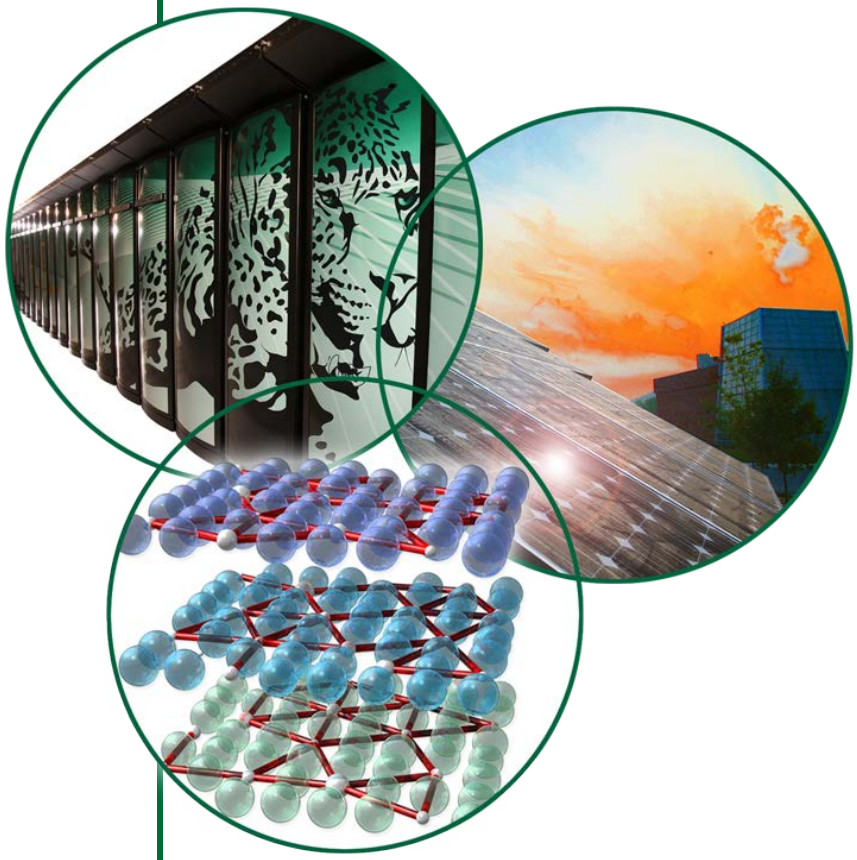
Application of SCALE for HTR-10 Spent Fuel Safeguards



Ian Gauld, Germina Ilas
Bryan Broadhead

Reactor and Nuclear Systems Division

RNSD
Reactor and Nuclear Systems Division

U.S. DEPARTMENT OF ENERGY

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Motivation

- What's the importance of fuel depletion to safeguards?

  Design of an effective safeguards approach for pebble bed spent fuel requires the capability to accurately predict the properties and radiation signatures of the fuel pebbles under a wide range of potential operating conditions, storage configurations, and fuel path scenarios

  – Spent fuel fissile inventories
  – Spent fuel verification
  – NDA using neutron and gamma detector design and optimization
  – Interpretation of other measurement techniques

- Also required to support
  – Burnup monitoring
  – Spent fuel monitoring and handling
  – Interim storage
  – Reprocessing or final repository

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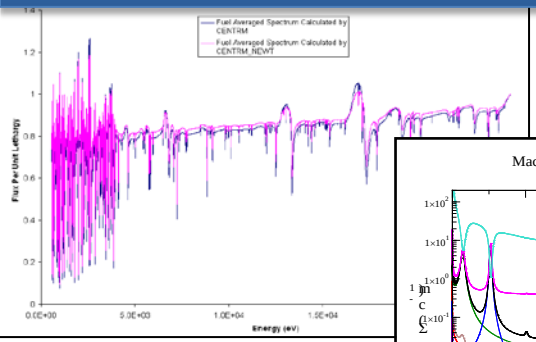
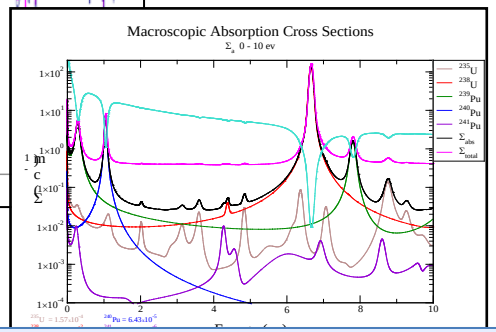
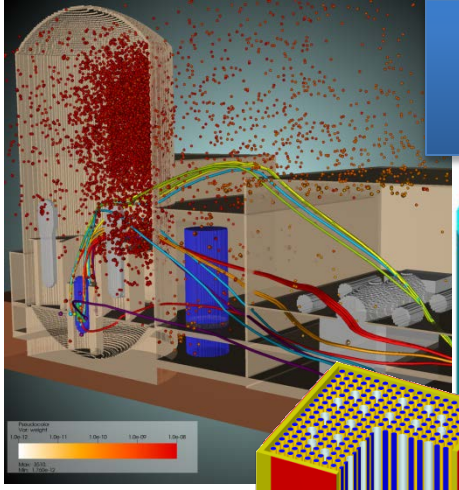
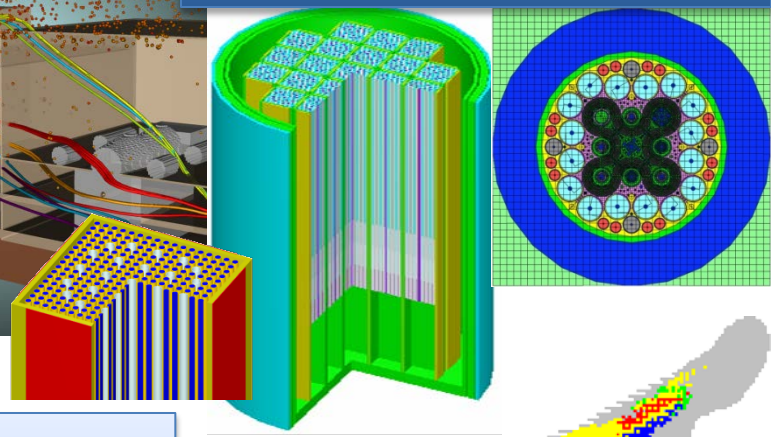
Convenient Material Input and Current Nuclear Data with Continuous-Energy Resonance Processing





High-Resolution Geometry Modeling in Monte Carlo and Deterministic Transport

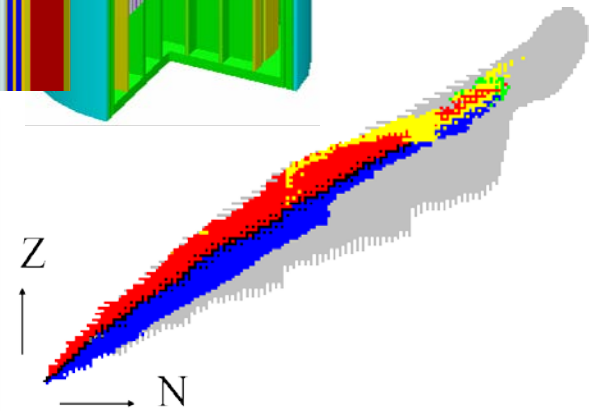


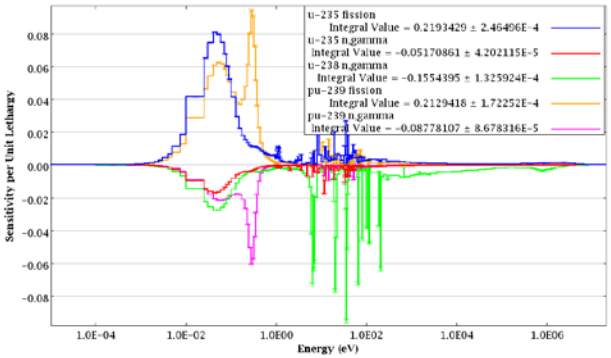


Radiation Shielding with Automated Variance Reduction

SCALE Capabilities

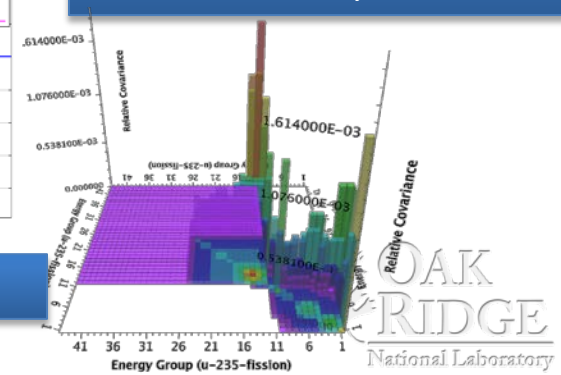
- Criticality safety
- Radiation shielding
- Cross-section processing
- Reactor physics
- Sensitivity and uncertainty analysis
- Spent fuel and HLW characterization





