years)
  - $\Delta k_{eff\text{-}max}$ = 0.0153 (1,000,000 years)
- k_{eff} results for time-dependent actinide and FP compositions
  - $\Delta k_{eff\text{-}min}$ = 0.0059 (20 and 40 years)
  - $\Delta k_{eff\text{-}max}$ = 0.0112 (45,000 years)
- k_{eff} uncertainty due to covariance data
  - Min $\%\Delta k_{eff}/k_{eff}$ = 0.4845 (100,000 years)
  - Max $\%\Delta k_{eff}/k_{eff}$ = 0.7601 (100 years)

Next steps

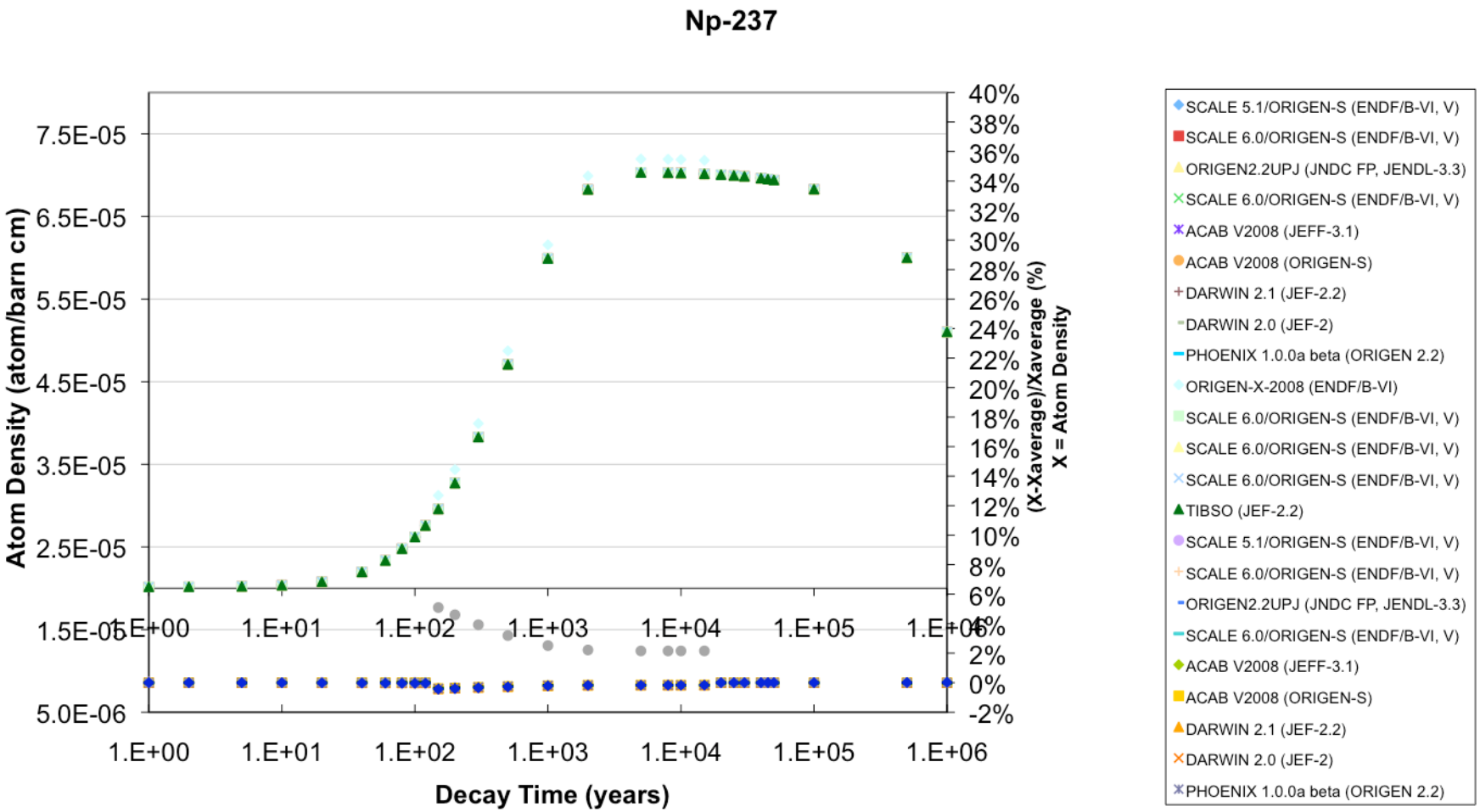
- Complete analysis of participant's results
  - Communicate with participants about their results, as needed
- Perform sensitivity calculations for isotopic predictions
- Complete and circulate draft report to participants for review
- Propose follow-up activity, if identified
- Publish benchmark report

