V&V for Radiation Characterization Codes at Oak Ridge National Laboratory

Past experience and benchmark needs

IAEA Consultancy meeting on the International Radiation Characterization Benchmark Experiment Project (IRCBEP)

Ian Gauld

General Thoughts

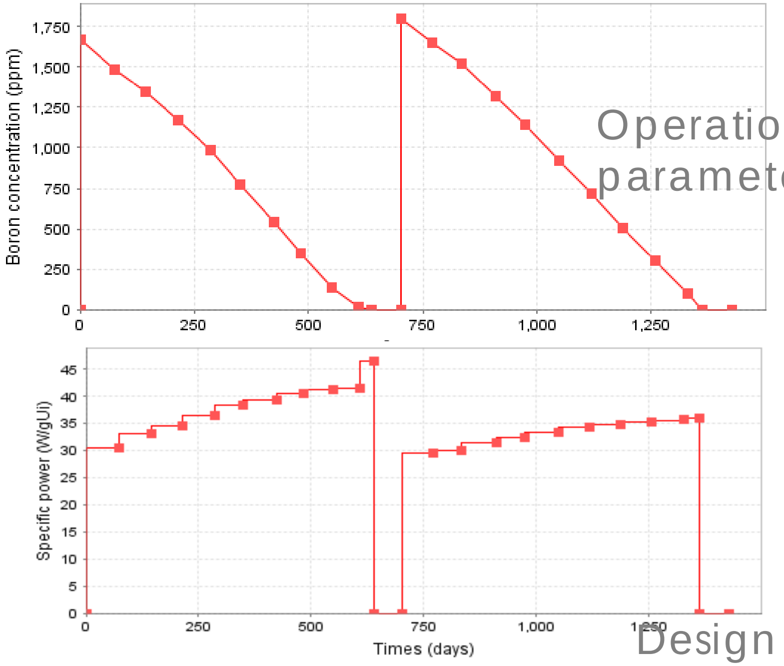
- What do we mean by "Radiation Characterization" and what class of codes/data should this include?
- Who are our end users? Code developers (code testing), application users, data evaluators, all?
- There are other databases (DBs) under active development (e.g. ICSBE, IRPhE, SINBAD, and SFCOMPO) that cross into Radiation Characterization applications.
- There is currently only limited coordination between these DBs. What gaps exist in compiled experimental data? In addition to adding data, is there a needed role to better support end users by cross linking experiments in different DBs?
- Benchmark experiments in SINBAD and SFCOMPO are largely unevaluated (volunteer efforts). Model development, benchmark specifications, and evaluations are also needed.
- How can the integration benchmarks be used to better assess the nuclear data performance and contribute to data testing and evaluation?

International Databases for V&V

- ICSBEP (Dice) – Critical experiments (~4700)
- IRPhEP (iDAT) – Reactor physics experiments (136) include criticality, buckling, spectral characteristics, reactivity effects, reactivity coefficients, kinetics, reaction rates, and power distributions (also contains calculated quantities, such as neutron flux/capture/fission spectrum data, neutron balance data)
- SFCOMPO 2.0 – Reactor spent fuel compositions (750)
- SINBAD – Reactor (47), Fusion (31), Accelerator (23) shielding benchmarks. Data are largely unevaluated collection of drawings, reports and experimental data
- IRCBEP Roles
  - Address gaps in current experimental databases?
  - Enhance use of integral benchmarks for data testing?
  - Improve coordination/integration with existing DBs for code/nuclear data testing?

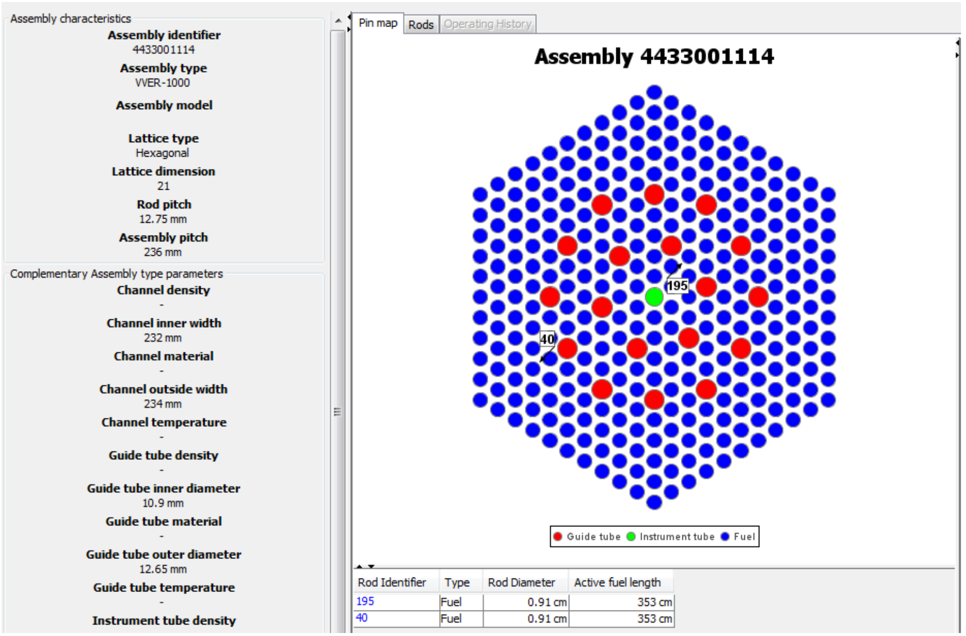
SFCOMPO 2.0 Database

- NEA Database of Spent Nuclear Fuel Assay Data
  http://www.oecd-nea.org/sfcompo/
- Preserve publicly available destructive radiochemical assay data
- Organize, Standardize, Centralize and access via the SFCOMPO-2.0 Java application
  - Measured data and uncertainties
  - All design and operating information
  - Links to primary experimental reference reports
- Includes data for 8 reactor types, 40 reactors, 116 fuel assemblies, 750 samples, 24000 measurement entries, 91 isotopes