Sensitivity and Uncertainty Analysis

Depletion and Decay, Radiation Source Terms, and Decay Heat



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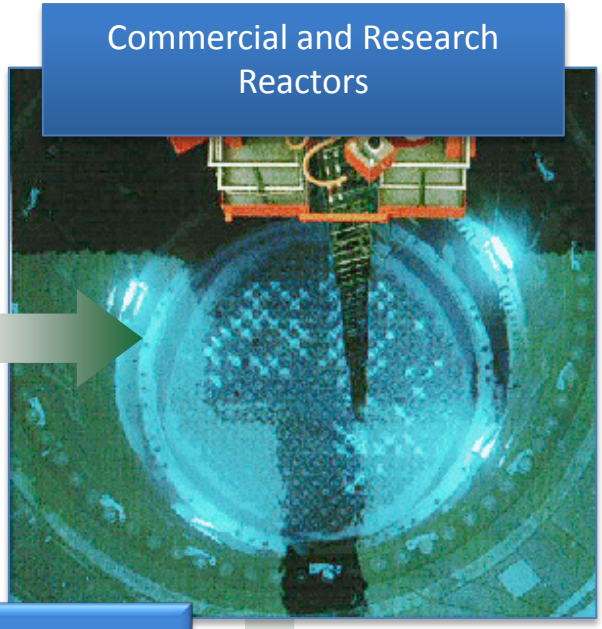
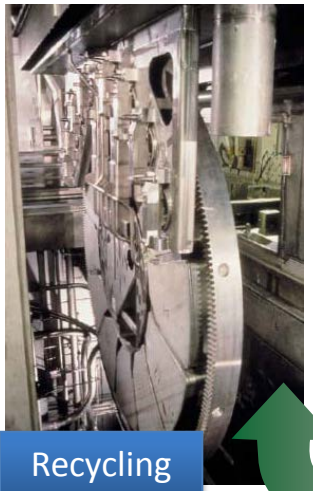
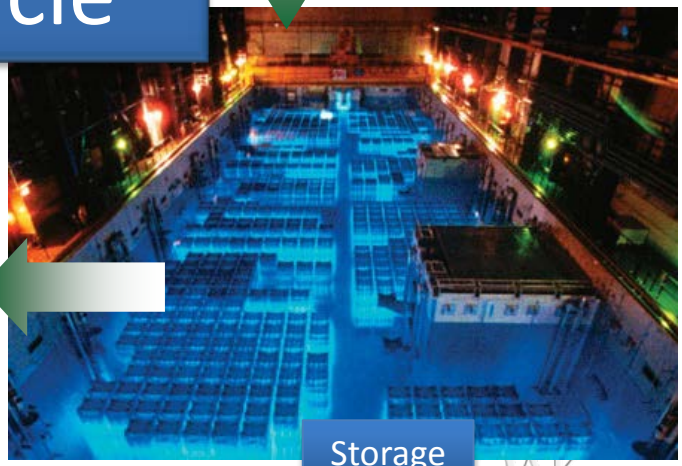
Applications of SCALE: The Nuclear Fuel Cycle







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SCALE 0.0 – SCALE 4.4a

1980 – 2000

Established for Nuclear Regulatory Commission

Provides an independent rigorous nuclear safety analysis capability for out-of-reactor license reviews

Key Capabilities

Criticality safety

Radiation source term characterization

Radiation shielding

Heat transfer

scale

Nuclear Systems Modeling & Simulation

SCALE 5.0 – SCALE 6.1

2004 – 2011

Expanded Capabilities to Address a Broader Class of Problems & Sponsors

Reactor physics

Shielding analysis with automated variance reduction

Sensitivity and uncertainty analysis

High-fidelity criticality safety in continuous energy

Graphical user interfaces and visualization tools

Expanding Use

Used in 40 nations by regulators, vendors, utilities, and researchers

SCALE 6.2 – SCALE 7.0

2012 – 2014

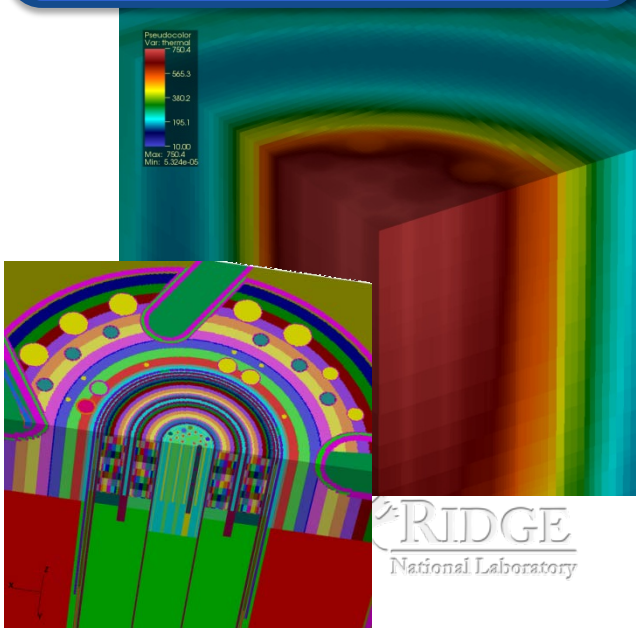
HPC Integration, Architecture Modernization, Further Expansion of Capabilities

Solutions for extremely complex systems

High-fidelity shielding, reactor physics and sensitivity analysis in continuous energy

Scalable from single core PCs to massively parallel machines

Integration with CASL Virtual Environment for Reactor Analysis



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SCALE Users

Regulators

Industry vendors

Utilities

Research laboratories

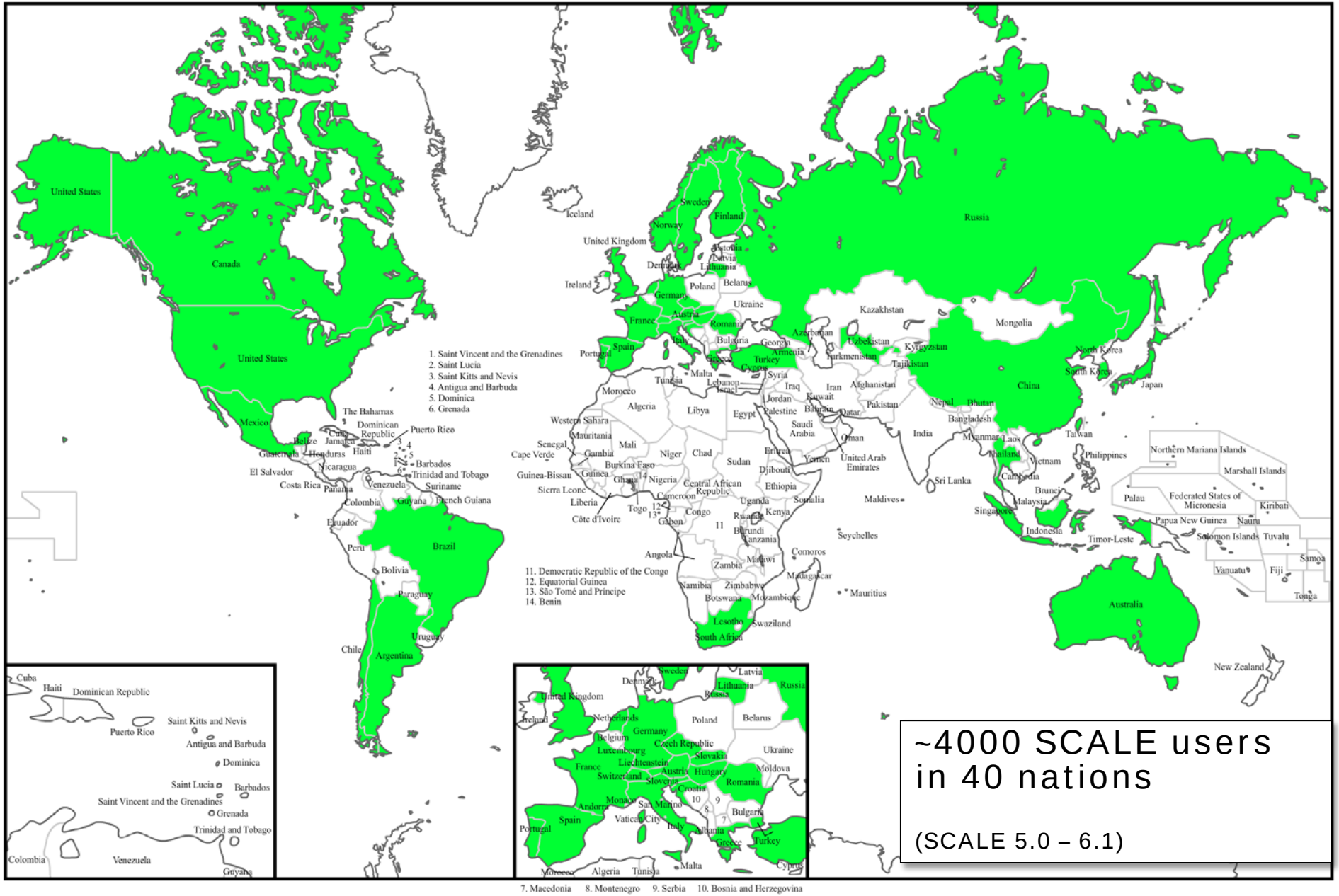
Government agencies

Universities

Software Distribution Process

- Releases provided to:
  - RSICC (Radiation Safety Information Computational Center)
  - OECD/NEA Data Bank (Organization for Economic Cooperation and Development – Nuclear Energy Agency)
- All users must apply to RSICC or NEA Data Bank for individual license for new version
- Full version (includes source code) and executable-only version are distributed
- International users are encouraged to request executable-only version