Backup Slides

Comparison of Decay Calculation Results for U-234

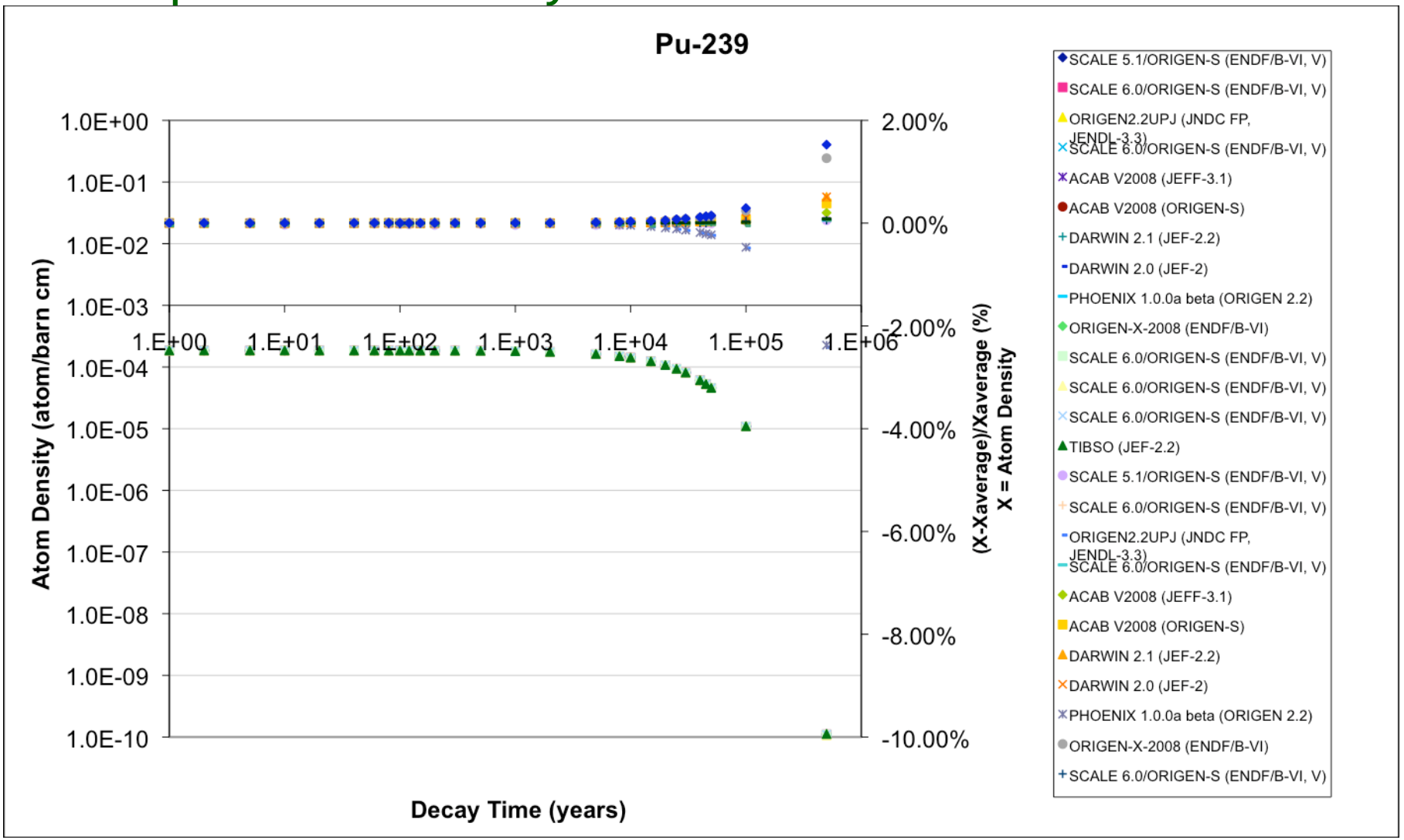


Comparison of Decay Calculation Results for Np-237

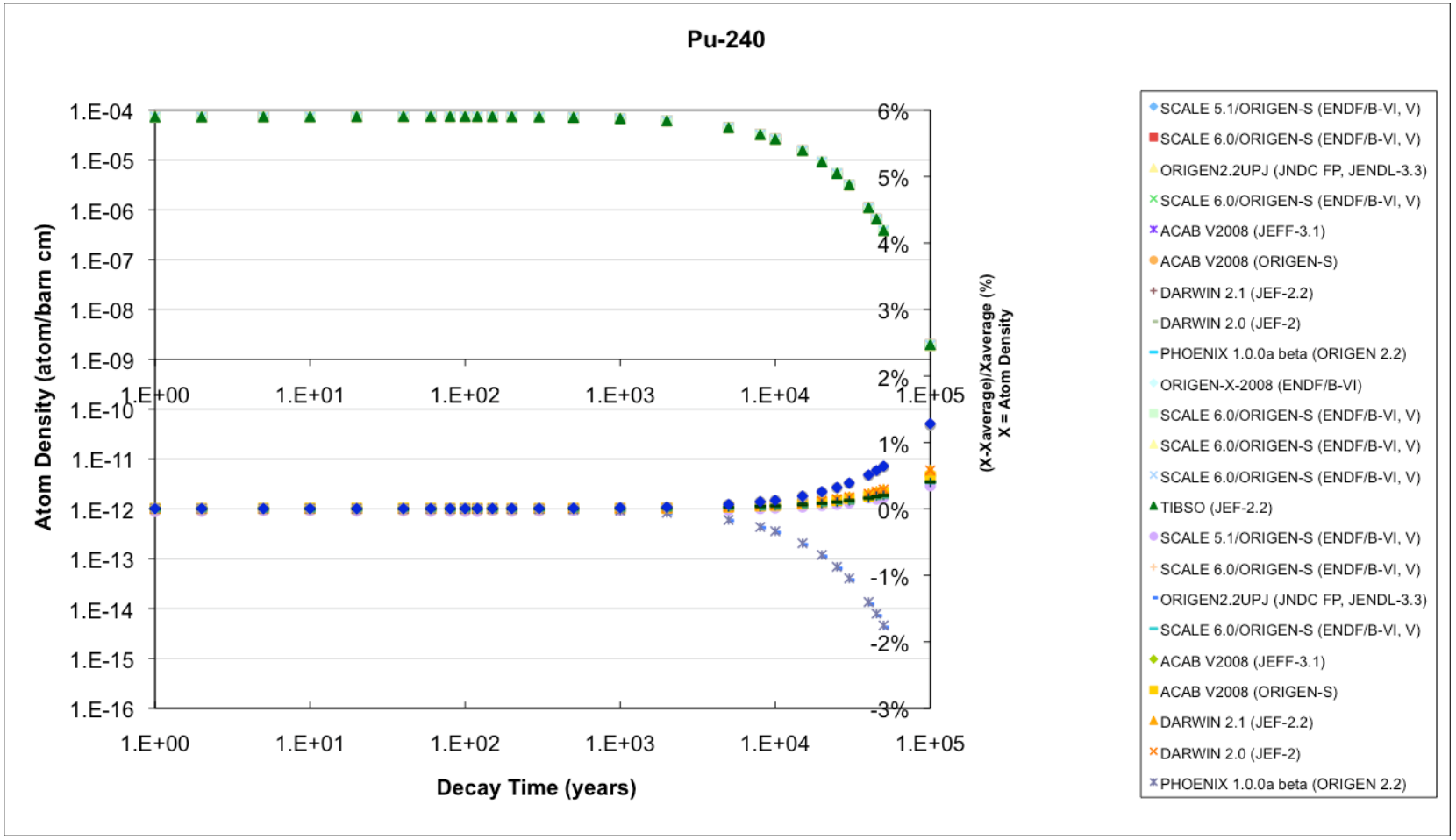


^{241}Pu (14.4y) → ^{241}Am (432.7y) → ^{237}Np (2.14E6y)