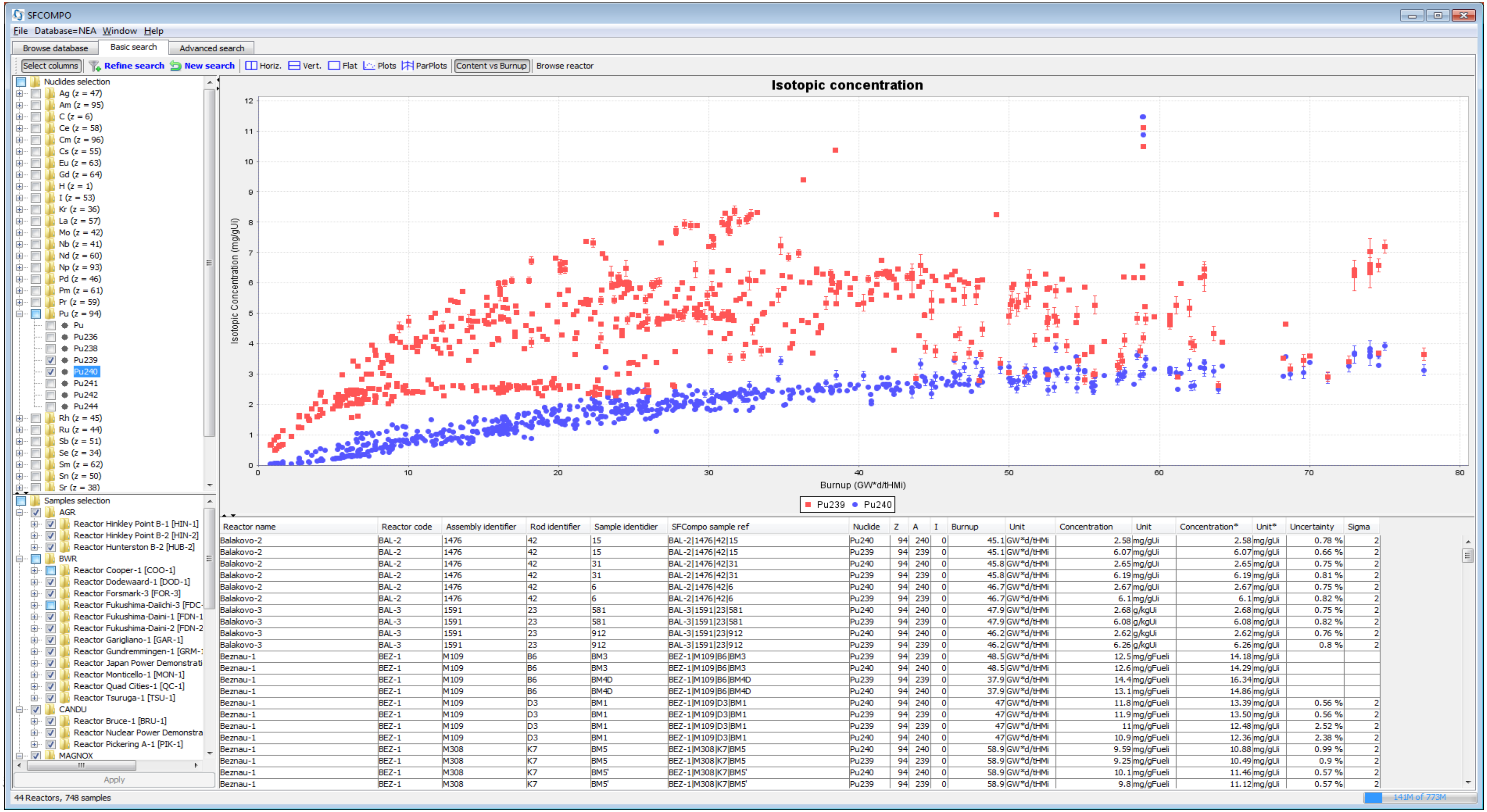


Operational parameters

Design data

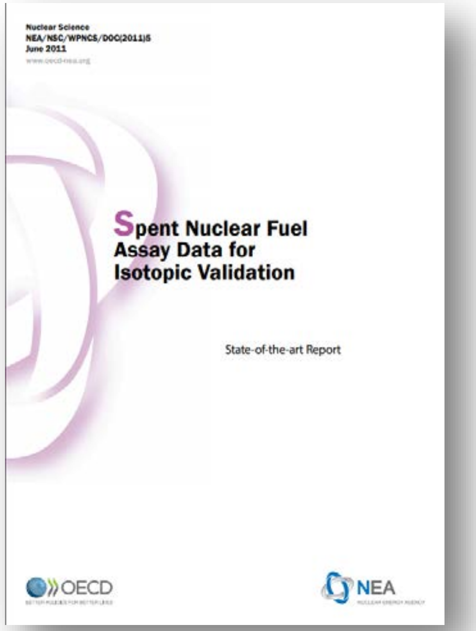


SFCOMPO Web Interface



Reactor name	Reactor code	Assembly identifier	Rod identifier	Sample identidier	SFCompo sample ref	Nuclide	Z	A	I	Burnup	Unit	Concentration	Unit	Concentration*	Unit*	Uncertainty	Sigma
Balakovo-2	BAL-2	1476	42	15	BAL-2|1476|42|15	Pu240	94	240	0	45.1	GW*d/tHMi	2.58	mg/gUi	2.58	mg/gUi	0.78 %	2
Balakovo-2	BAL-2	1476	42	15	BAL-2|1476|42|15	Pu239	94	239	0	45.1	GW*d/tHMi	6.07	mg/gUi	6.07	mg/gUi	0.66 %	2
Balakovo-2	BAL-2	1476	42	31	BAL-2|1476|42|31	Pu240	94	240	0	45.8	GW*d/tHMi	2.65	mg/gUi	2.65	mg/gUi	0.75 %	2
Balakovo-2	BAL-2	1476	42	31	BAL-2|1476|42|31	Pu239	94	239	0	45.8	GW*d/tHMi	6.19	mg/gUi	6.19	mg/gUi	0.81 %	2
Balakovo-2	BAL-2	1476	42	6	BAL-2|1476|42|6	Pu240	94	240	0	46.7	GW*d/tHMi	2.67	mg/gUi	2.67	mg/gUi	0.75 %	2
Balakovo-2	BAL-2	1476	42	6	BAL-2|1476|42|6	Pu239	94	239	0	46.7	GW*d/tHMi	6.1	mg/gUi	6.1	mg/gUi	0.82 %	2
Balakovo-3	BAL-3	1591	23	581	BAL-3|1591|23|581	Pu240	94	240	0	47.9	GW*d/tHMi	2.68	g/kgUi	2.68	mg/gUi	0.75 %	2
Balakovo-3	BAL-3	1591	23	581	BAL-3|1591|23|581	Pu239	94	239	0	47.9	GW*d/tHMi	6.08	g/kgUi	6.08	mg/gUi	0.82 %	2
Balakovo-3	BAL-3	1591	23	912	BAL-3|1591|23|912	Pu240	94	240	0	46.2	GW*d/tHMi	2.62	g/kgUi	2.62	mg/gUi	0.76 %	2
Balakovo-3	BAL-3	1591	23	912	BAL-3|1591|23|912	Pu239	94	239	0	46.2	GW*d/tHMi	6.26	g/kgUi	6.26	mg/gUi	0.8 %	2
Beznau-1	BEZ-1	M109	B6	BM3	BEZ-1|M109|B6|BM3	Pu239	94	239	0	48.5	GW*d/tHMi	12.5	mg/gFueli	14.18	mg/gUi		
Beznau-1	BEZ-1	M109	B6	BM3	BEZ-1|M109|B6|BM3	Pu240	94	240	0	48.5	GW*d/tHMi	12.6	mg/gFueli	14.29	mg/gUi		
Beznau-1	BEZ-1	M109	B6	BM4D	BEZ-1|M109|B6|BM4D	Pu239	94	239	0	37.9	GW*d/tHMi	14.4	mg/gFueli	16.34	mg/gUi		
Beznau-1	BEZ-1	M109	B6	BM4D	BEZ-1|M109|B6|BM4D	Pu240	94	240	0	37.9	GW*d/tHMi	13.1	mg/gFueli	14.86	mg/gUi		
Beznau-1	BEZ-1	M109	D3	BM1	BEZ-1|M109|D3|BM1	Pu240	94	240	0	47	GW*d/tHMi	11.8	mg/gFueli	13.39	mg/gUi	0.56 %	2
Beznau-1	BEZ-1	M109	D3	BM1	BEZ-1|M109|D3|BM1	Pu239	94	239	0	47	GW*d/tHMi	11.9	mg/gFueli	13.50	mg/gUi	0.56 %	2
Beznau-1	BEZ-1	M109	D3	BM1	BEZ-1|M109|D3|BM1	Pu239	94	239	0	47	GW*d/tHMi	11	mg/gFueli	12.48	mg/gUi	2.52 %	2
Beznau-1	BEZ-1	M109	D3	BM1	BEZ-1|M109|D3|BM1	Pu240	94	240	0	47	GW*d/tHMi	10.9	mg/gFueli	12.36	mg/gUi	2.38 %	2
Beznau-1	BEZ-1	M308	K7	BM5	BEZ-1|M308|K7|BM5	Pu240	94	240	0	58.9	GW*d/tHMi	9.59	mg/gFueli	10.88	mg/gUi	0.99 %	2
Beznau-1	BEZ-1	M308	K7	BM5	BEZ-1|M308|K7|BM5	Pu239	94	239	0	58.9	GW*d/tHMi	9.25	mg/gFueli	10.49	mg/gUi	0.9 %	2
Beznau-1	BEZ-1	M308	K7	BM5'	BEZ-1|M308|K7|BM5'	Pu240	94	240	0	58.9	GW*d/tHMi	10.1	mg/gFueli	11.46	mg/gUi	0.57 %	2
Beznau-1	BEZ-1	M308	K7	BM5'	BEZ-1|M308|K7|BM5'	Pu239	94	239	0	58.9	GW*d/tHMi	9.8	mg/gFueli	11.12	mg/gUi	0.57 %	2

SFCOMPO Outcomes


Nuclear Science
NEA/NSC/WPNCS/DOC(2011)5
June 2011

Spent Nuclear Fuel Assay Data for Isotopic Validation

State-of-the-art Report

OECD

NEA

- State-of-the-art report https://www.oecd-nea.org/science/wpncs/ADSNF/SOAR_final.pdf
- Compilation and archiving of experimental data
- Database and interface program development https://www.oecd-nea.org/sfcompo/
- Database population and independent review
- Evaluation guidance https://www.oecd-nea.org/science/docs/2015/nsc-r2015-8.pdf (rev. 0)
- Preliminary evaluations completed for 7 datasets - most data sets are still unevaluated
- Activities now managed under an NEA Technical Review Group

Shielding Integral Benchmark Archive and Database (SINBAD)

- SINBAD evaluations are generally not formalized documents except for a few quality reviews
- Most are collections of drawings, reports and experimental data that need to be evaluated
- Fusion Neutronics Source (FNS) Experiments
  - [FNS/JAEA, Japan] FNS Experimental data for fusion neutronics benchmark
  - [FNS/JAEA, Japan] FNS Integral Experiment on Graphite Cylindrical Assembly
  - [FNS/JAEA, Japan] FNS Liquid Oxygen
  - [FNS/JAEA, Japan] FNS Vanadium Cube
  - [FNS/JAEA, Japan] FNS Tungsten
  - [FNS/JAEA, Japan] FNS Skyshine
  - [FNS/JAEA, Japan] FNS Dogleg Duct Streaming
  - [FNG/ENEA, Italy] FNG-SS Shield (integral meas.)
  - [FNG/ENEA, Italy] FNG-ITER Blanket Bulk Shield (integral meas.)
  - [FNG/ENEA, Italy] FNG-ITER Neutron Streaming (integral)
  - [FNG/ENEA, Italy] FNG-ITER Dose Rate Experiment
  - [FNG/ENEA, Italy] FNG Silicon Carbide (integral)
  - [FNG/ENEA, Italy] FNG Tungsten (integral)
  - [FNG/ENEA, Italy] FNG HCPB Tritium Breeder Module (integral measurements)
  - [FNG/Italy, TUD/Germany] FNG/TUD ITER Blanket Bulk Shield (spectra measurements)
  - [FNG/Italy, TUD/Germany] FNG/TUD Silicon Carbide (spectra)
  - [FNG/Italy, TUD/Germany] FNG/TUD Tungsten (spectra measurements)