SCALE Map of the World

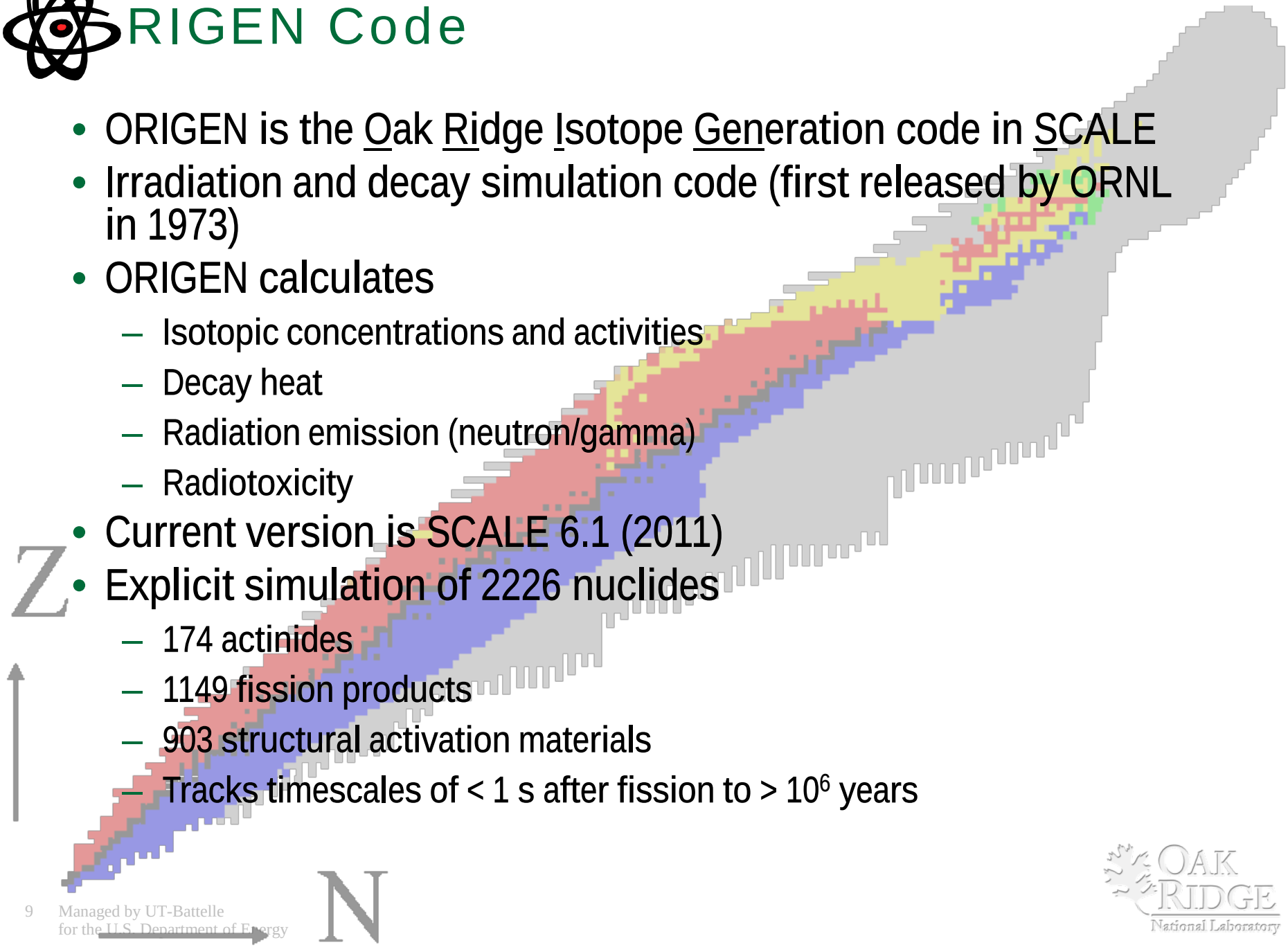


~4000 SCALE users in 40 nations

(SCALE 5.0 – 6.1)

ORIGEN Code

- ORIGEN is the Oak Ridge Isotope Generation code in SCALE
- Irradiation and decay simulation code (first released by ORNL in 1973)
- ORIGEN calculates
  - Isotopic concentrations and activities
  - Decay heat
  - Radiation emission (neutron/gamma)
  - Radiotoxicity
- Current version is SCALE 6.1 (2011)
- Explicit simulation of 2226 nuclides
  - 174 actinides
  - 1149 fission products
  - 903 structural activation materials
  - Tracks timescales of < 1 s after fission to > 10^6 years



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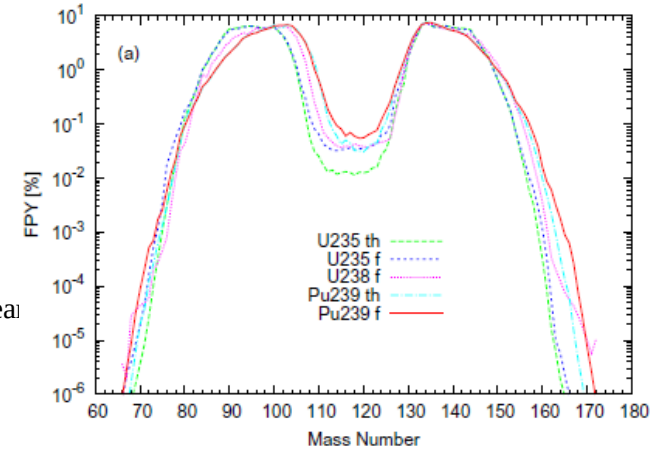
for the U.S. Department of Energy

Nuclear Data

- Decay data compiled entirely from ENDF/B-VII*
  - T ½
  - Decay modes β^-, β^+, EC, α, IT, $\beta^-\beta^-$, β^-n, SF, n, β^-α
- Neutron cross section libraries
  - ENDF/B-V, -VI, and –VII
  - Multigroup cross sections from JEFF-3.1/A activation file
  - 774 target nuclei, 12,617 neutron-induced reactions

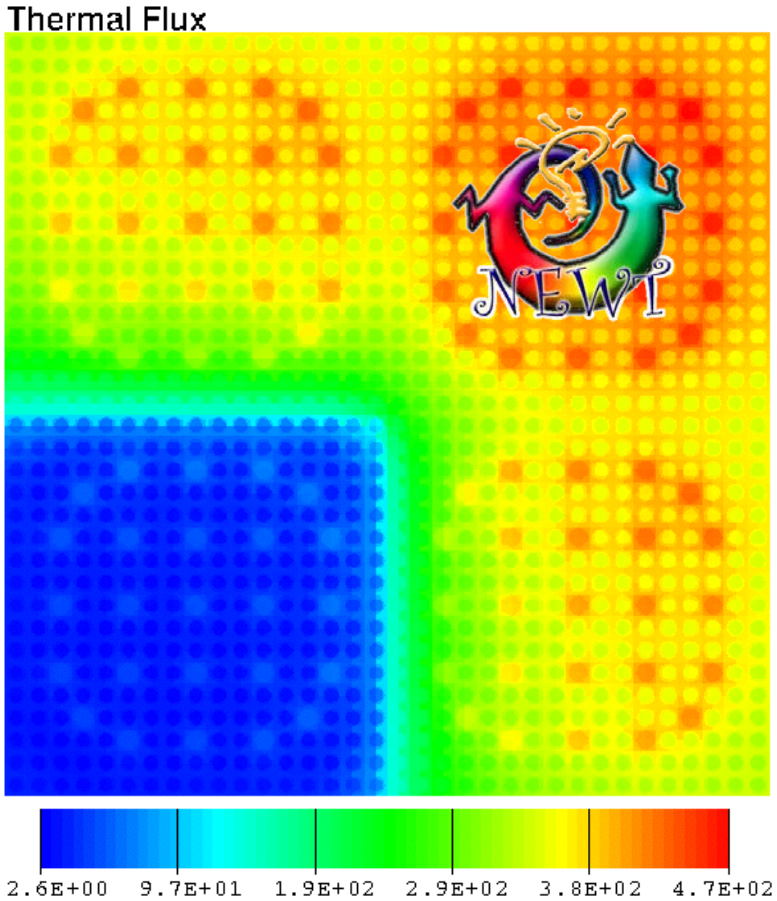
    (n,2n), (n,3n), (n,f), (n,nα), (n,n3α), (n,2nα), (n,3n α), (n,np), (n,n2α), (n,2n2α), (n,nd), (n,nt), (n,n ^{3}He), (n,nd2α), (n,nt2α), (n,4n), (n,g), (n,p), (n,d), (n,t), (n,^{3}He), (n,α), (n,2α), (n,3α), (n,2p), (n,pα), (n,t2α), (n,d2α), (n,n')
  - Available in 44-, 47-, 49-, 200-, and 238-energy groups
- Energy-dependent fission yields
  - ENDF/B-VII



* M. B. Chadwick, P. Oblozinsky, M. Herman et al., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nuclear Data Sheets* **107**, 2931–3060 (2006)..

ORIGEN Cross Section Generation

- Neutron cross sections are generated dynamically using fuel design and operating conditions
- SCALE couples ORIGEN calculations with detailed transport calculations
  - XSDRN (1-D SN)
  - NEWT (2-D SN)
  - KENO-V and –VI (3-D Monte Carlo)



Example of 2-D MOX-UOX lattice configuration

PBR Reactor Physics Studies

- 2002-2003: PBMR depletion benchmark
- 2007-2009: HTR-10 physics for depletion modeling
- 2009-2011: NGNP physics and depletion
  - Prismatic fuel design
  - Pebble fuel design

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PBMR Depletion Modeling (2003)

- Early work based on studies by Stoker, Reitzma, and Karriem (HTR 2002)
  - Developed SCALE procedure to create an ORIGEN library
  - Static cross section values (no burnup dependence)
  - C. Stoker (NECSA) provided technical data
- ORNL studies expanded this methodology to include time (burnup) dependent cross sections

I. C. Gauld, "Automated Depletion Analysis of PBMR Fuel Using SCALE," American Nuclear Society Transactions, vol. 91, p. 673–674 (November 2004).