Comparison of Decay Calculation Results for Pu-239

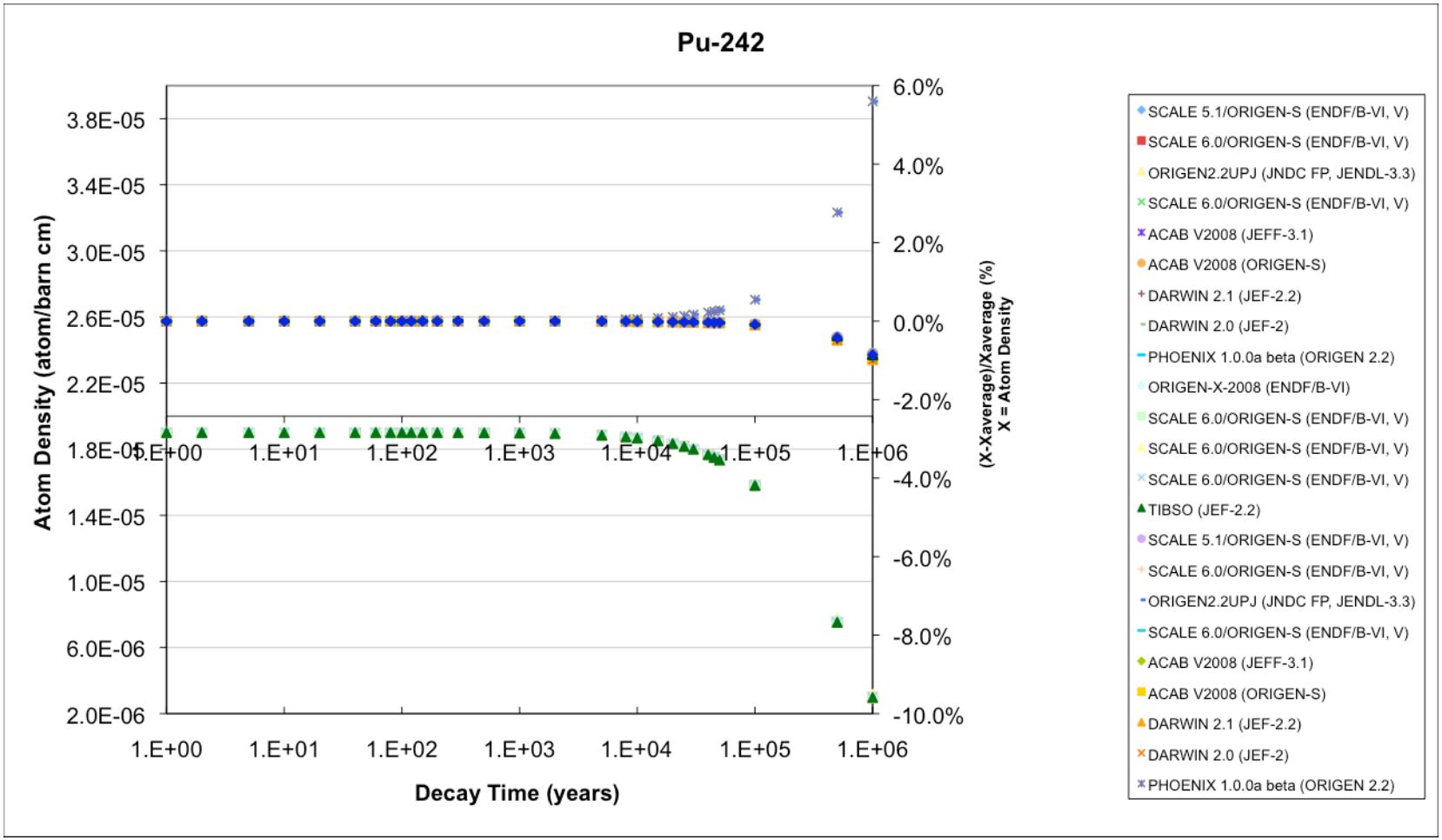


Comparison of Decay Calculation Results for Pu-240



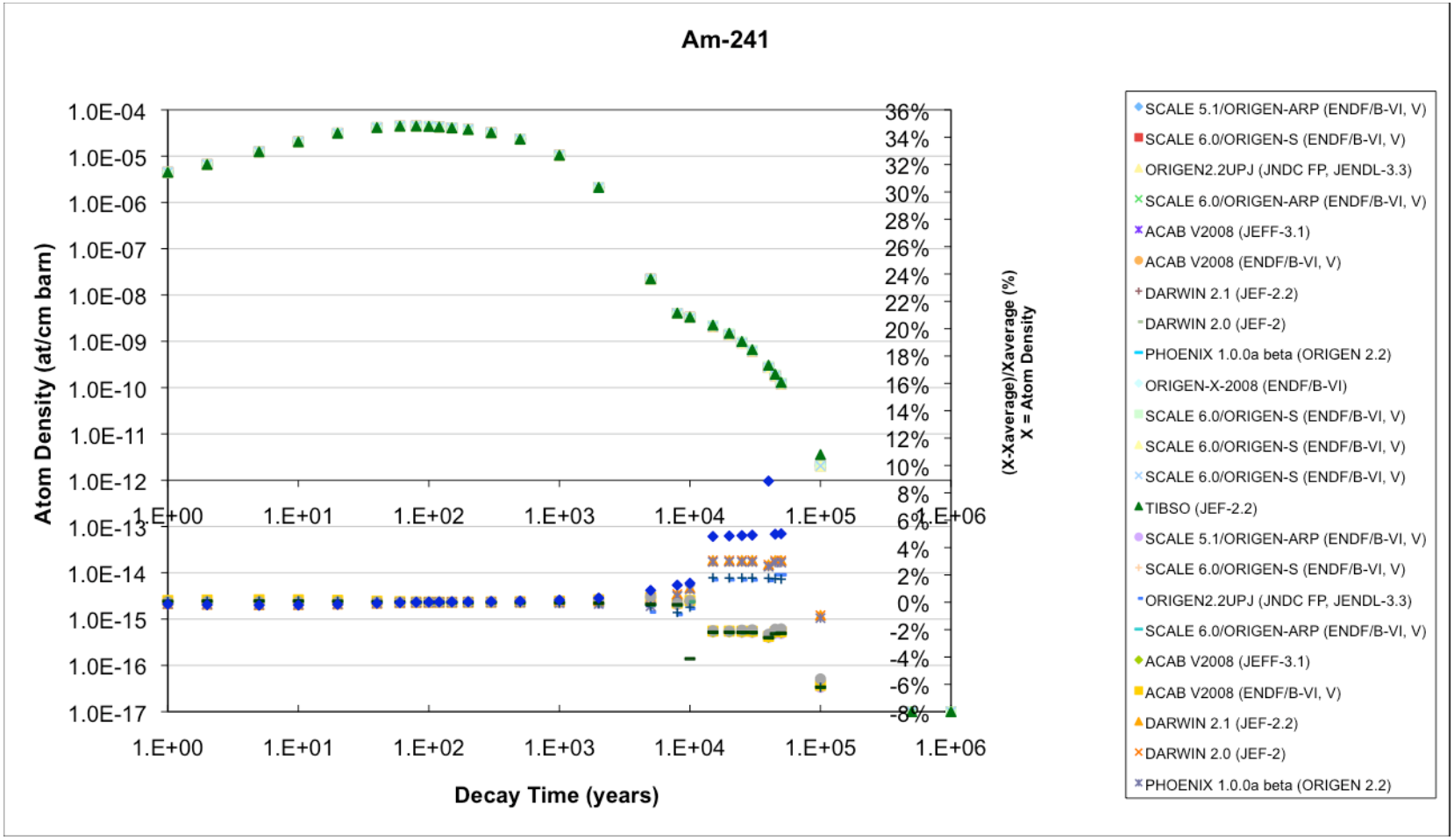
Note: Different trends between ORIGEN2.2UPJ and PHONIX 1.0.0a beta results and the results of the other calculations for long decay times.

