Karlsruhe Institute of Technology

Monte Carlo neutronics investigations of VVER-1000 fuel assemblies

L. Mercatali[1]***, A. Venturini***[2]***, V.H. Sanchez***[1]

[1]**KIT- Institute for Neutron Physics and Reactor Technology (Germany)**
[2]**University of Pisa (Italy)**

Annual Meeting on Nuclear Technology (Berlin, May 5-7 2015)

Institute for Neutron Physics and Reactor Technology

luigi.mercatali@kit.edu

Outline

- Introduction & motivation
- The *“OECD VVER-1000 LEU and MOX Assemblies Burnup Computational Benchmark”*
  1. Specifications
  2. Modeling of the benchmark exercises
  3. Results
     - Monte Carlo & deterministic static solutions
     - Burn-up
       - k_{inf}
       - Nuclide concentrations
     - Pin-by pin fission rates
- Summary and conclusions

Introduction & motivation

- The loading of <u>M</u>ixed Uranium Plutonium <u>OX</u>ide (MOX) and <u>L</u>ow <u>E</u>nriched <u>U</u>ranium (LEU) fuels in commercial nuclear reactors requires well validated computational methods and codes capable to provide reliable predictions of the neutronics characteristics of such fuels in terms of reactivity conditions (k_{inf}), nuclide inventory and pin power generation over the entire fuel cycle length

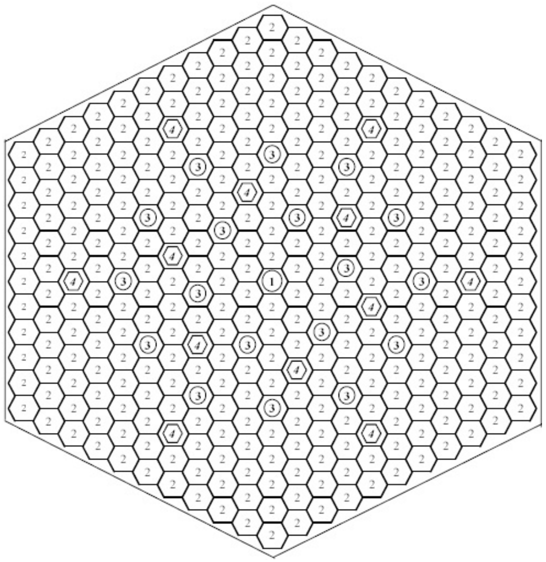
- Within the framework of Joint United States/Russian Fissile Materials Disposition Program an important task is to verify and validate neutronics codes for the use of MOX fuel in VVER-1000 reactors

- In this work new solutions for the (UO_2+Gd) and (UO_2+PuO_{2+}Gd) fuel assemblies proposed within the *"<u>OECD VVER-1000 LEU and MOX Assemblies Burnup Computational Benchmark</u>"* have been produced

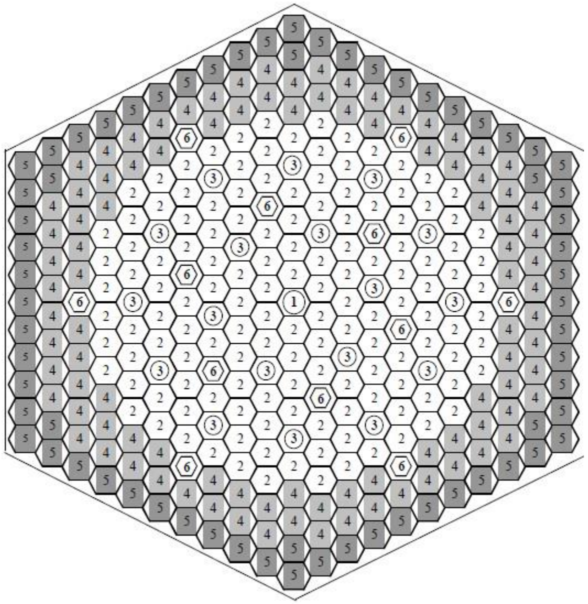
- The SCALE and SERPENT codes have been used with ENDF/B-VII and JEFF3.1 nuclear data libraries (NDLs)

OECD VVER-1000 burnup computational benchmark – LEU/MOX assemblies

- **The LEU assembly consists of low enriched fuel rods (3.7 wt %) and 12 rods poisoned with 4.0 wt % of gadolinium (3.6 wt % ^{235}U)**
- **The MOX assembly contains fuel rods with three different plutonium loadings: the central region with 4.2 wt % of fissile plutonium (93 wt % ^{239}Pu), two outer rings a 3.0 wt % and the outermost ring a 2.0 wt %**