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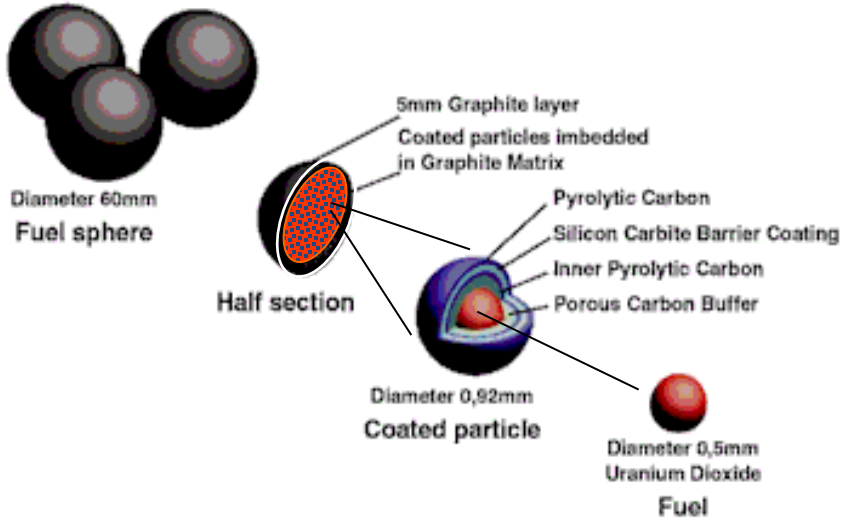
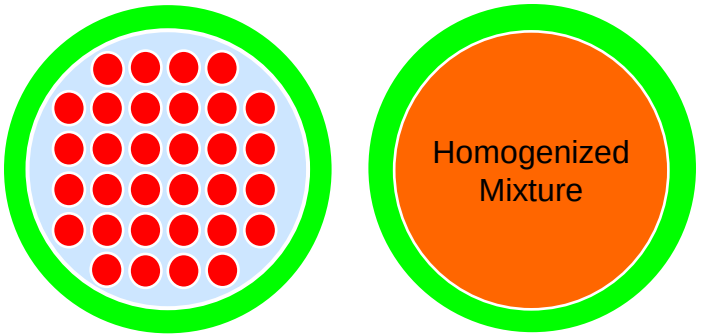
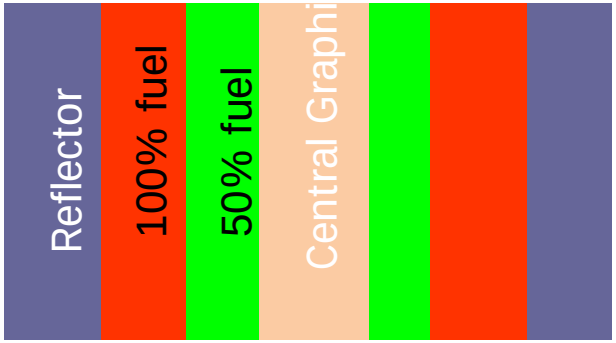
Fuel element design for PBMR



- XSDRN 1-D homogenization used for PBMR fuel cross section generation
- Level-1: UO_2 fuel grain and carbon/graphite grain coating
- Level-2: Pebble exterior coating, helium coolant / moderator

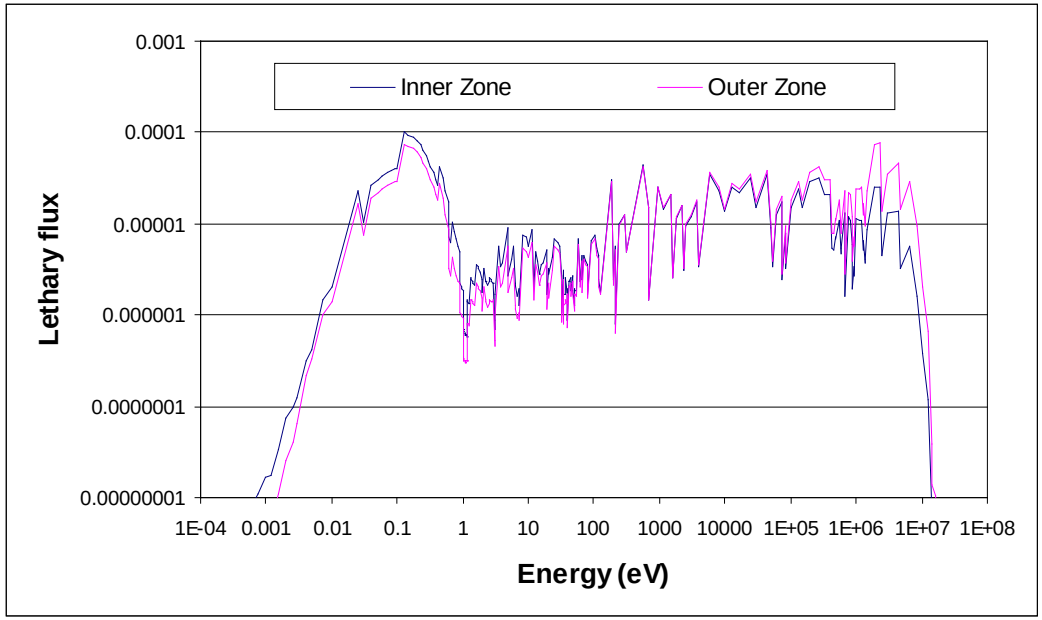




Simplified reactor model (cylindrical)

Benchmark - VSOP code

- South African PBMR fuel calculational model
  - 10 cycles (874 days)
  - 80,048 GWd/MTU discharge burnup
  - Enrichment of 8.07 wt % ^{235}U
  - 9 g U per pebble
  - Average power, 91.5 W/g U
  - Core design
    - Central graphite reflector region
    - External reflector
    - Inner fuel zone 50% fuelled pebbles
    - Outer fuel zone all fuelled pebbles



Benchmark Results

Neutron spectrum (normalized to 1.0)

Upper Energy	SCALE			VSOP	MCNP
	Fuel Core Avg	Inner Core Zone	Outer Core Zone		
10 MeV	0.162	0.123	0.175	0.167	0.183
100 keV	0.261	0.210	0.278	0.287	0.288
29 eV	0.068	0.061	0.070	0.070	0.072
1.86 eV	0.509	0.605	0.477	0.476	0.457

Pebble contents (grams)

Isotope	ORIGEN (Outer)	ORIGEN (Average)	VSOP	% Diff
^{235}U	0.125	0.120	0.119	< 1
^{238}U	7.90	7.91	7.92	< 1
^{239}Pu	0.0384	0.0370	0.0374	1.1
^{241}Pu	0.0174	0.0177	0.0199	11.1

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Cooperative Task 3

HTR-10 Safeguards Depletion Code Library (2007)

- Development with Tsinghua University
- Objective:
  - Develop improved computer modeling of spent fuel composition of PBMR reactor type for safeguards analysis
  - Generate HTR-10 libraries for the ORIGEN code
  - If possible, develop code benchmark and include results from Chinese codes and validate models/libraries using measured fuel data
- Accomplishments:
  - ORNL and LANL developed benchmark pebble bed fuel models using MCNPX and SCALE/ORIGEN
  - Technical reports on models and results issued

HTR-10 Modeling and Simulation

- Development and application of full-core 3-D models
- Monte Carlo transport (multigroup and continuous-energy cross sections)
- ORNL
  - SCALE Nuclear Modeling and Simulation Code System
  - KENO-VI coupled to ORIGEN for depletion
- LANL
  - MCNPX
  - CINDER depletion
- China

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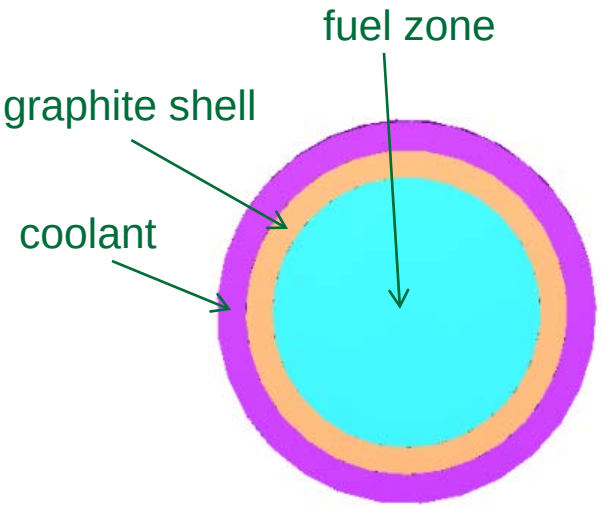
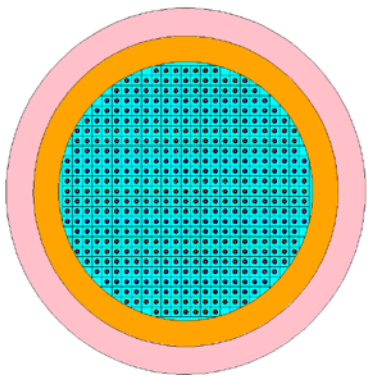
HTR-10 Fuel Models
SCALE Cross Sections for PBR Analysis





- **Fuel typical of HTR-10**
- **Temperature conditions:**
  300K fuel and coolant
  1200K fuel + 900K coolant
- **Analyzed parameters:**
  - **spectral indices**
  - **few-group xs for ^{235}U, ^{238}U**
  - **K_{inf}**

SCALE
238-gr ENDF/B-VII cross sections
DOUBLEHET option for self-shielding

MCNP
CE ENDF/B-VII cross sections
Explicit particle representation

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HTR-10 Fuel Models – Spectral indices at 1200K

Parameter	Significance	MCNP5	SCALE	Difference (%)
ρ_{28}	fast-to-thermal ^{238}U capture ratio	**10.218**	**10.414**	**1.9**
$\delta_{25} \times 10^2$	fast-to-thermal ^{235}U fission ratio	**12.319**	**12.279**	**-0.3**
$\delta_{28} \times 10^4$	^{238}U fission to ^{235}U fission ratio	**14.519**	**14.058**	**-3.2**
C^*	^{238}U capture to ^{235}U fission ratio	**0.254**	**0.258**	**1.7**