Validation Experience with the ORIGEN Code

- Oak Ridge Isotope Transmutation and Radiation Characterization code
- Neutron transmutation analysis focusing on spent nuclear fuel and component activation (E_n < 20 MeV)
- Matrix exponential solvers for large systems – Taylor series expansion (+ Bateman) and Chebyshev Rational Approximation solvers
- Couples with 1-D, 2-D, and 3-D neutron transport solvers
- ENDF/B nuclear data plus activation data from JEFF-3.0/A, ENDF/B-VII.1 decay data and *adjusted* ENDF/B fission product yields
- Source terms and radiation emissions
  - Activities and decay heat (large decay time range)
  - Gamma radiation sources – plus bremsstrahlung, spontaneous fission (SF), alpha,n (a,n)
  - Neutron source and energy spectra – delayed neutron, (a,n), SF
  - Beta source and spectra
  - Alpha particle emission source and spectra

Other US Radiation Source Characterization Codes

- SOURCES 4C (LANL)
  - (a,n) and spontaneous fission neutrons (and delayed neutrons)
- MISC (LANL) MCNP Intrinsic Source Constructor (ISC)
  - Bateman decay solution
  - Includes SOURCES plus gamma and beta
  - Bremsstrahlung calculation (thick target)
  - https://mcnp.lanl.gov/pdf_files/la-ur-16-27265.pdf
- RASTA (SRNL) Radiation Source Term Analysis Code
  - Neutrons and photons from (a,n) using SOURCES
  - Photons from nuclide decay
  - Neutrons and photons from Spontaneous Fission
  - Photons from bremsstrahlung
  - https://www.ipen.br/biblioteca/cd/physor/2000/physor/033.pdf
- RadSrc Library (LLNL) Gamma source distribution code

Benchmark Experiments

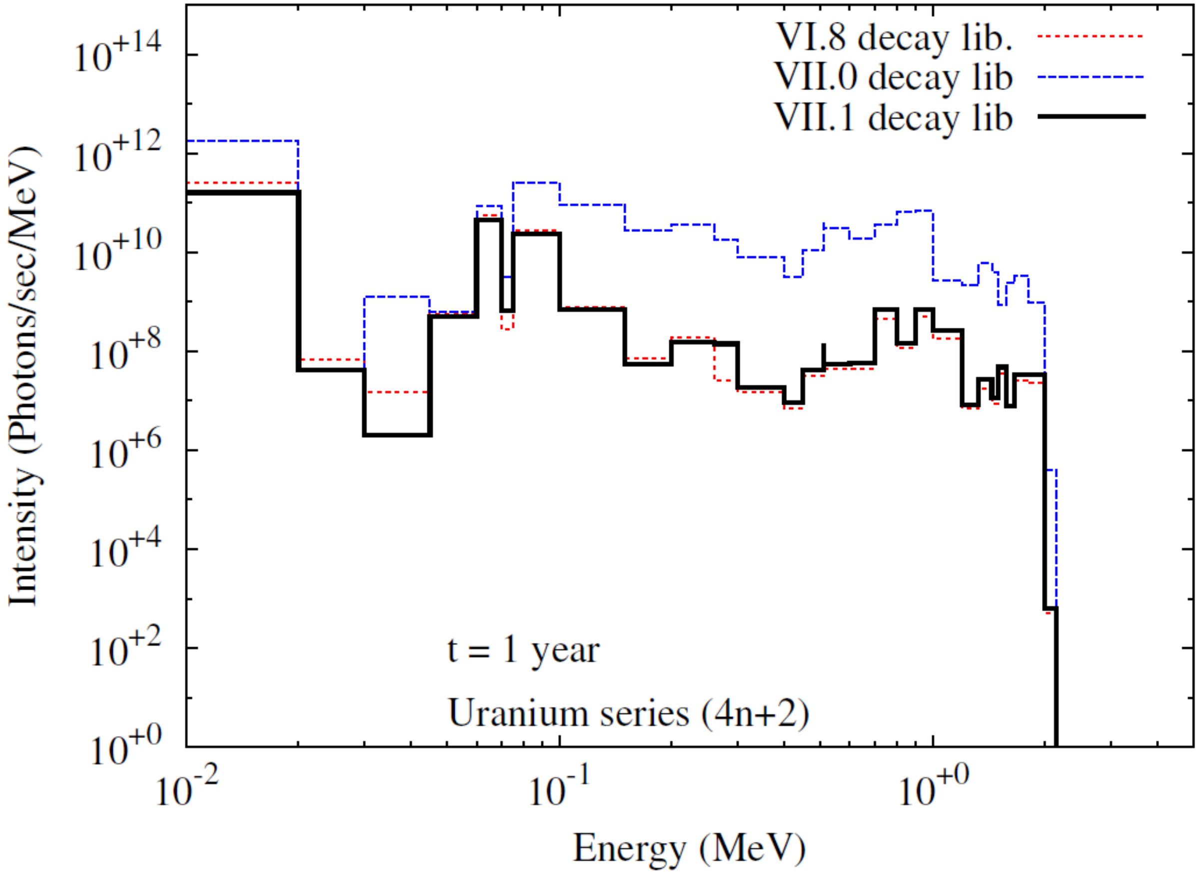
- Different benchmarks can exercise very different classes of data
- Commonly used experiment classes

Measurement	Nuclear Data
Spent fuel calorimetry	cross sections, decay data, fission yields
Burst fission experiments	decay data, fission yields (gamma/beta)
Spent fuel compositions	cross sections, fission yields, decay data
Gamma emission	gamma decay data (emission yields)
Neutron emission	(a,n) cross sections, stopping powers, branching
Beta emission	beta decay data

- Nuclear data is a significant component of code V&V

Benchmarks – Start Simple

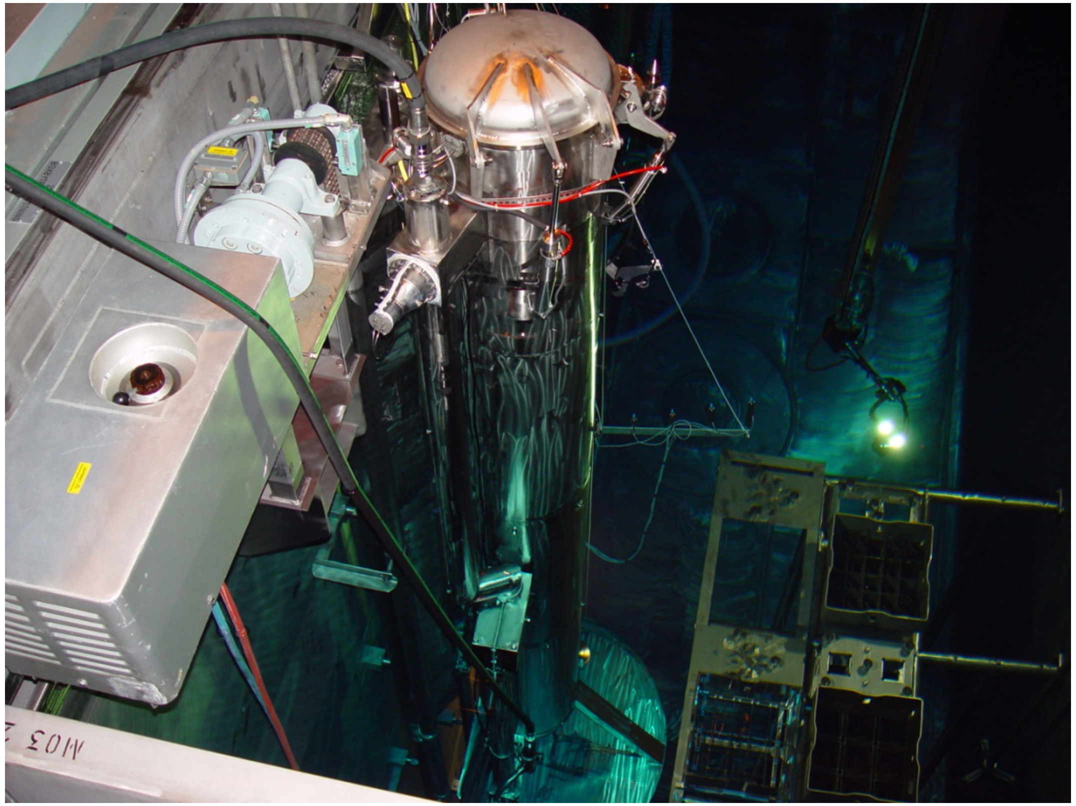
- Nuclear decay data testing
- Systematic errors found in the ENDF/B-VII.0 decay data release
- Initially identified in decay branch of ^{234}Th during analysis of an unirradiated fuel transportation package
- Errors not identified in ORIGEN testing (irradiation experiments)
- ^{235}U, ^{238}U, and ^{232}Th decay series now added to test suite



I.C. Gauld, M. Pigni, G. Ilas, "Validation and Testing of ENDF/B-VII Decay Data," *Nuclear Data Sheets* **120** (2014). https://doi.org/10.1016/j.nds.2014.06.134