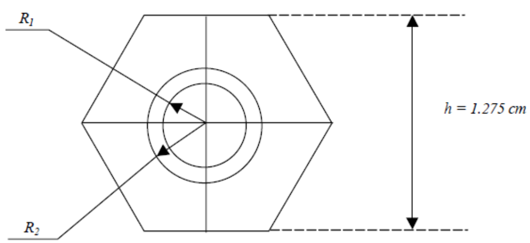
LEU



MOX

OECD VVER-1000 benchmark – specifications

Karlsruhe Institute of Technology



S1 - S2: Poisons (Xe + Sm) effects

S2 - S3: Doppler coefficient

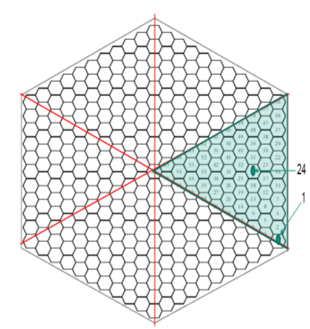
S3 - S4: Boron effect

S4 - S5: Moderator temperature coefficient

Operational states

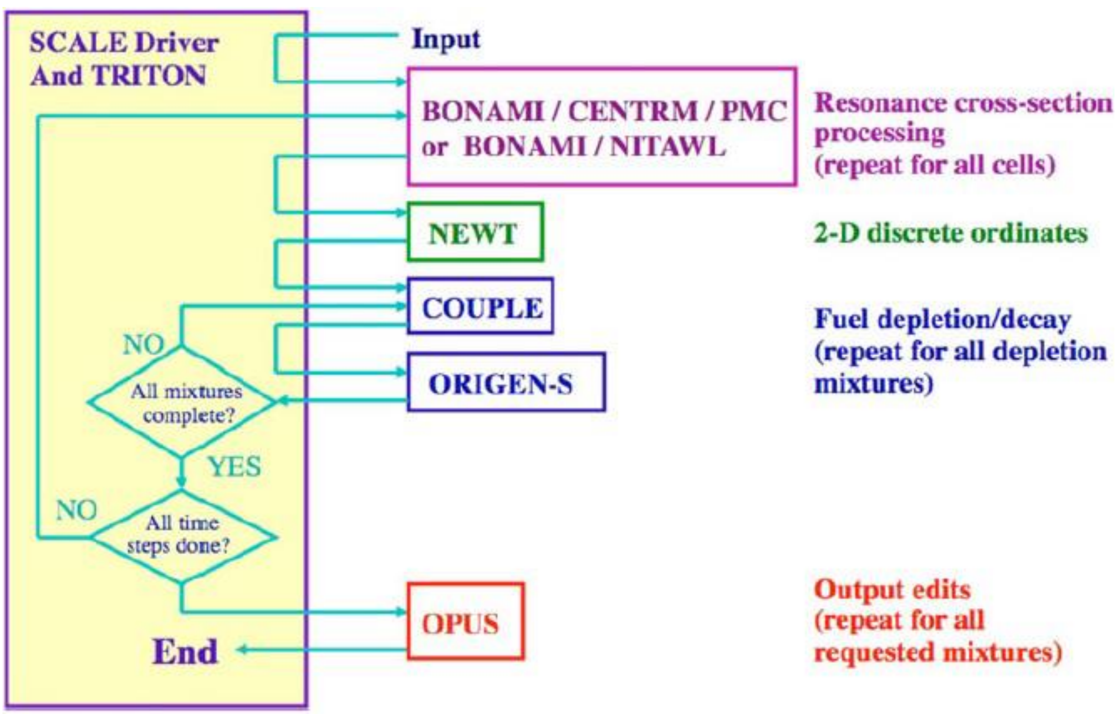
State	Fuel temp. K	Non-fuel temp. K	^{135}Xe,^{149}Sm	Boron [ppm]	Moderator density [g/cm^3]
S1	1027	575	Eq.	600	0.7235
S2	1027	575	0.0	600	0.7235
S3	575	575	0.0	600	0.7235
S4	575	575	0.0	0.0	0.7235
S5	300	300	0.0	0.0	1.0033