Good agreement for fuel cross sections obtained with SCALE and MCNP

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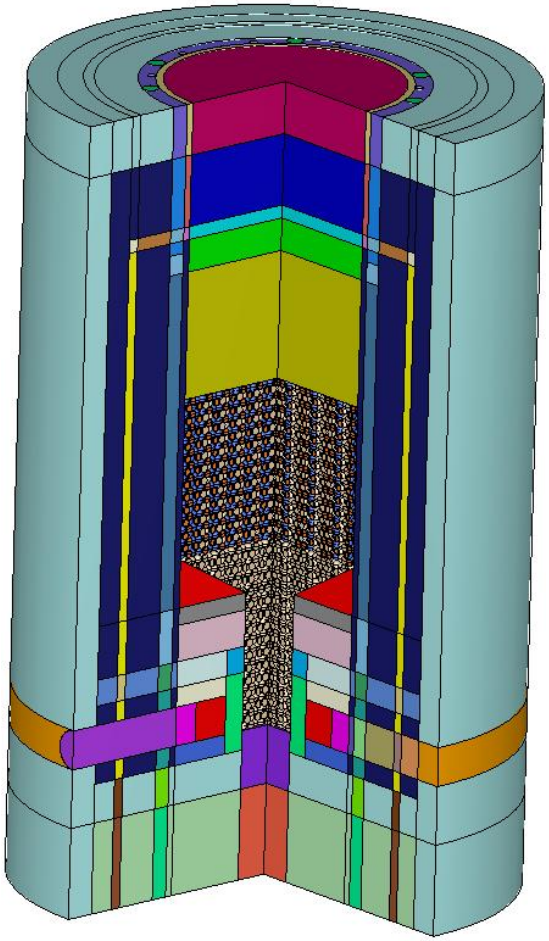
Benchmark - HTR-10 First Critical Core

- OECD/NEA International Reactor Physics Experiments (IRPhE) 2009 benchmark
  - High-fidelity HTR-10 model

- Fuel specifications:
  - 61% pebble packing fraction
  - 16,890 fuel and moderator pebbles in the active core region
  - 57:43 fuel-to-moderator pebble ratio
  - 5.0 g U loading in each fuel pebble
  - 17 wt% ^{235}U enrichment



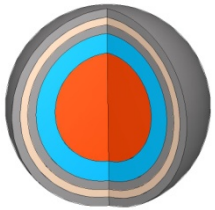
SCALE/KENO-VI model for HTR-10

Challenge: An accurate model of the doubly-heterogeneous fuel region

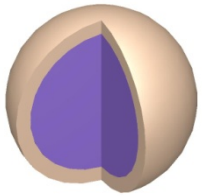
Thousands of particles in fuel region

Fuel and graphite pebbles packed in a unit cell

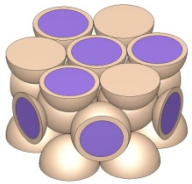
Unit cells arranged into a layer



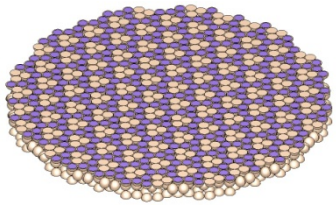
TRISO Particle
Radius = 0.0455 cm
(First level of Heterogeneity)



Fuel Pebble
Radius = 3 cm
(Second level of Heterogeneity)

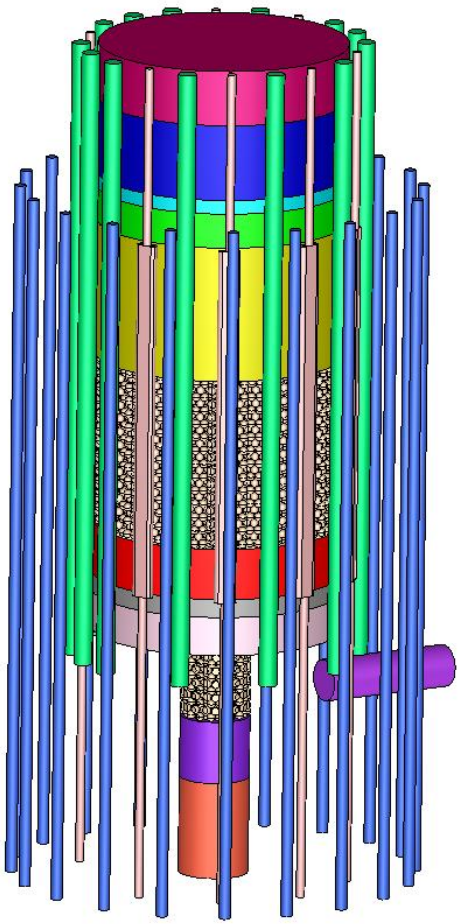


Hexagonal Prism Unit Cell



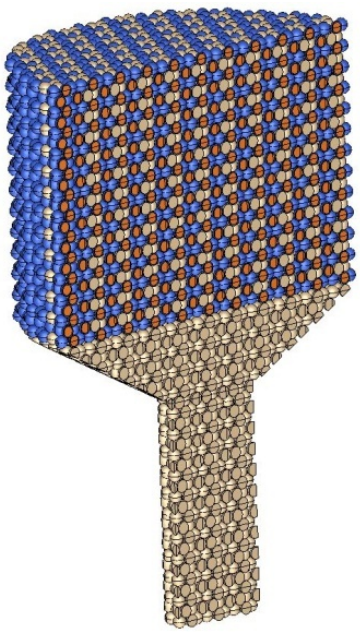
Hexagonal Lattice

HTR-10 Benchmark – Modeling details

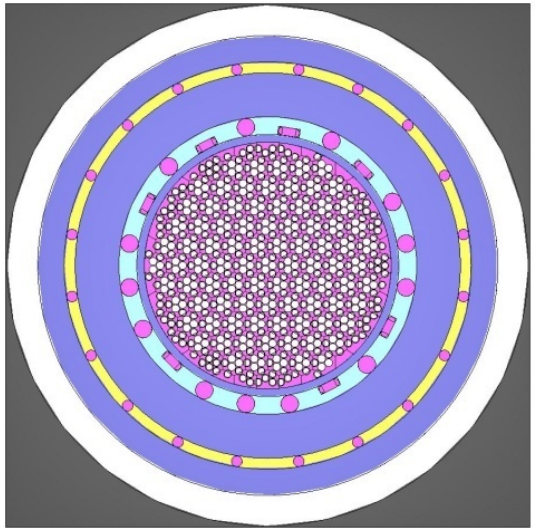


Details of the reflector region

High-fidelity benchmark



Details of the fuel and moderator pebbles region



Horizontal cross-sectional view of High-Fidelity Model

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HTR-10 First Critical Core Benchmark – Results

High-Fidelity Model	Data Library	K_{eff}	Standard deviation	ΔK_{eff} (pcm)
SCALE/KENO-VI (ORNL model)	238-group ENDF/B-VII.0	1.01311	0.00025	-162 ± 33
MCNP5 (IRPhE model, revised by ORNL)	CE ENDF/B-VII.0	1.01473	0.00021	

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Unique challenges for PBR depletion

- Modeling of approach to equilibrium
  - Initial fresh fuel (uniform compositions)
  - At equilibrium fresh pebble introduced to equilibrium core (heterogeneous challenge to double het problem)
  - Stoker et al. demonstrated importance of surrounding fuel on pebble cross sections: *C. C. STOKER, F. REITSMA and Z. KARRIEM, "Creation of the Equilibrium Core PBMR ORIGEN-S Cross Section Library," Proceedings of the Conference on High Temperature Reactors, HTR 2002, Petten, Netherlands, April 22-24 (2002)*

    Pebble cross sections dominated by compositions of surrounding fuel
  - Depletion calculations using a reflected pebble unit cell will be highly inaccurate (unlike typical LWR simulations with assembly models)
- Sensitivity of cross sections to location in reactor core (random)
  - Long neutron path length

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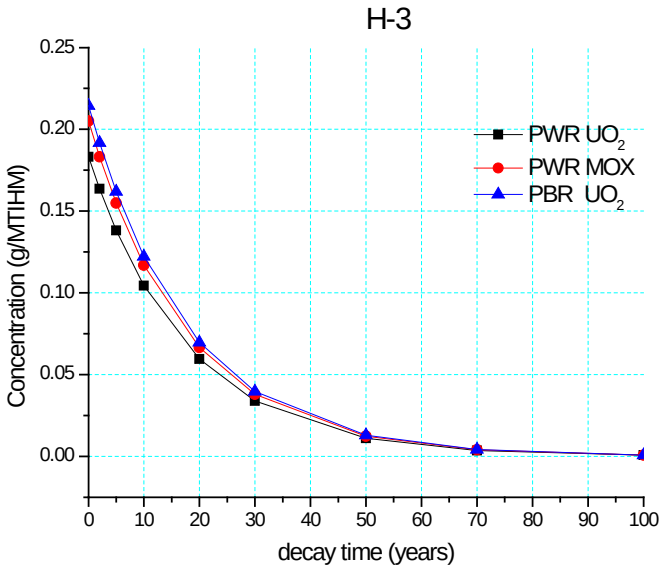
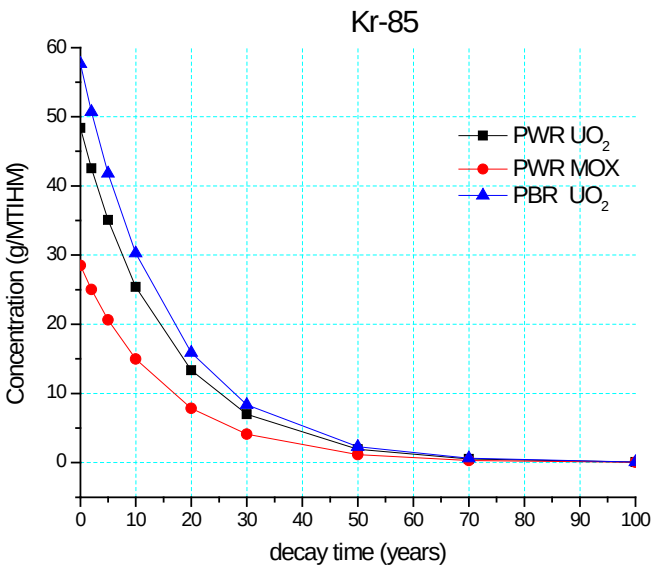
Unique challenges for PBR depletion (cont.)