Decay Heat Experiments – Spent Nuclear Fuel

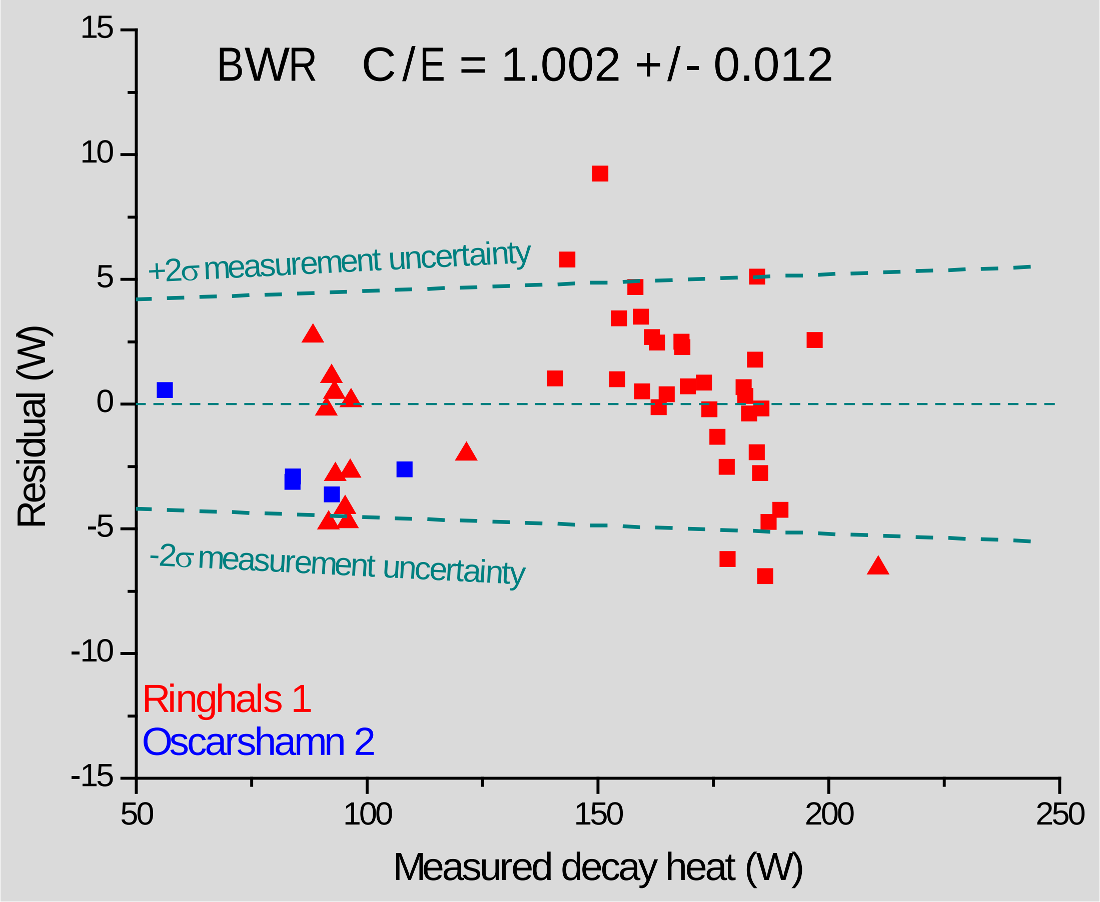
- Calorimeter measurements of full-length assemblies conducted in US (GE-Morris and Hanford) and Sweden
  - 200 assemblies measured
  - Cooling time range ~ 1 year to 30 years.
- New OECD/NEA Blind decay heat benchmark organized by SKB Sweden
- Measurement data currently planned for inclusion in the OECD/NEA Spent Fuel Database (SFCOMPO)

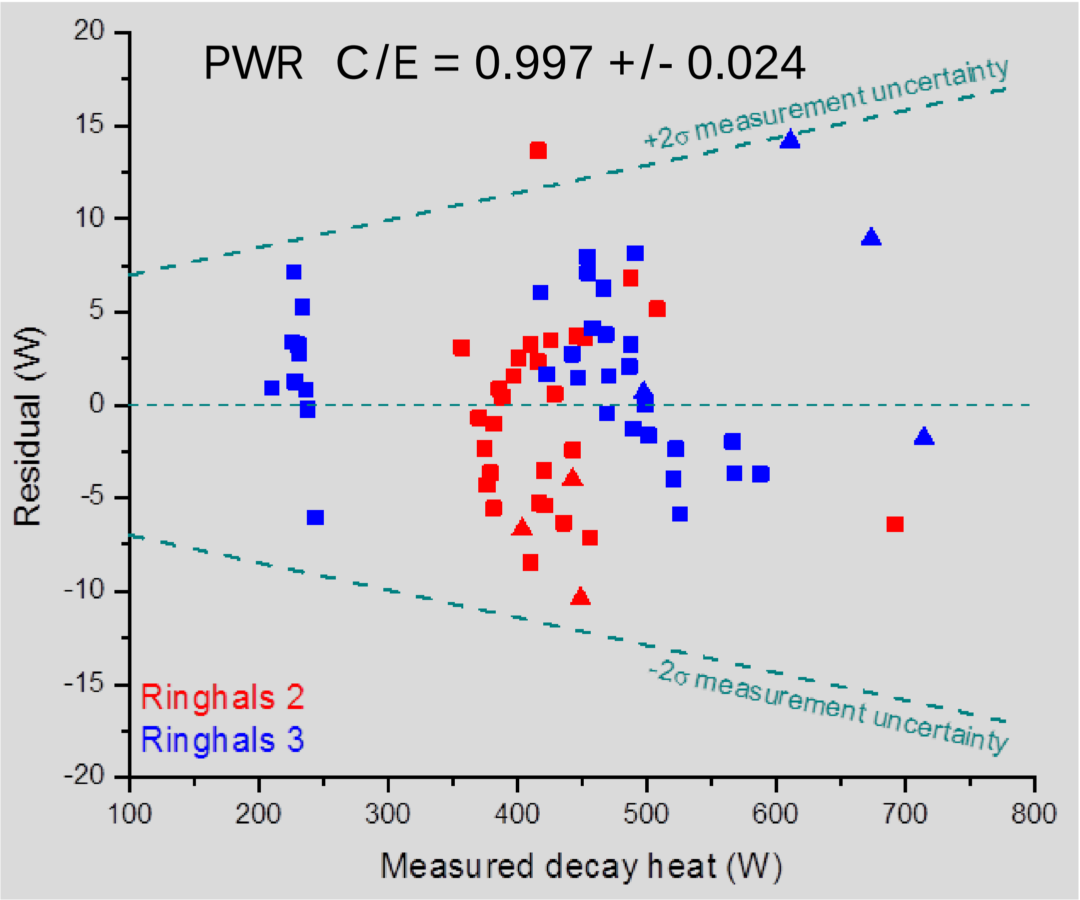


Spent fuel assembly calorimeter at the SKB CLAB facility Sweden

Validation Results (SCALE 6.1.2 / ENDF/B-VII.0)

Measurements at the SKB Swedish Central Interim Storage Facility for Spent Nuclear Fuel (Clab)





* Germina Ilas, Ian C. Gauld, Henrik Liljenfeldt, "Validation of ORIGEN for LWR used fuel decay heat analysis with SCALE," *Nuclear Engineering and Design* **273** (2014). https://doi.org/10.1016/j.nucengdes.2014.02.026

Decay Heat Experiments – Fission Burst

- Measurements performed to support development of decay heat data and standards for loss-of-coolant accident analysis
- Short irradiation of small actinide samples with measurement times from 0.4 s up to 5 hours after fission
- Experiments test fission product yields and decay data (decay constants and recoverable energy Q values)
- These experiments have been used extensively for ORIGEN V&V and applications to decay heat analysis at short cooling times
- Current standards ANSI/ANS-5.1-2014 and ISO 10645(1992) do not include measurements from UML (1997) covering very short decay times
- Data gap between 5 hours and 1 year – MERCI experiments for longer times (CEA) are not public – UO_2 fuel sample measured using MOSAÏC calorimeter https://doi.org/10.13182/NT12-A13328

OAK RIDGE National Laboratory

Decay Heat Burst Fission Experiments (> 1980)

Data set	Isotopes	Method[a]	Author(s)	Institute	Year (circa)
1	^{235}U, ^{239}Pu, ^{241}Pu	γ, β	Dickens et al.	Oak Ridge National Laboratory	1980
2	^{235}U	calorimeter	Baumung	Karlsruhe	1981
3	^{233}U, ^{235}U, ^{238}U, ^{239}Pu	γ, β	Akiyama et al.	Tokyo University YAYOI fast reactor	1982
4	^{235}U	γ, β	Johansson	Uppsala University / Studsvik	1987
5	^{235}U, ^{238}U, ^{239}Pu	γ, β	Schier and Couchell et al.	University of Massachusetts, Lowell	1997