Comparison of Decay Calculation Results for Pu-242



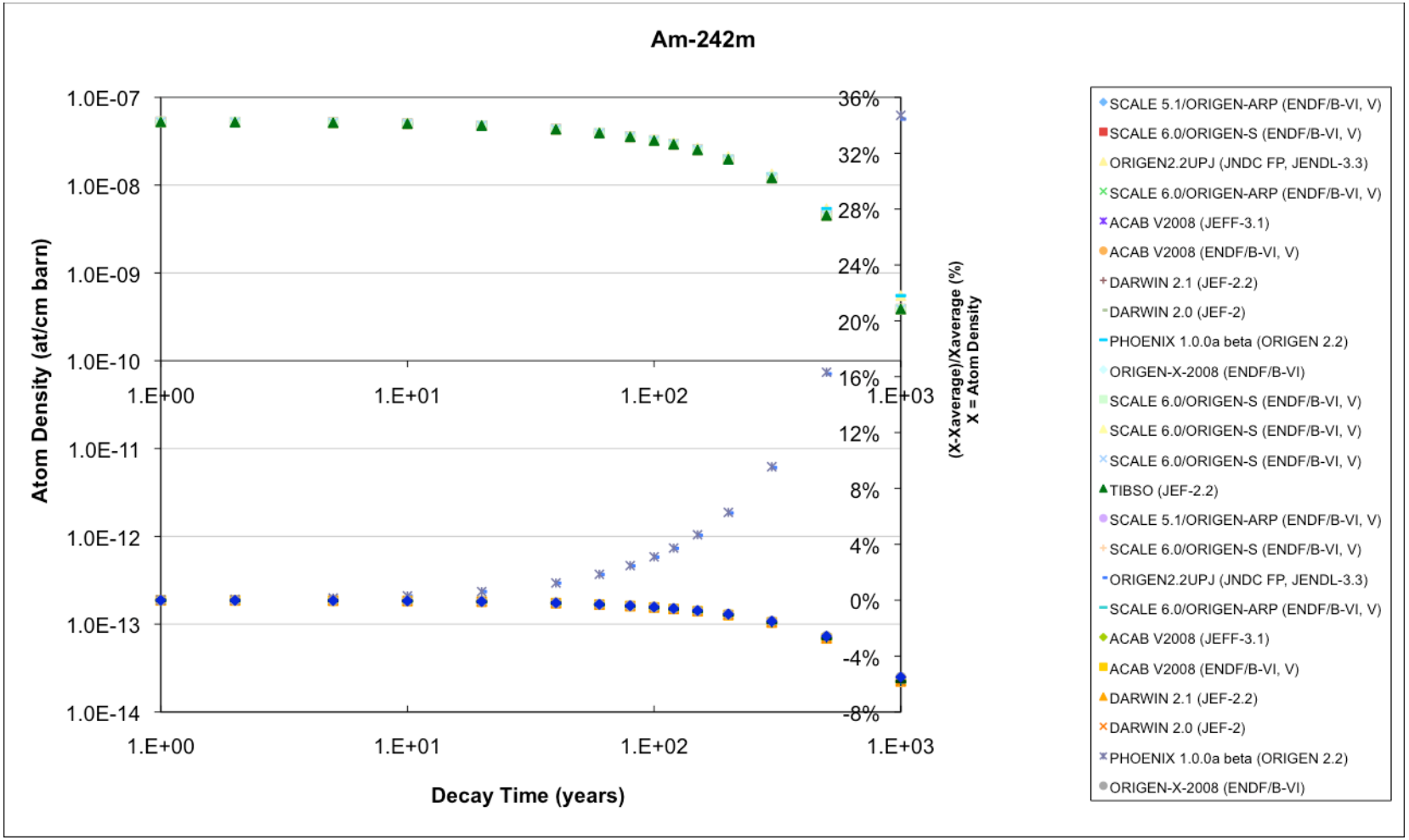
Note: Different trends between ORIGEN2.2UPJ and PHONIX 1.0.0a beta results and the results of the other calculations for long decay times.