- Limited validation data
  - Code performance experience with LWR fuel can not be automatically extended to PBR design



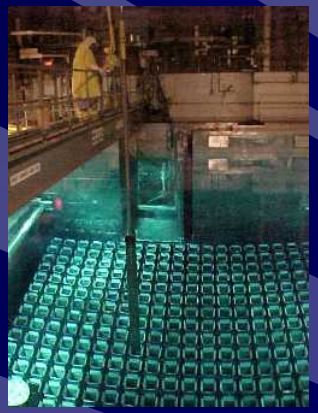


Example - Comparison of H-3 and Kr-85 content vs. decay time for three reactor fuels (PBR NGNP fuel considered)

Applications of Depletion Analysis to Safeguards

Spent Fuel Safeguards

Spent fuel stored in water pools



Spent fuel dry storage cask

ORIGEN Code has been integrated as an automated spent fuel Data Analysis Module for the EURATOM RADAR (Remote Acquisition of Data and Review software) System for Unattended Measurements

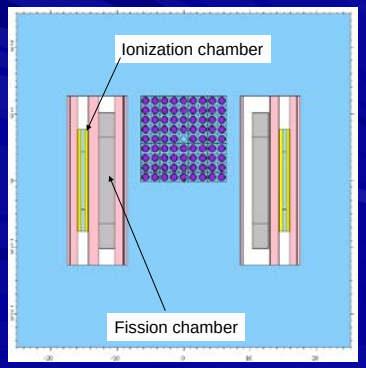
This approach is being considered for implementation by the IAEA

IAEA requires spent fuel assembly measurements (neutron-gamma) detector prior to storage

Fuel declarations

ORIGEN

Perform fuel burnup and neutron-gamma source analysis

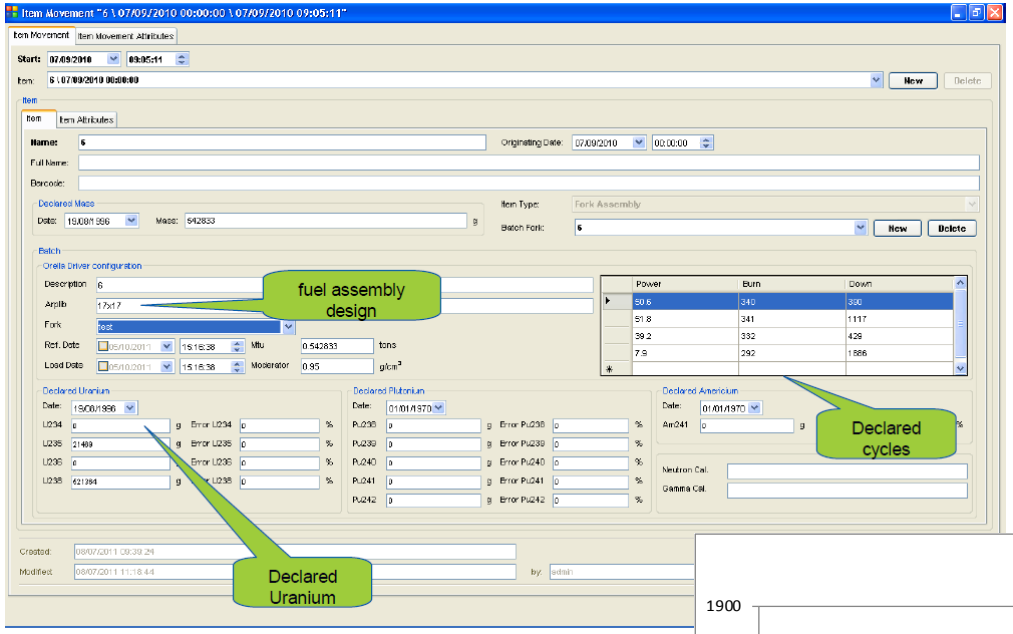


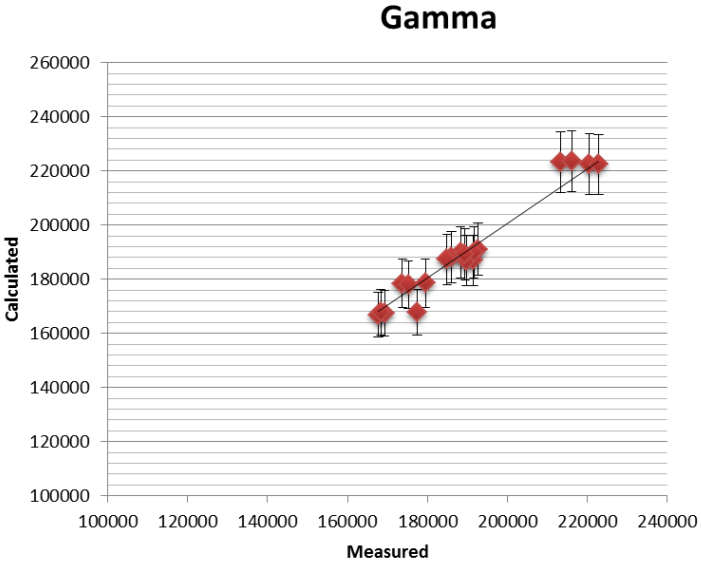
Apply detector responses simulated for the Fork detector measurement configuration

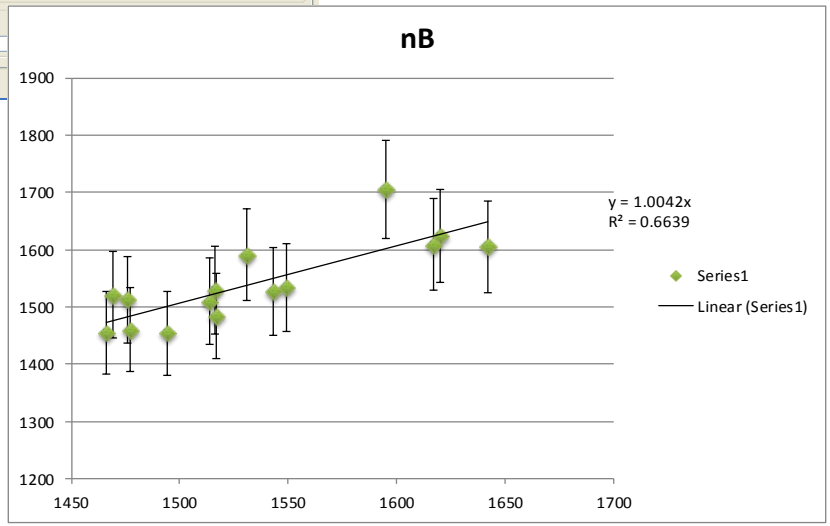
Declared material is independently verified by comparing measured detector signals and expected signals based on declared assembly information

RADAR - Analysis of Operator Declaration

CASTOR cask loading







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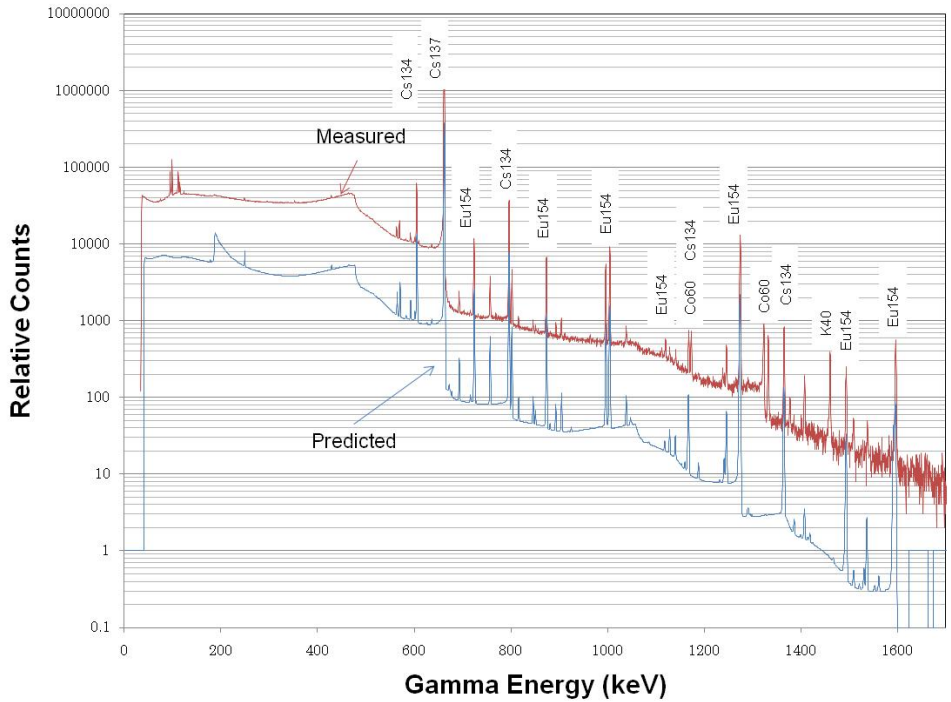
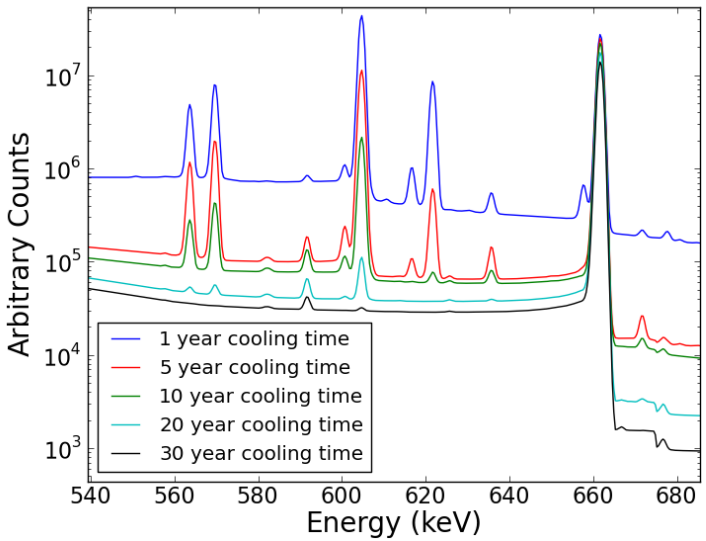
Gamma Spectroscopy
Detector Response Simulation