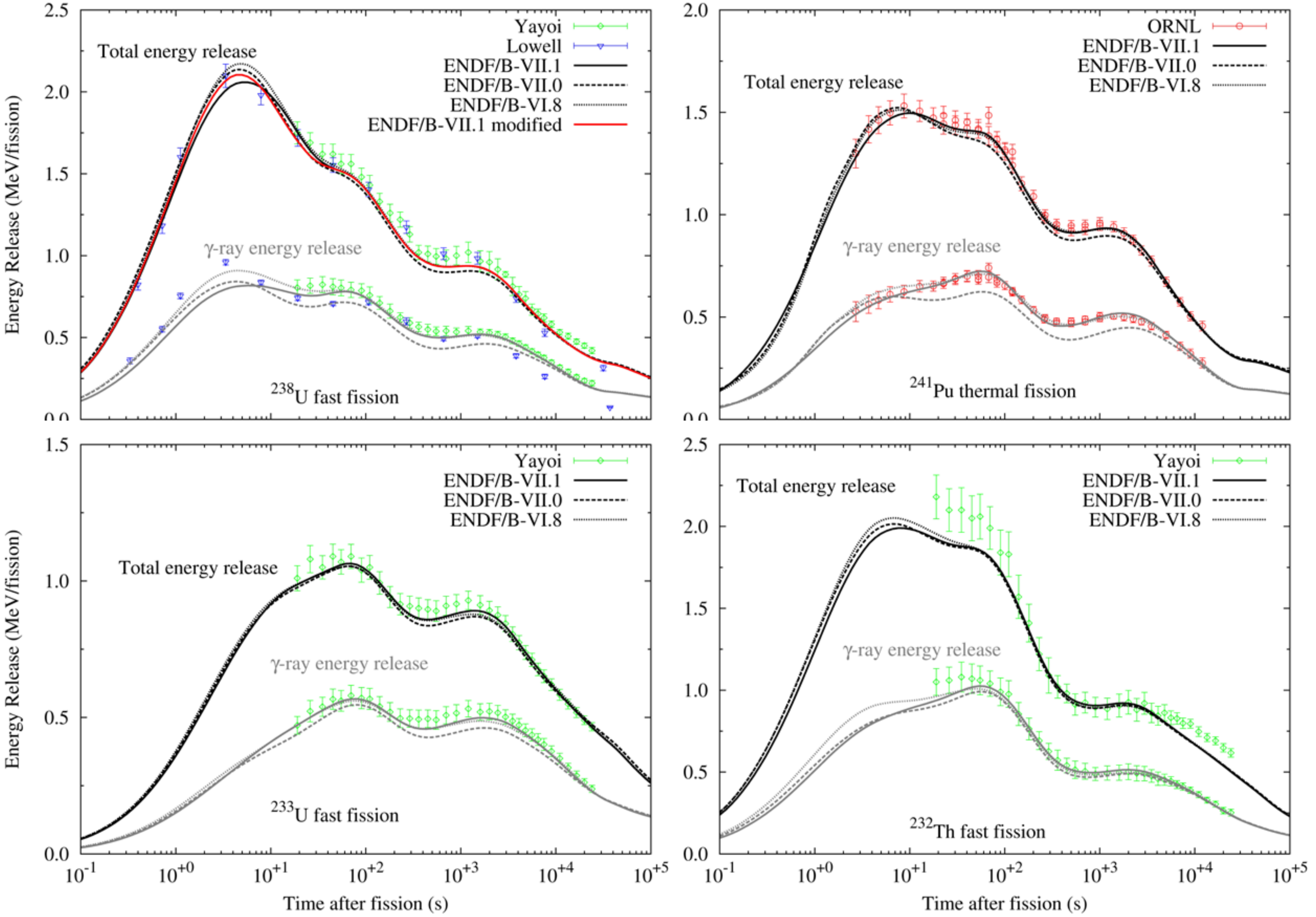
[a] γ, β = spectroscopic measurements

Burst Fission Experiments used at ORNL

- Calorimeter and spectroscopic (gamma and beta) measurement methods
- Experiments are not collected in a central location (useful for decay heat standards development)
- Some UM Lowell measurement data acquired from personal communications (Schier)
- ORNL measurement data (Dickens et al.) are archived at RSICC on DLC-061 for ^{235}U (KDDK) and DLC-074 (PUDK) for ^{239}Pu and ^{241}Pu
  - https://rsicc.ornl.gov/codes/dlc/dlc0/dlc-061.html
  - https://rsicc.ornl.gov/codes/dlc/dlc0/dlc-074.html
- Data compilation needed to support decay heat standard revisions (ISO 10645)

Burst Fission Experiment Benchmarks

- ^{238}U
- ^{235}U
- ^{239}Pu
- ^{241}Pu
- ^{233}U
- ^{232}Th
- Fast and thermal systems



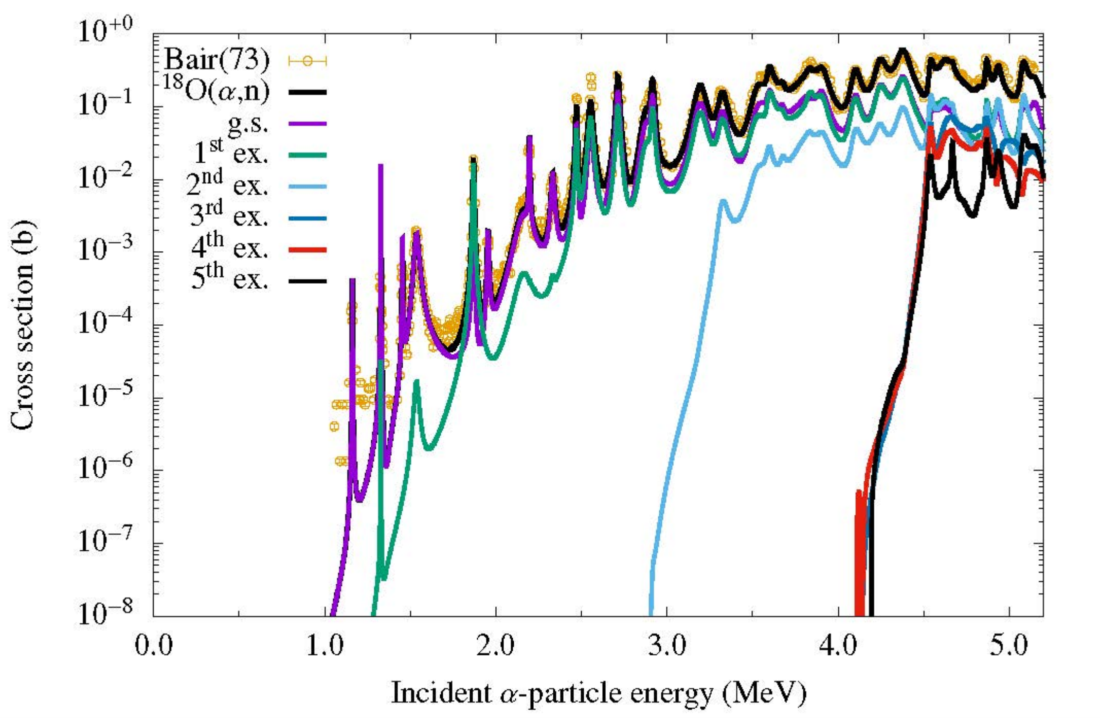
M. Pigni, M. W. Francis, **I. C. Gauld**, "Investigation of Inconsistent ENDF/B-VII.1 Independent and Cumulative Fission Product Yields with Proposed Revisions," *Nuclear Data Sheets* **1** (2015), https://doi.org/10.1016/j.nds.2014.12.040

Neutron Sources

- SOURCES 4C code developed by Los Alamos National Laboratory is widely used in US (integrated into ORIGEN)
- Spontaneous fission and (a,n) neutron source calculations
- Nuclear data:
  - Watt fission spectrum parameters, half lives, nubar
  - (a,n) cross sections
  - Alpha particle stopping powers
  - Alpha reaction branching levels
- Little uncertainty information or covariances are available with data to perform uncertainty analysis
- Experimental data are available for neutron yields and energy spectra
  - Thick target integral (a,n) neutron yield measurements
  - Spontaneous fission spectral measurements