Comparison of Decay Calculation Results for Am-241



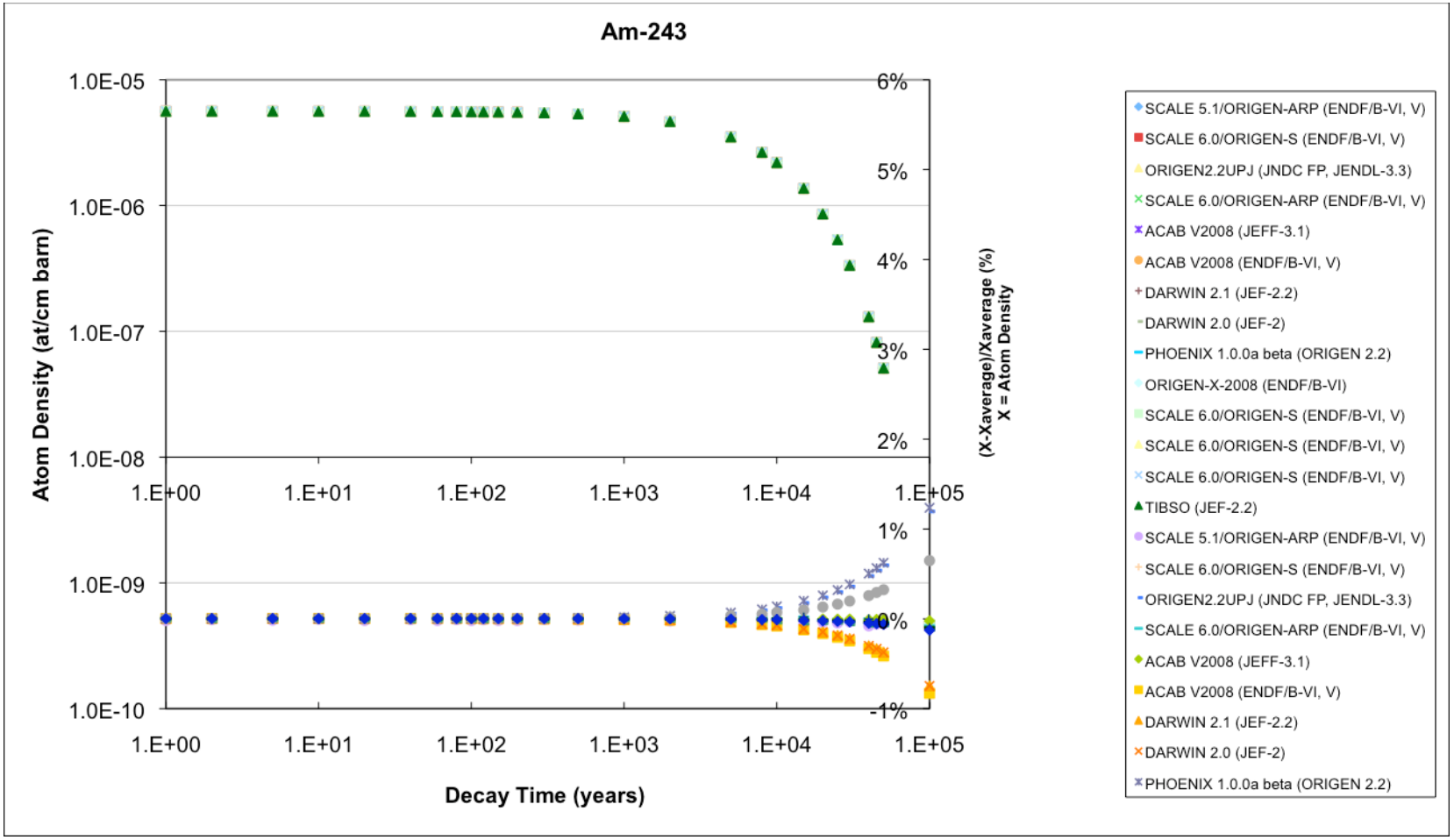
^{241}Pu (14.4y) → ^{241}Am (432.7y)