- Simulate HPGe gamma detector response to support NDA measurements
  - GADRAS code (Sandia National Laboratory) for detector simulation
  - ORIGEN code for gamma spectra
  - 2000 simulated energy channels





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ORIGEN Validation for LWR Fuel Depletion Analysis

Summary of PWR data for isotopic validation

Reactor	Measurement Laboratory	Experimental Program	Assembly Design	Enrichment (wt % ^{235}U)	No. of Samples/ Fuel Rods	Burnup (GWd/MTU)
Trino Vercellese	Ispra, Karlsruhe	JRC	15 × 15	2.72, 3.13, 3.897	15/5	7.2–17.5
	Ispra, Karlsruhe	JRC	15 × 15	3.13	16/5	12.8–25.2
Obrigheim	Ispra, Karlsruhe	JRC	14 × 14	2.83, 3.00	22/6	15.6–38.1
	ITU, IRCh, WAK, IAEA	ICE	14 × 14	3.13	5/5	27.0–29.2
H. B. Robinson-2	PNNL	ATM-101	15 × 15	2.561	4/1	16.0–31.7
Turkey Point-3	Battelle-Columbus	NWTS	15 × 15	2.556	5/1	30.5–31.6
Calvert Cliffs-1	PNNL, KRI	ATM-104	14 × 14	3.038	3/1	27.4–44.3
	PNNL	ATM-103	14 × 14	2.72	3/1	18.7–33.2
	PNNL, KRI	ATM-106	14 × 14	2.453	3/1	31.4–46.5
Takahama-3	JAERI	JAERI	17 × 17	2.63, 4.11	16/3	14.3–47.3
TMI-1	ANL	DOE YMP	15 × 15	4.013	11/1	44.8–55.7
	GE-VNC	DOE YMP	15 × 15	4.657	8/3	22.8–29.9
Gösgen	SCK•CEN, ITU	ARIANE	15 × 15	3.5, 4.1	3/2	29.1–59.7
	SCK•CEN, PSI, CEA	MALIBU	15 × 15	4.3	3/1	47.2—70.4
GKN II	SCK•CEN	REBUS	18 × 18	3.8	1/1	54.0

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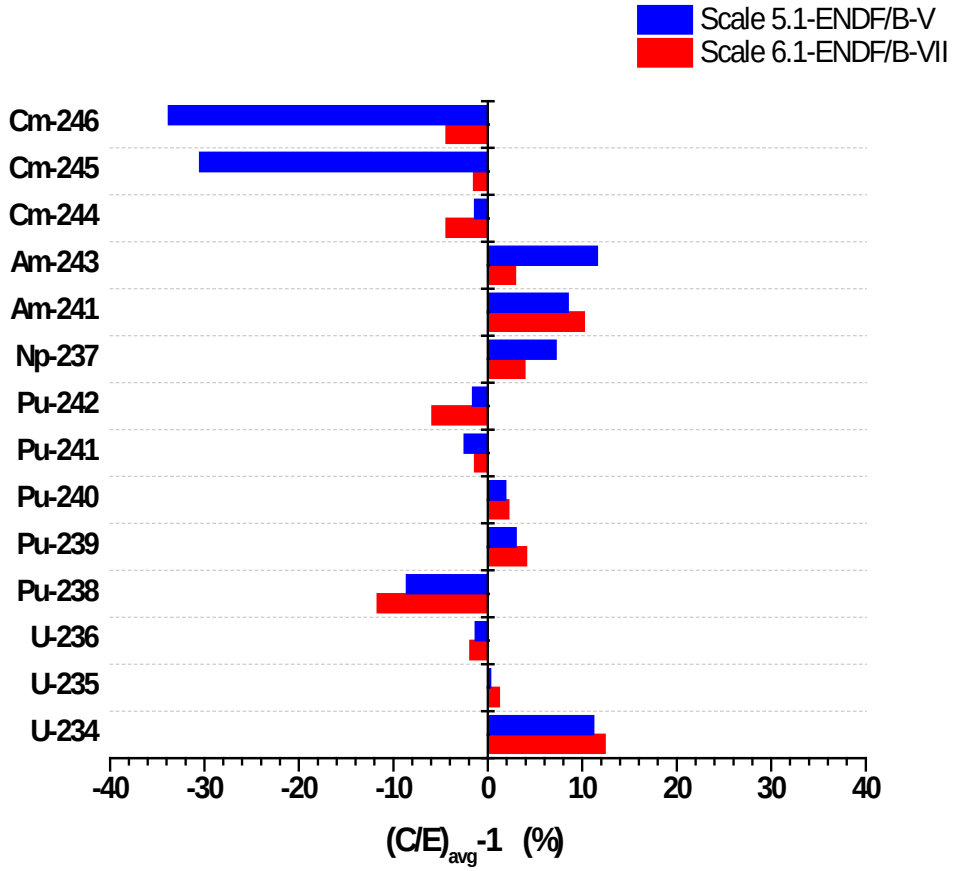
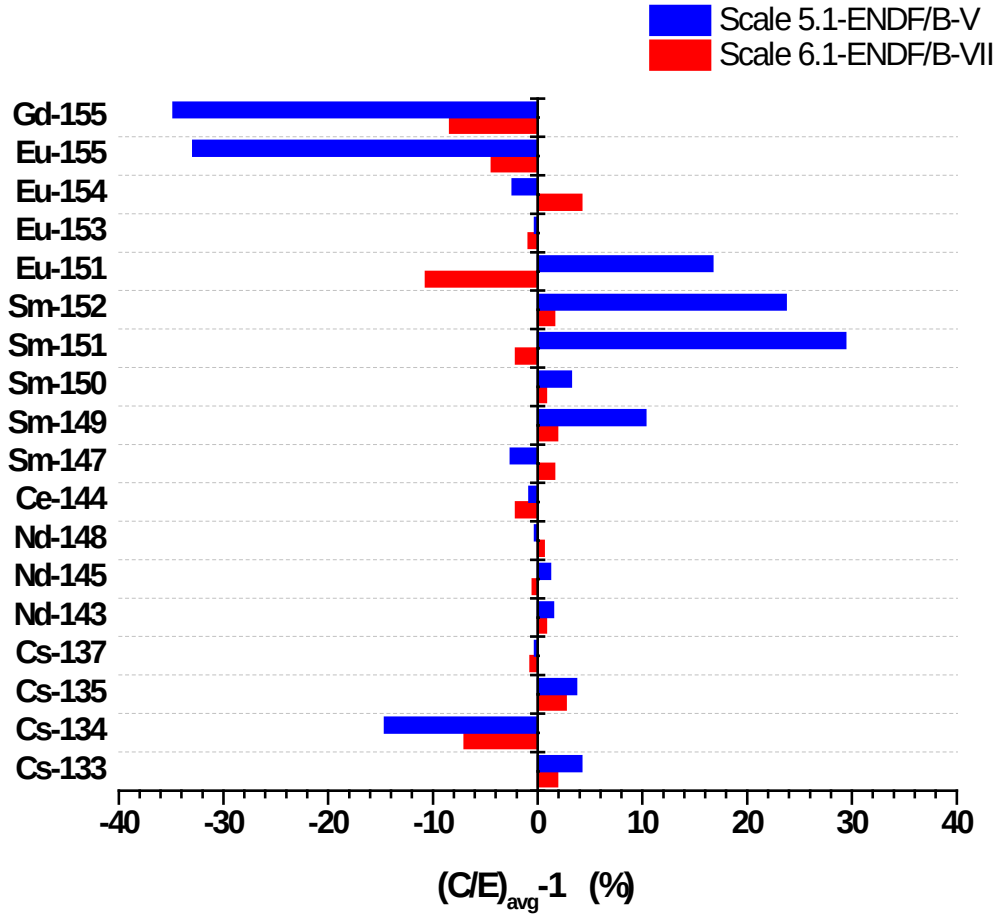
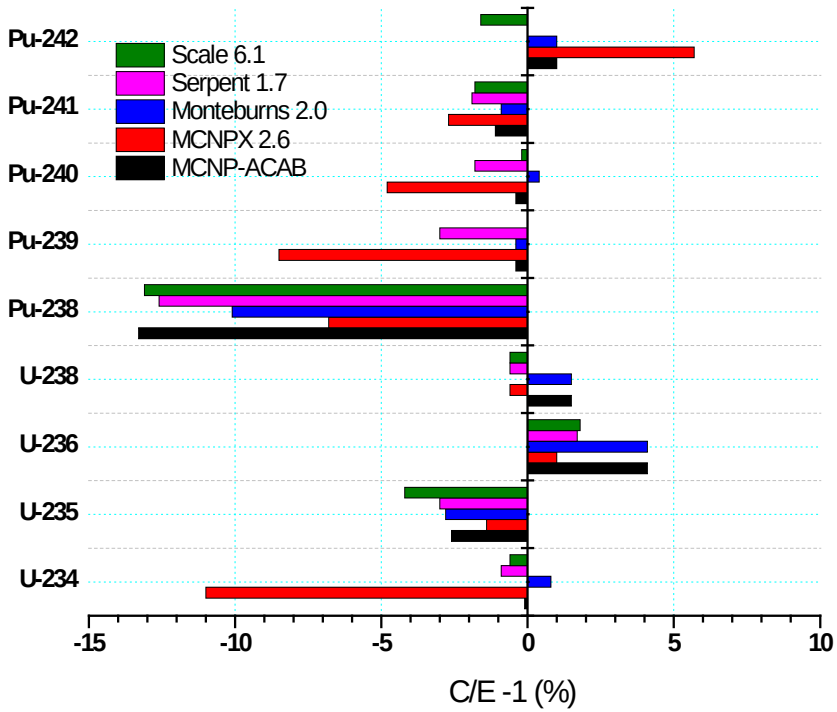
Actinides – comparison calculation-experiment