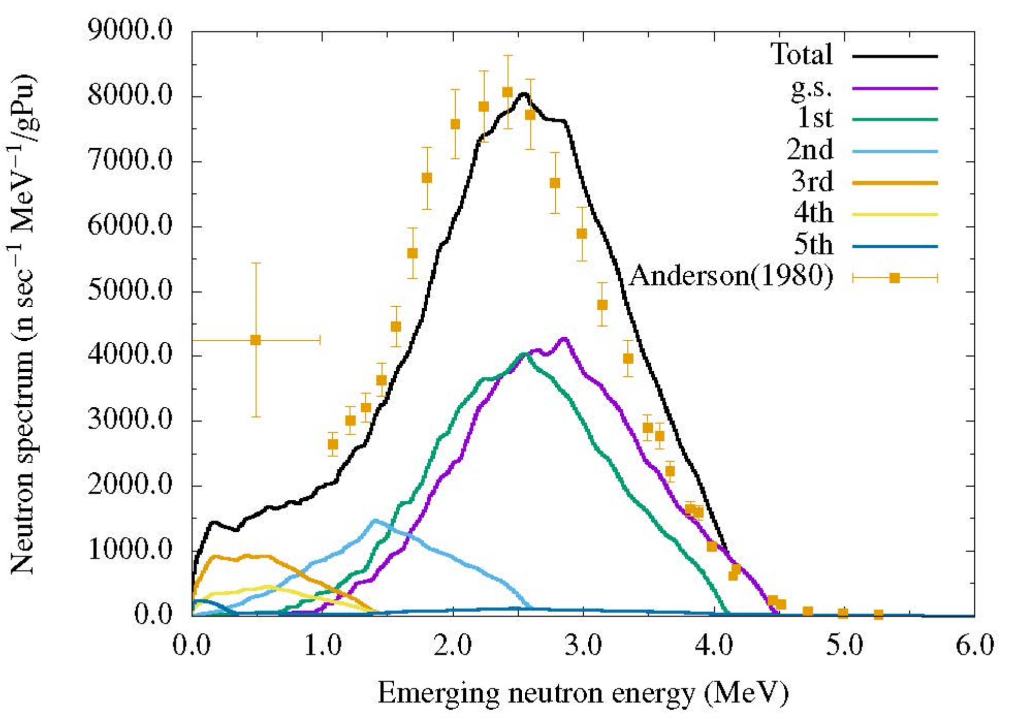
(a,n) Neutron Source Characterization

Partial (a,n) cross section evaluation



- In SOURCES 4C code, partial cross sections are based on Hauser Feshbach calculations performed by the GNASH code
- The partial cross sections (branching) to each level define the neutron emission spectrum

Impact on (a,n) emission spectrum

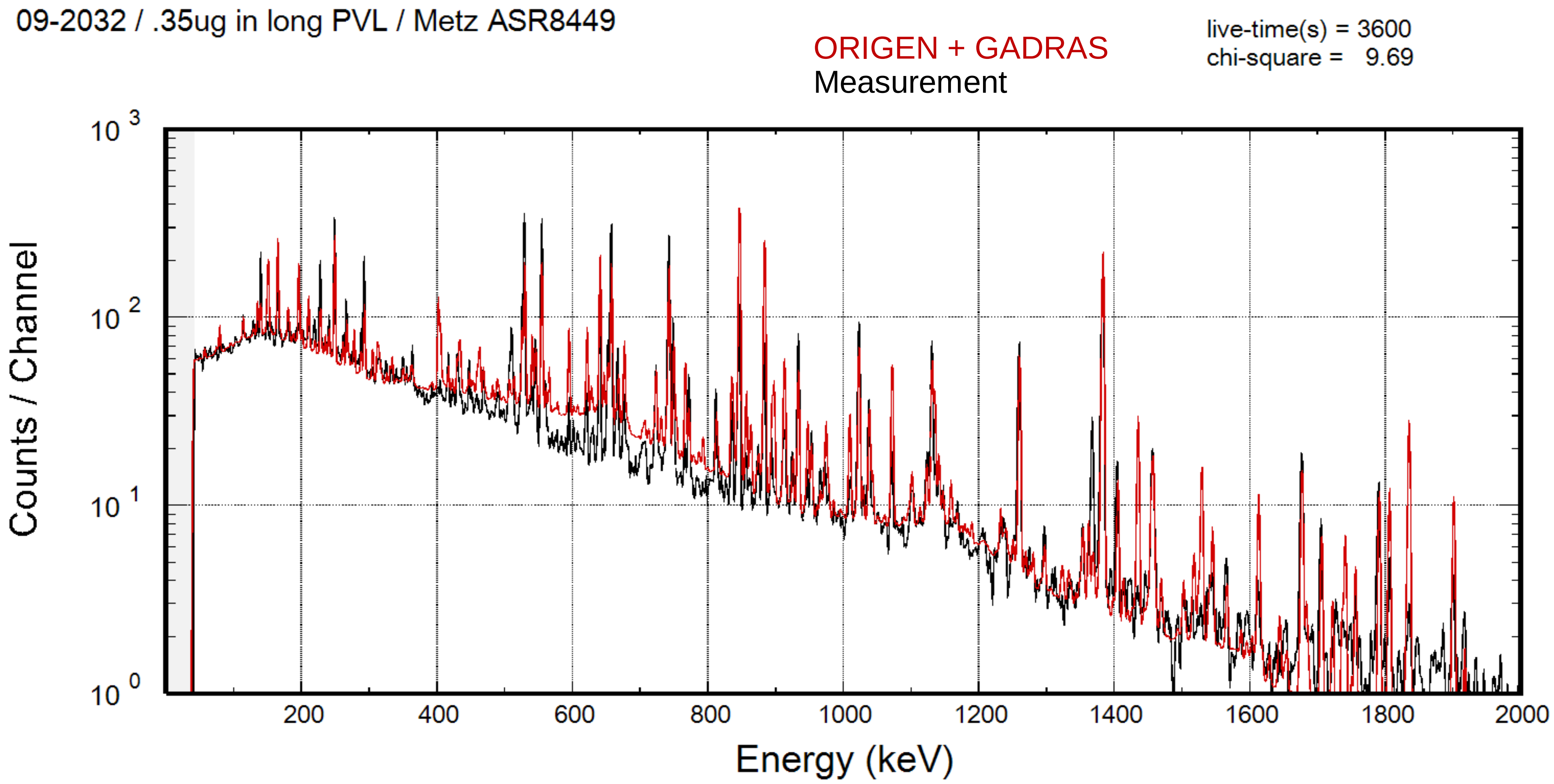


- The spectrum contribution from each level can be simulated
- Discrepancies in total spectrum can be used to inform nuclear models to improve predictions
- There is no consolidated resource for these experiments

Short-Lived Fission Product Gamma Spectra (PNNL)

- High Resolution HPGe gamma spectra following fission of ^{233}U, ^{235}U, ^{238}U, ^{237}Np, ^{239}Pu samples (~1 µg to 1 mg)
- Thermal, epithermal and fast neutron spectra
- Counting times 4 min to 1 week after fission
- Reported in PNNL-20141(2011)
- Data accessible online from https://spcollab.pnnl.gov/sites/gammadata/

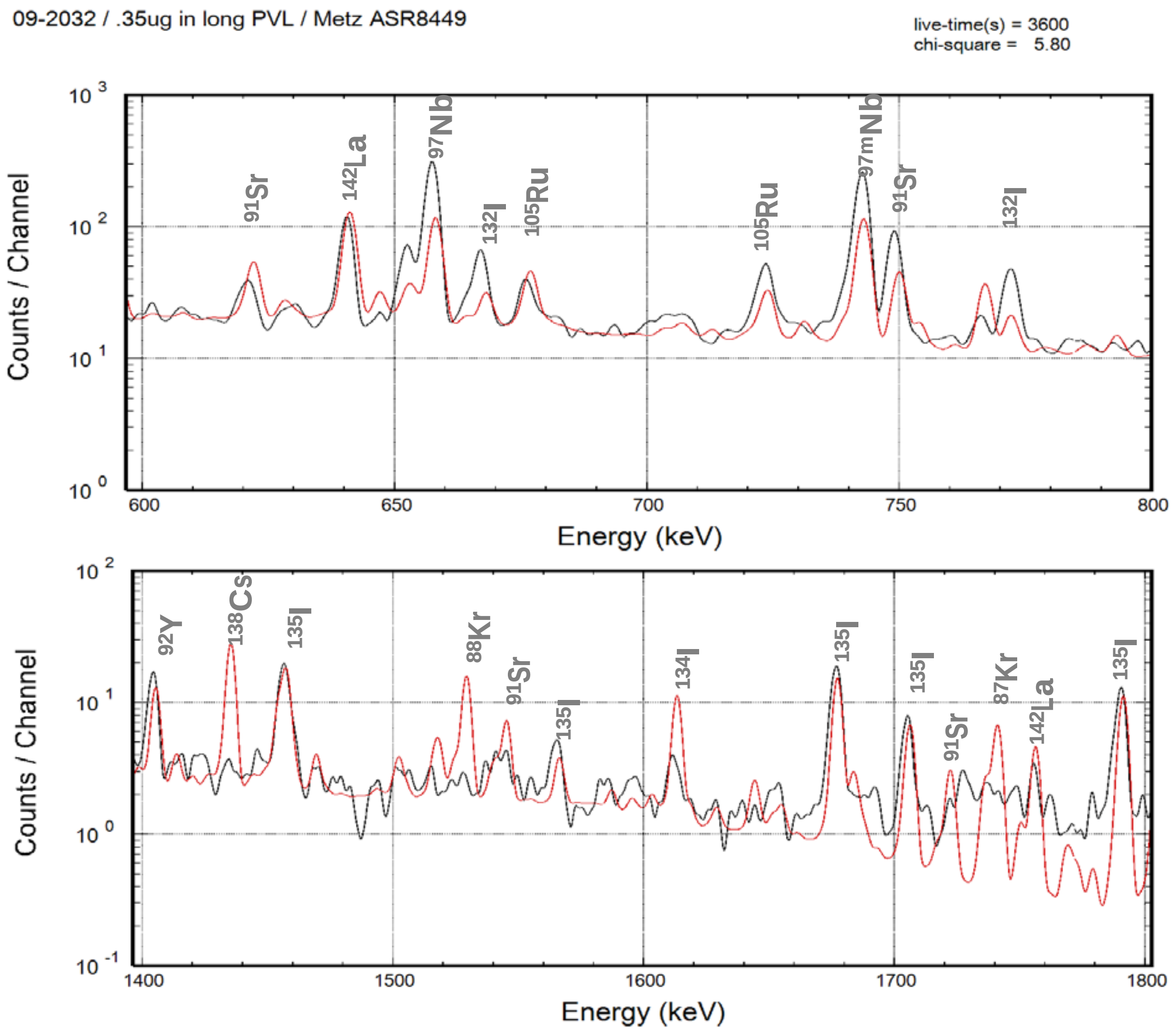
^{235}U Fission γ-Spectrum – 7 hour data