Comparison of Decay Calculation Results for Am-242m

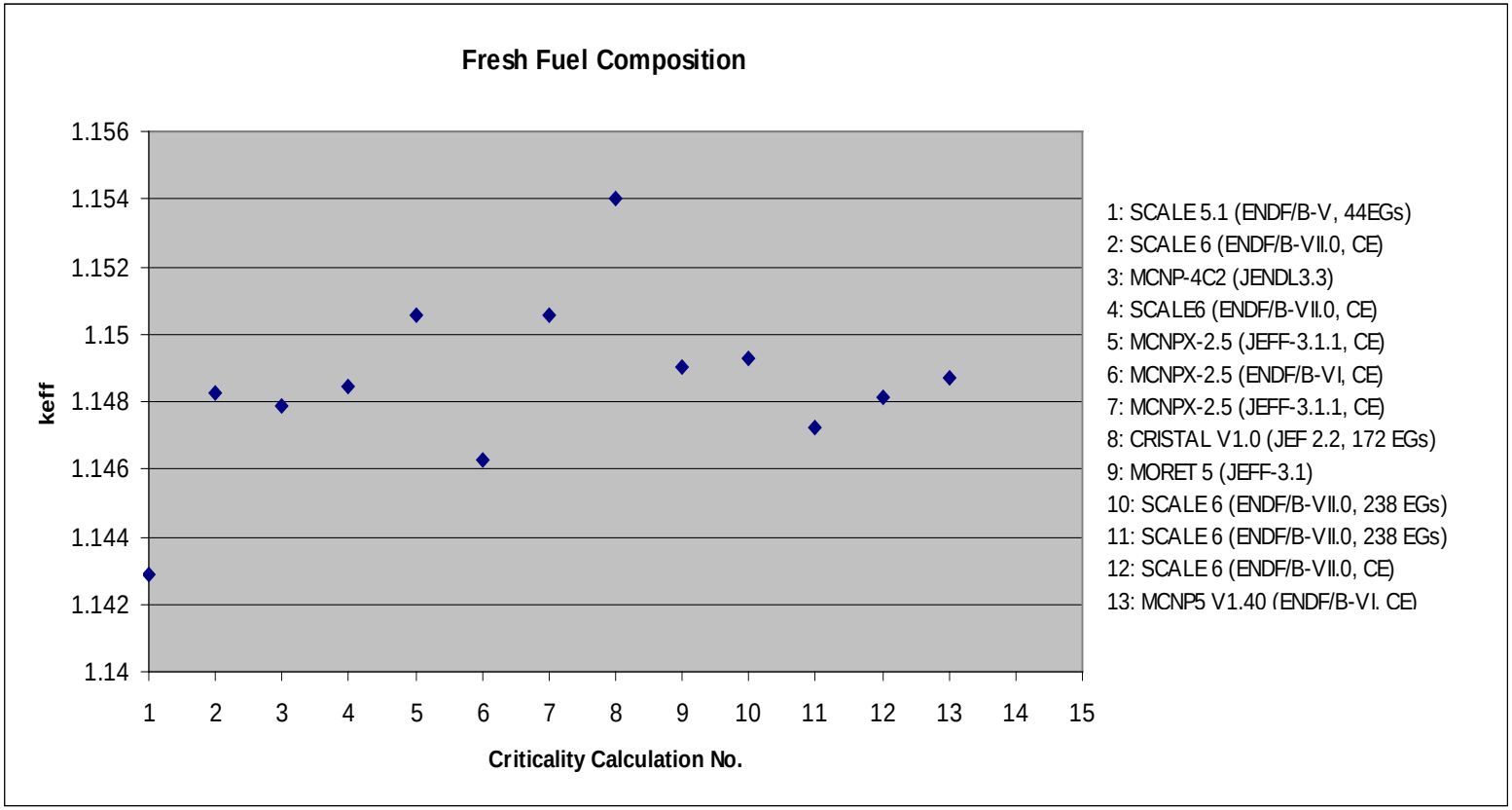


Note: Different trends between ORIGEN2.2UPJ and PHONIX 1.0.0a beta results and the results of the other calculations for long decay times.