Fission products – comparison calculation-experiment

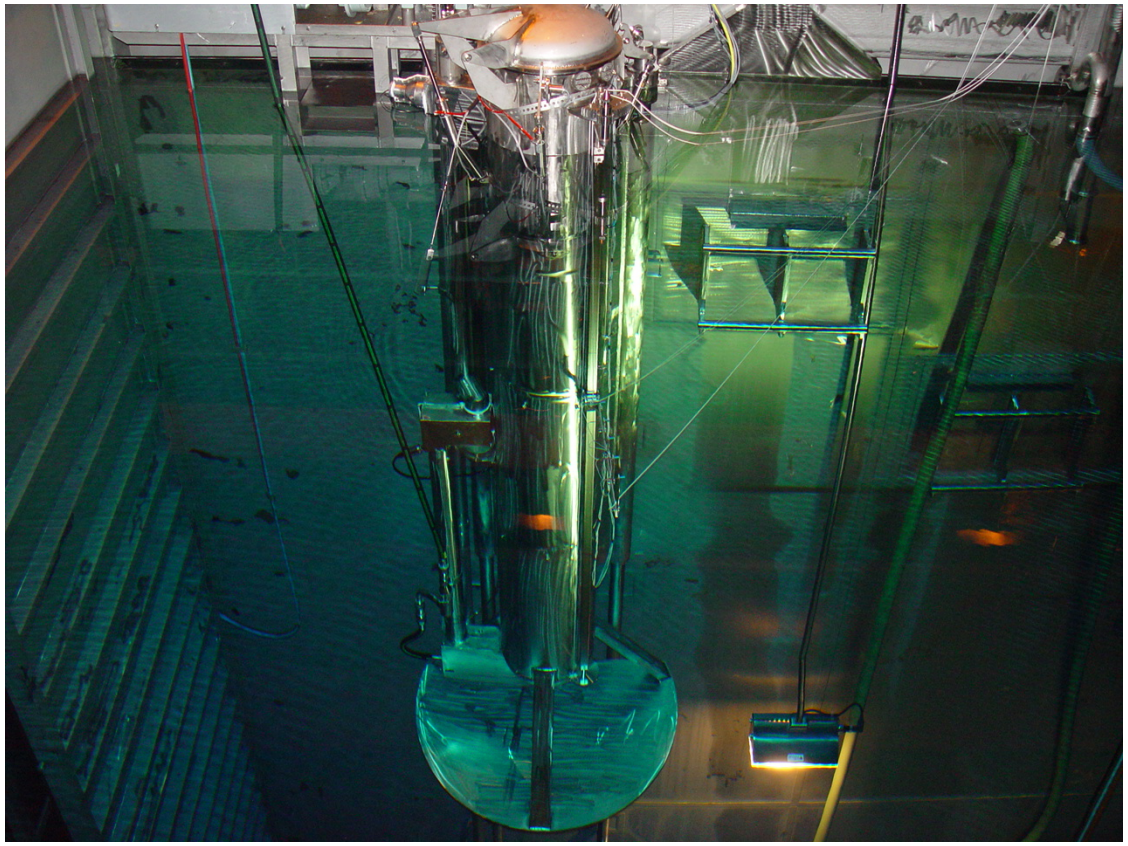


How well does SCALE perform compared to other codes?



C/E comparison for OECD/NEA burnup credit computational benchmark phase I-B, case A

Decay Heat Validation –long decay time



Spent fuel assembly calorimeter at the Swedish CLAB facility

SCALE Decay Heat Validation – Results

- Comparison calculation – experiment
  - 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

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Relevant references on ORIGEN methods and applications

I. C. Gauld, G. Radulescu, G. Ilas, B. D. Murphy, M. L. Williams, and D. Wiarda, *Isotopic Depletion and Decay Methods and Analysis Capabilities in SCALE*, Nuclear Technology, vol.174, no.2, p.169 (May 2011).

G. Ilas, I. C. Gauld, and G. Radulescu, *Validation of new depletion capabilities and ENDF/B-VII data libraries in SCALE*, to be published in Annals of Nuclear Energy (accepted March 2012).

C. McGraw and G. Ilas, *PWR ENDF/B-VII Cross-Section Libraries for ORIGEN-ARP*, CD Proceedings, PHYSOR 2012, Knoxville, TN (April 2012).

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S. M. Bowman and I. C. Gauld, *OrigenArp Primer: How to Perform Isotopic Depletion and Decay Calculations with SCALE/ORIGEN*, ORNL/TM-2010/43, Oak Ridge National Laboratory, Oak Ridge, TN (2010).

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G. Ilas, I. C. Gauld, F. C. Difilippo, and M. B. Emmett, *Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—Calvert Cliffs, Takahama, and Three Mile Island Reactors*, NUREG/CR-6968, U.S. Nuclear Regulatory Commission Office of Nuclear Regulatory Research (2010).

G. Ilas, I. C. Gauld, and B. D. Murphy, *Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—ARIANE and REBUS Programs (UO_2 Fuel)*, NUREG/CR-6969 (ORNL/TM-2008/072), U.S. Nuclear Regulatory Commission Office of Nuclear Regulatory Research (2010).

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G. Ilas, *On SCALE validation for PBR analysis*, CD Proceedings, PHYSOR 2010, Pittsburgh, PA (2010).

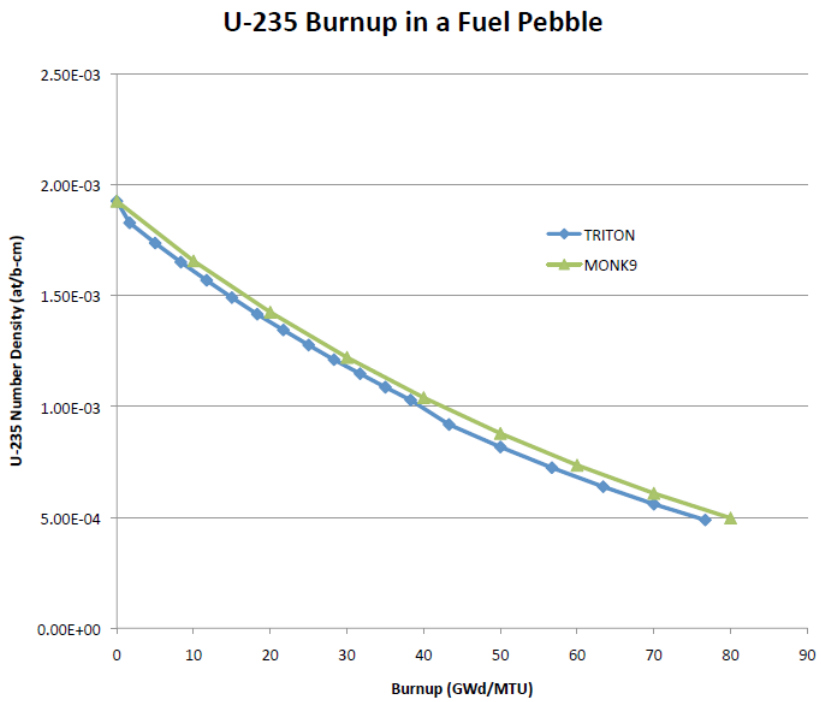
E. E. Sunny and G. Ilas, *SCALE 6 analysis of HTR-10 pebble-bed reactor for initial critical configuration*, CD Proceedings, PHYSOR 2010, Pittsburgh, PA (2010.)

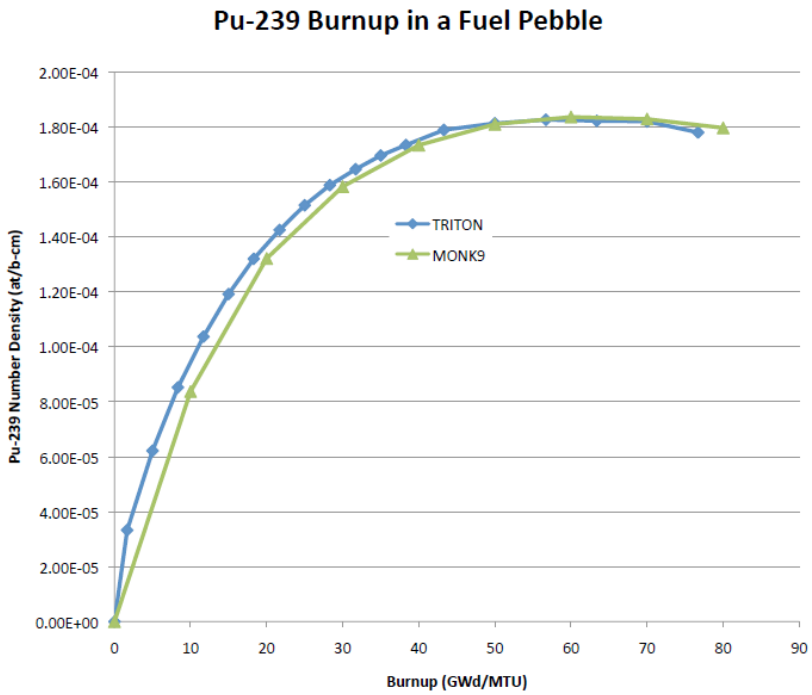
G. Ilas and I.C. Gauld, *SCALE analysis of CLAB decay heat measurements for LWR spent fuel assemblies*, Annals of Nuclear Energy vol.35, no.1 (January 2008).

I. C. Gauld, *Automated Depletion Analysis of PBMR Fuel Using SCALE*, American Nuclear Society Transactions, vol. 91, p. 673–674 (November 2004).

PBMR Depletion Studies

SCALE comparison with MONK Code (UK)





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