OAK RIDGE National Laboratory

^{235}U Fission γ-Spectrum – 7 hours

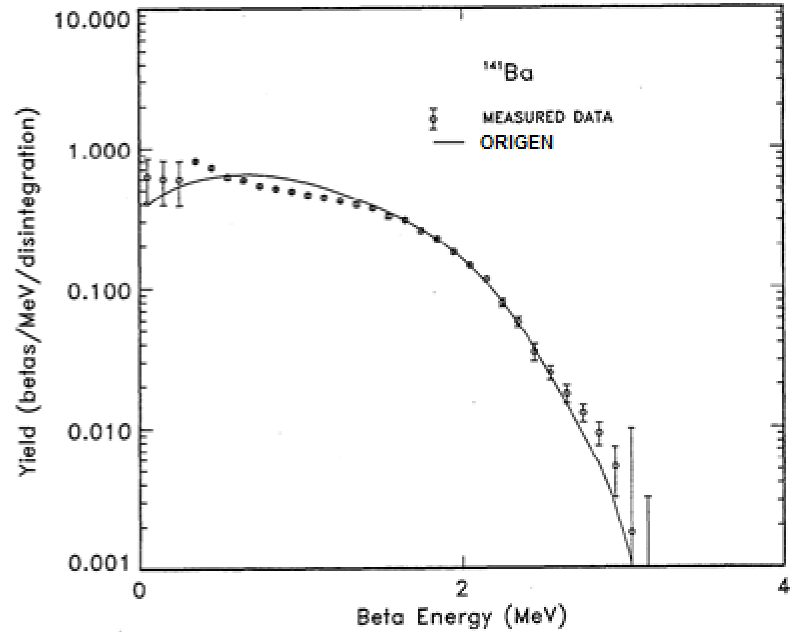
- High resolution spectra with individual nuclide lines
- Experiments provide V&V for short cooling times
- Test fission product yields (energy dependent), decay data, and gamma emission data

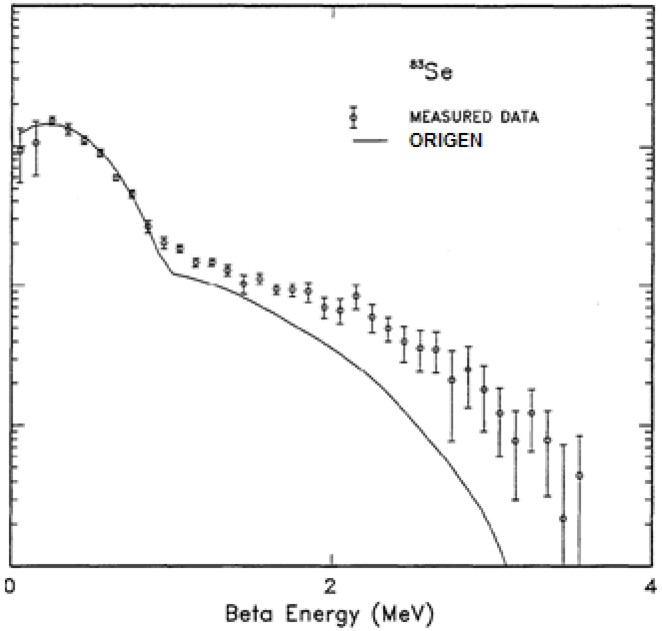


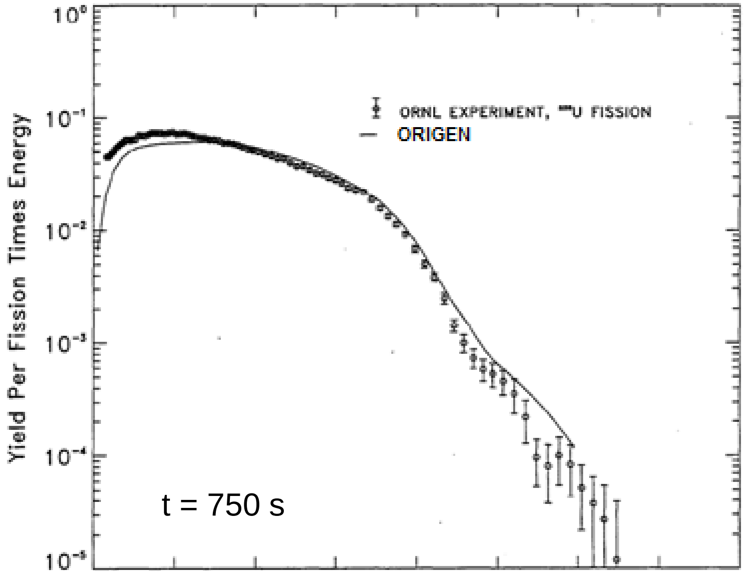
OAK RIDGE
National Laboratory

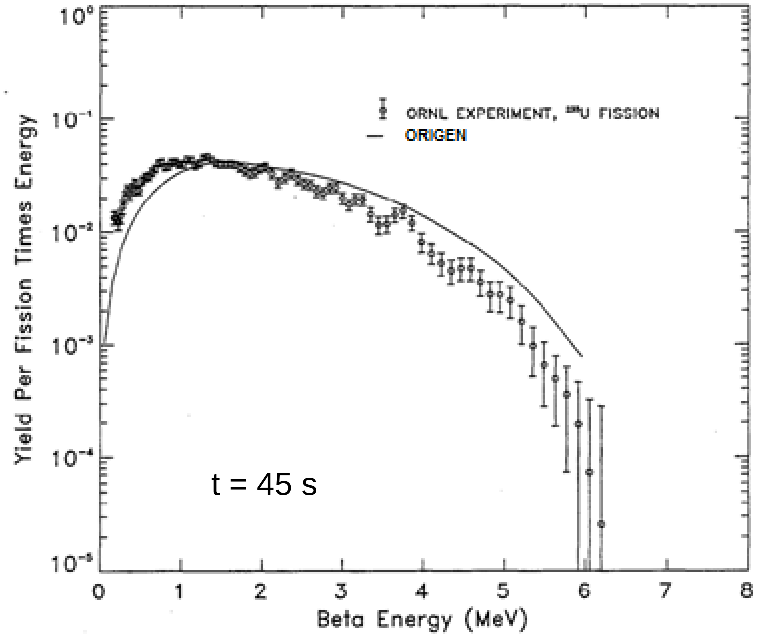
Beta Sources

- Beta spectra measured during burst fission experiments (ORNL 1979)
- Short-lived fission product measurements
  - OSIRIS Facility (Studsvik), ISOLDE (CERN)
  - Rudsdam et al. (1990)









Fission Product Yield Measurements

- Gap in consolidated experimental data for fission yield data analysis
- WPEC SG-37 and IAEA Technical Meetings and activities
- No central database of yield measurements for use in modeling
- Increased worldwide interest in improving fission yields
- In the US, no new evaluations since 1994
- Modeling of independent yields using cumulative yield measurements relies on nuclear decay data – as decay data evolves (delayed beta branching fractions), need to reassess yields more frequently