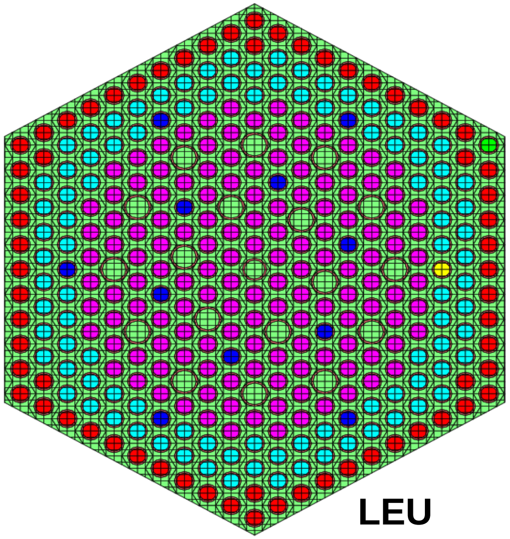
- Constant power density: 108 MW/m^3
- Requested responses: k_{inf} for state S1 at each burn-up step
  - k_{inf} for states S2-S5 at 0, 20, 40 MWd/kgHM
  - Pin-by-pin fission rate distribution
  - Nuclide assembly average concentrations + nuclide average concentrations in cell 1 and cell 24 for ^{235}U, ^{236}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{135}Xe, ^{149}Sm, ^{155}Gd and ^{157}Gd



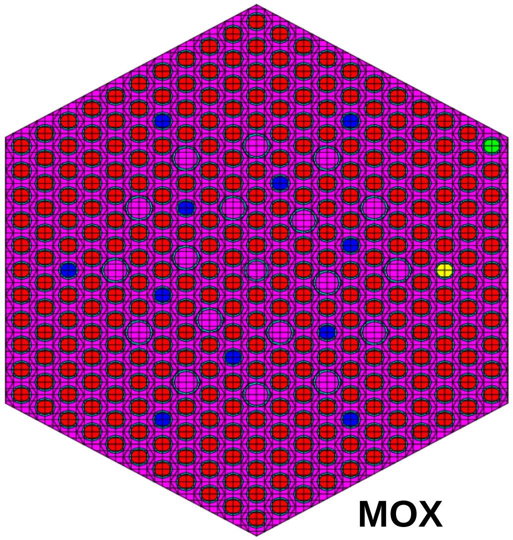
Modeling assumptions – SCALE 6.1

- Transport solutions (SN6)
- Boundary condition: white
- Convergence criterion (spatial/eigenvalue): ε=1E-6
- Predictor-corrector algorithms
- Cross-section library: ENDF/B-VII.0