Comparison of Decay Calculation Results for Am-243

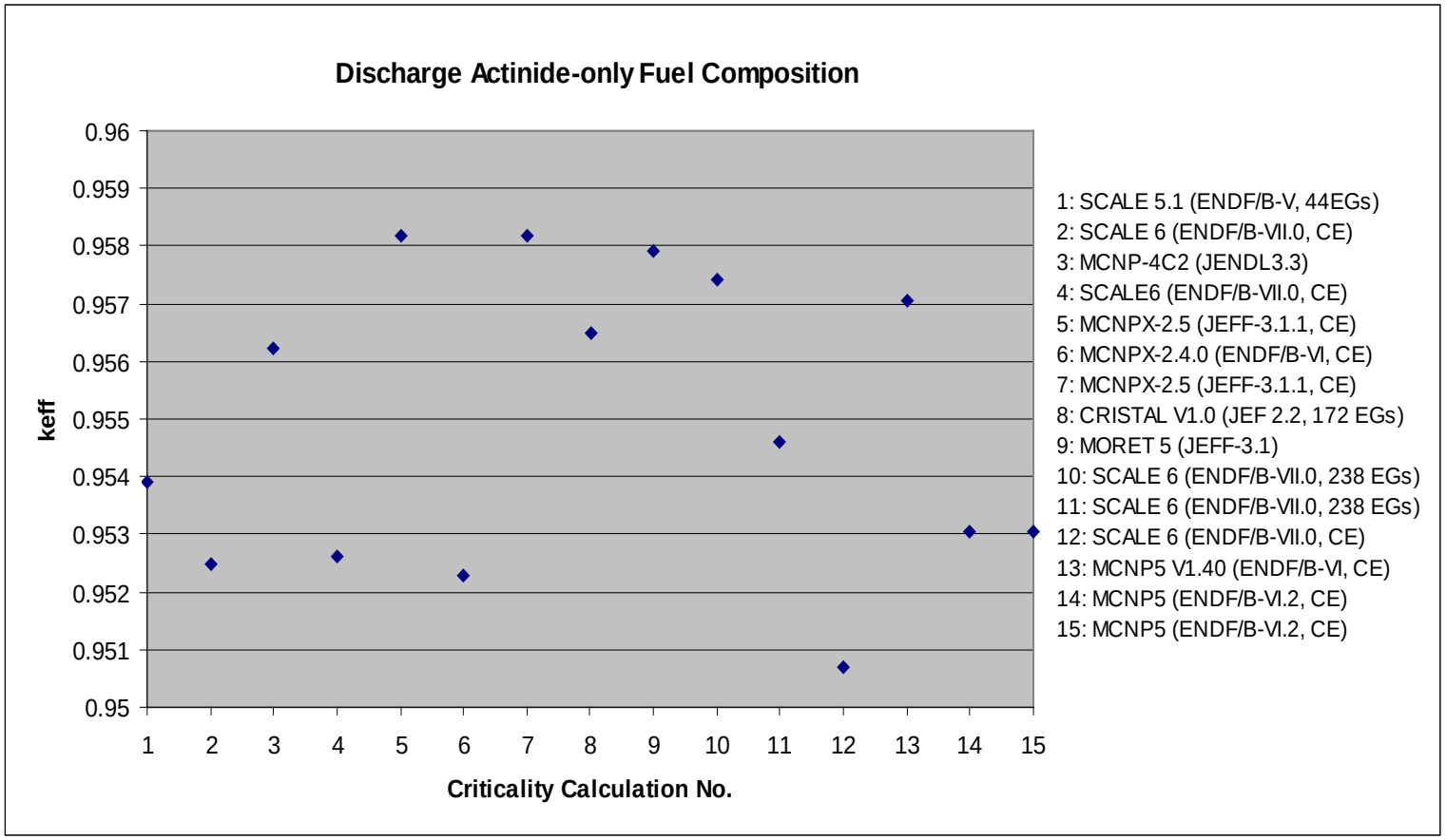


Comparison of k_{eff} Values for the Fresh Fuel Composition



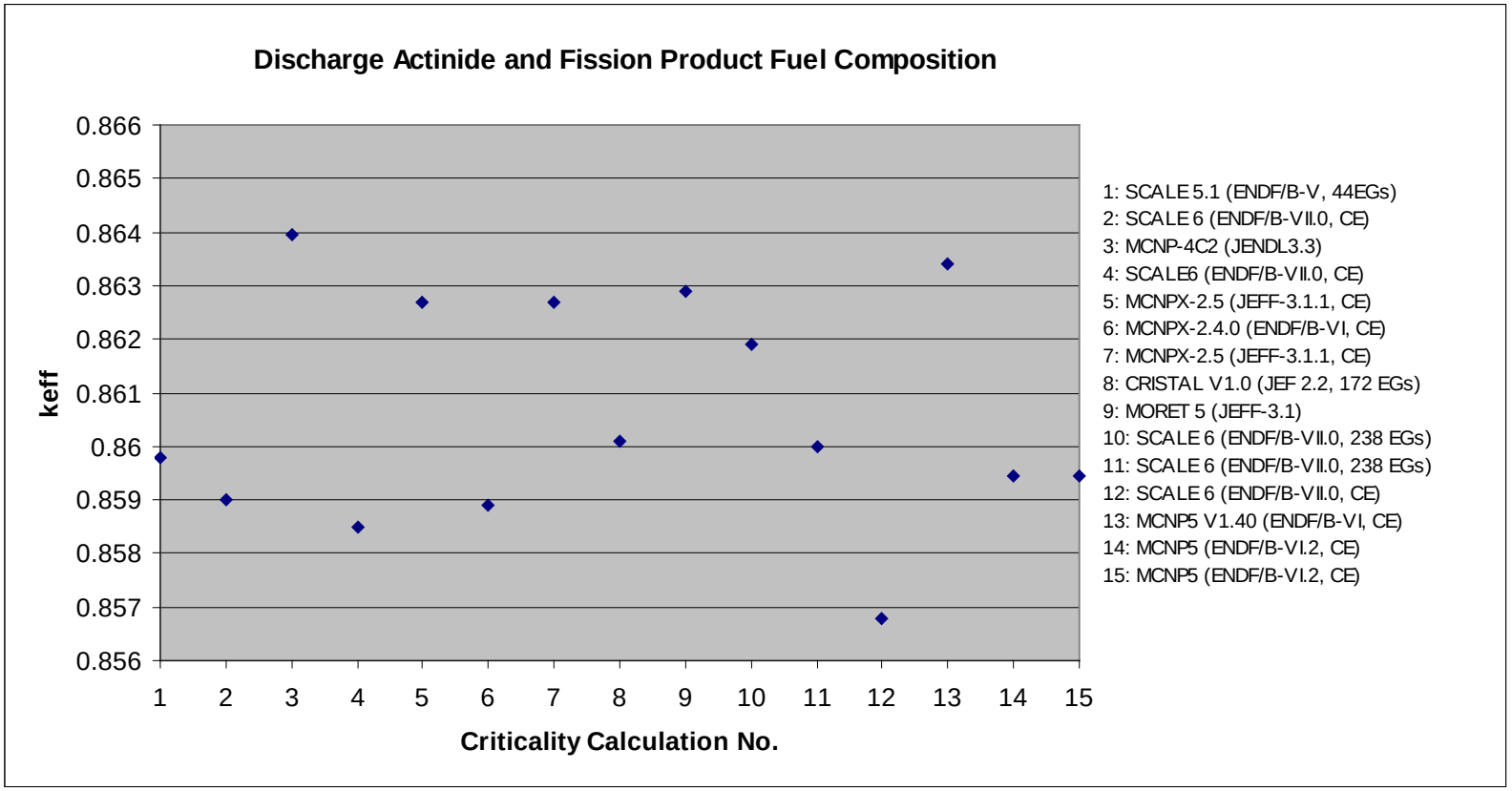
$k_{eff\text{-}max} - k_{eff\text{-}min} = 0.01109$

Comparison of k_{eff} Values for Discharge Actinide-only Fuel Composition



$k_{eff\text{-}max} - k_{eff\text{-}min} = 0.00749$

Comparison of k_{eff} Values for Discharge Actinide and FP Fuel Composition



$k_{eff\text{-}max} - k_{eff\text{-}min} = 0.00714$