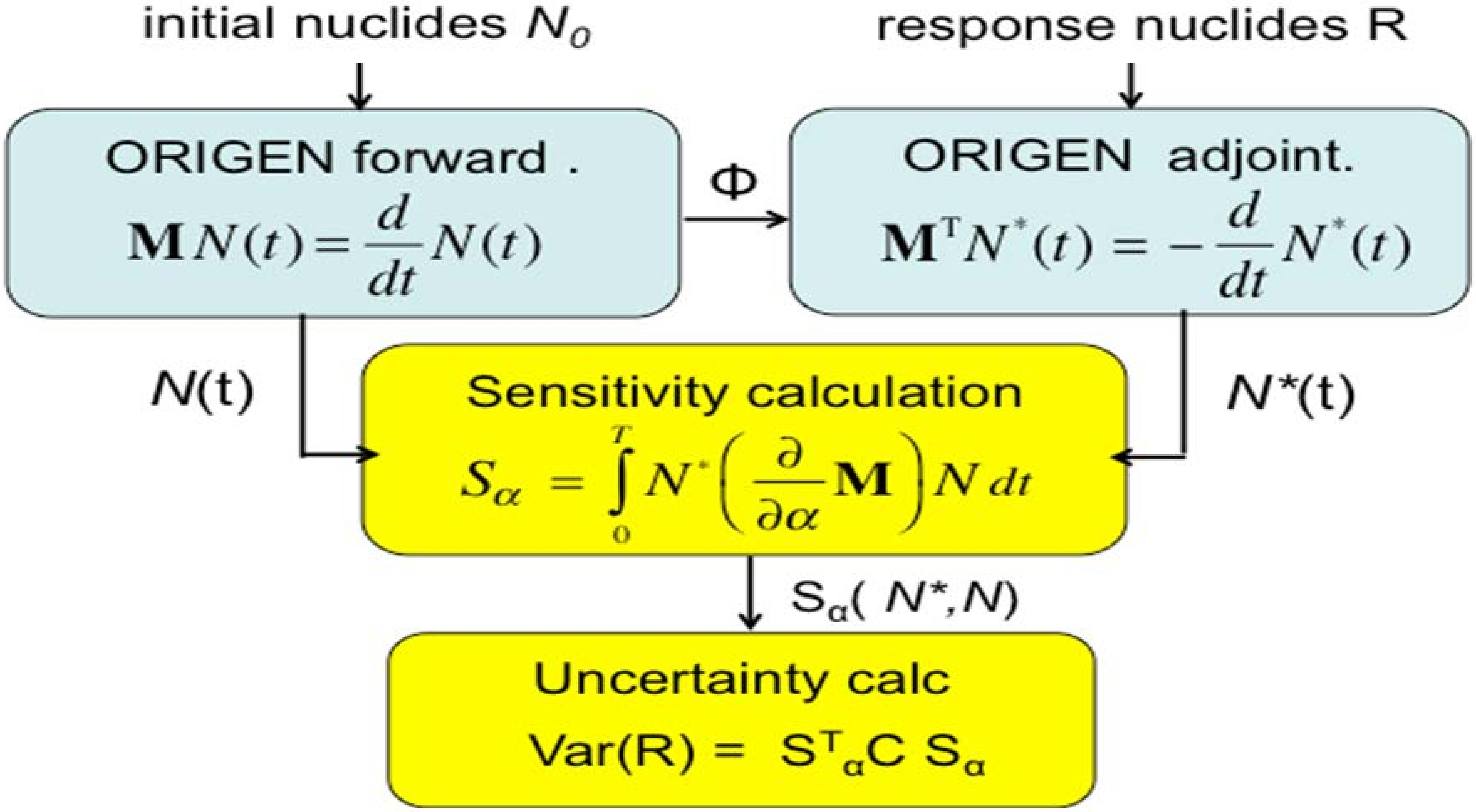
M. Pigni, M. W. Francis, **I. C. Gauld**, "Investigation of Inconsistent ENDF/B-VII.1 Independent and Cumulative Fission Product Yields with Proposed Revisions," *Nuclear Data Sheets* **1** (2015), https://doi.org/10.1016/j.nds.2014.12.040

Applying Integral Measurements for Data Evaluation

- Beyond code V&V and integral nuclear data library testing – can we use these measurements to target/improve specific nuclear data?
- Sensitivity coefficients useful for identifying responsible data
- Transmutation problems can be very complex due to time dependent nature of the coefficients (data importance)

I.C. Gauld, M.L. Williams, F. Michel-Sendis, and J.S. Martinez, “Integral Nuclear Data Validation Using Experimental Spent Nuclear Fuel Compositions,” *Nuclear Engineering and Technology 49 (2017) 1226-1233*. https://doi.org/10.1016/j.net.2017.07.002

Sensitivity/Uncertainty Calculations using Adjoints



Example: 3.5% Enriched PWR Fuel

Response= Pu-238 after 3-years irradiation to 30 GWd/tU and 3 year decay

Nuclear Data Relative Sensitivity Coefficients

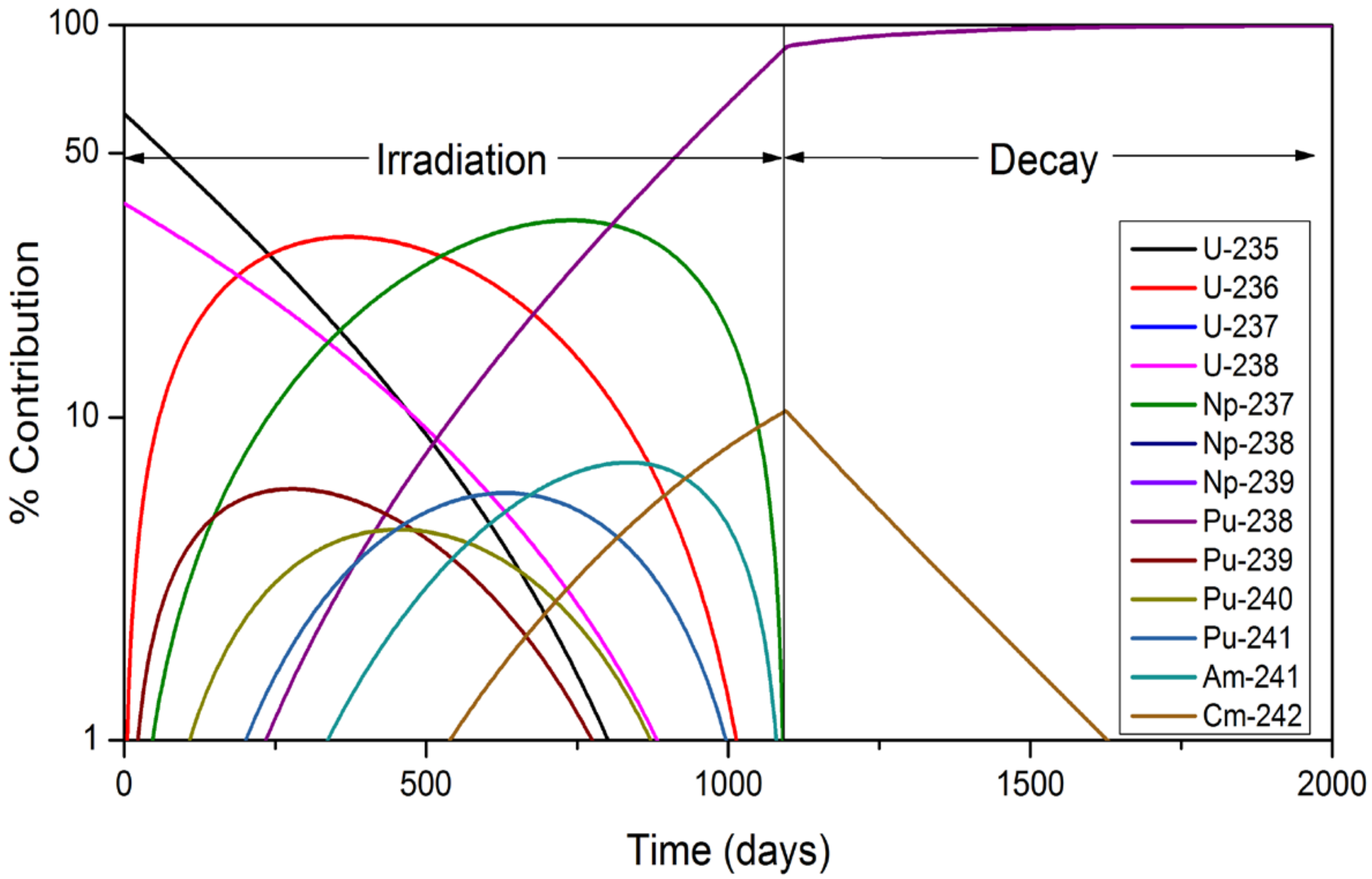
Parent nuclide	Product nuclide	Data type	S
^{237}Np	^{238}Np	(n,γ)	0.6136
^{235}U	^{236}U	(n,γ)	0.5928
^{236}U	^{237}U	(n,γ)	0.5877
^{241}Pu	^{241}Am	Half life	0.2132
^{238}U	^{239}U	(n,γ)	0.2155
^{242}Cm	^{238}Pu	Decay branch	0.2182
^{241}Pu	^{241}Am	Decay branch	0.2176
^{242}Am	^{242}Cm	Decay branch	0.2175
^{239}Pu	^{240}Pu	(n,γ)	0.1740
^{238}U	^{237}U	(n,2n)	0.1576
^{238}Pu	^{239}Pu	(n,γ)	-0.1475

Example: 3.5% Enriched PWR Fuel

Response= Pu-238 after 3-years irradiation to 30 GWd/tU and 3 year decay

- "*Contributon*" response:
  - $\mathbf{N}^T(t)\,\mathbf{N}^*(t) = R(T_F)$
  - Used for pathway analysis

$$\frac{d}{dt}\left[\mathbf{N}^{T}(t)\,\mathbf{N}^{*}(t)\right]\rightarrow 0$$



Looking Forward

- Define the application space and audience – what is entailed by “Radiation Characterization” codes/data.
- Identify additional benchmark data needs.
  - Many useful benchmarks are part of existing DBs (e.g., SINBAD, IRPhE, SFCOMPO)
  - Additional benchmarks missing from DBs?
  - Better coordination of existing databases helpful for end user V&V activities (e.g., link benchmarks to data/applications)
- Many radiation emission benchmarks and source characterization experiments have not been compiled/archived or do not easily fit in existing DBs.
- Evaluation, uncertainty analysis, and benchmark model development essential for the end users.
- Methods to apply integral benchmark testing for nuclear data evaluation.

Possible IRCBEP Organization/Roles