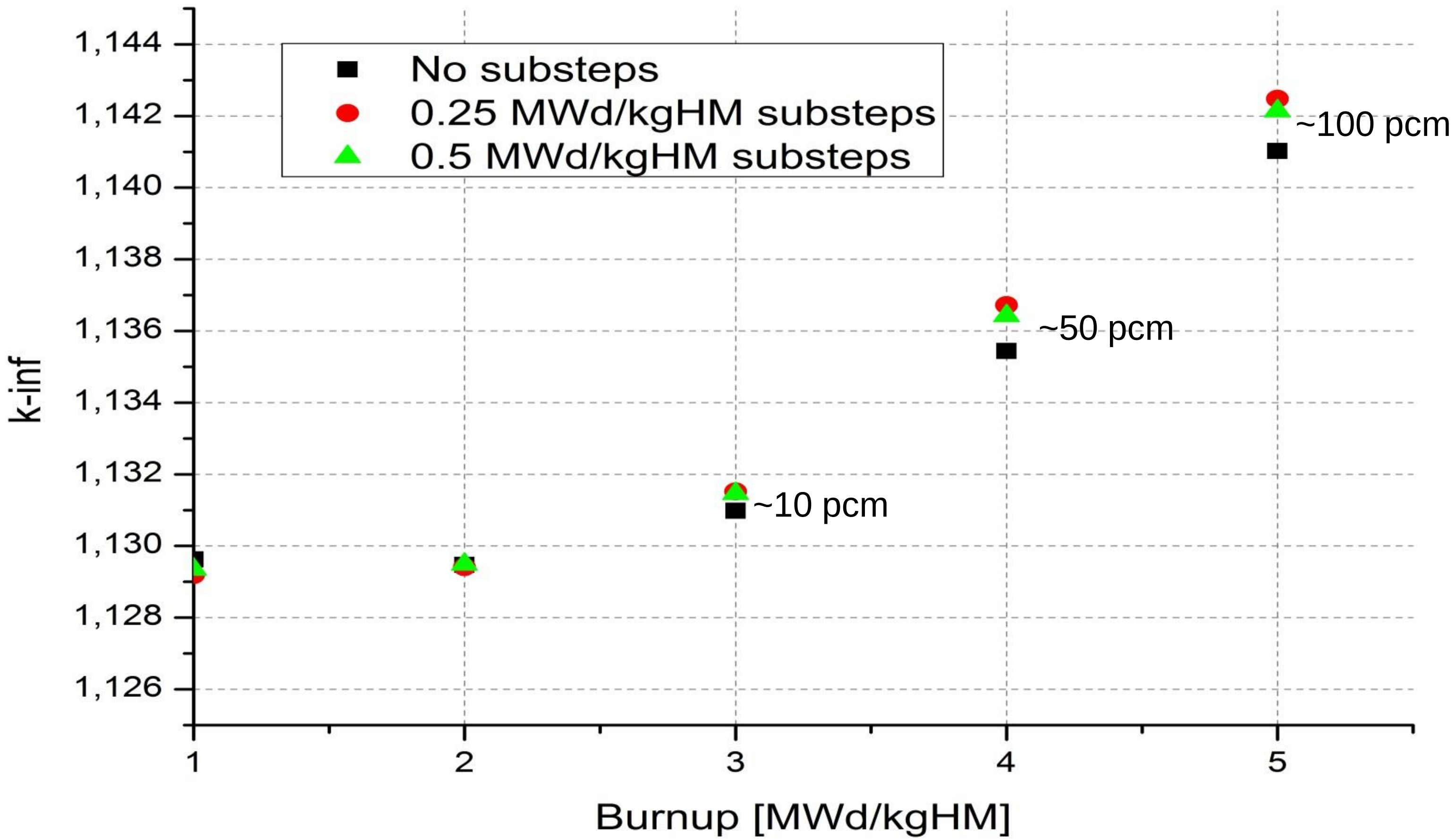


LEU



MOX

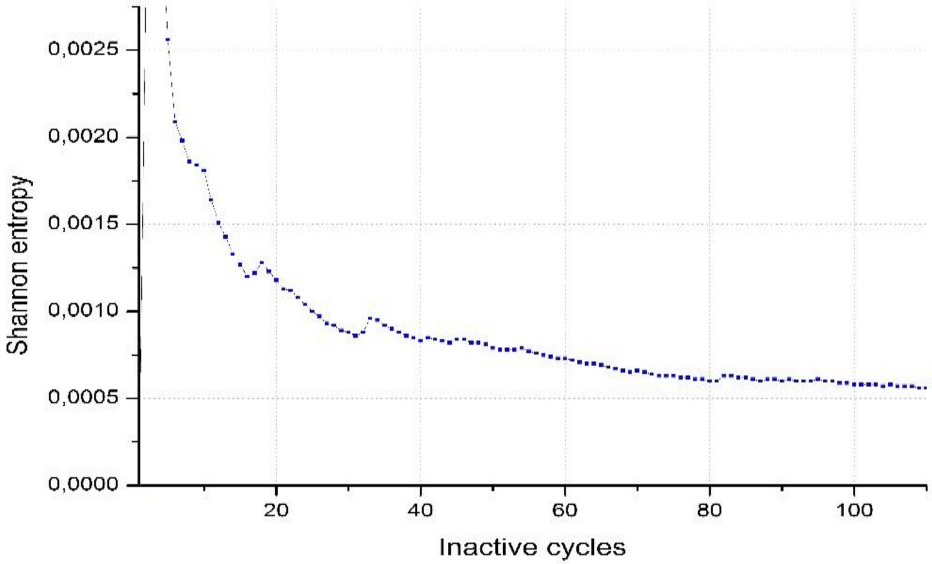
LEU – sensitivity studies on burn-up steps



Negligible effect of gadolinium mesh refinement (<20 pcm)

Modeling assumptions – SERPENT 2.1

- Solution of Depletion Equations**:** CRAM
- Predictor-corrector method (PC) vs Stochastic Implicit Euler (SIE)
- Pin-by-pin model
- Boundary condition: reflective
- Gadolinium refinement
- 10000 neutrons, 4000 cycles, 100 inactive cycles (Shannon enrtopy criterion)
- Tmp card (Doppler broadening) vs. Temperature weighted compositions (~200 pcm)
- Cross-section library: ENDF/B-VII.0, JEFF3.1, JEFF2.2



Monte Carlo solutions - k_{inf}

SERPENT and MCNP4B results for k_{inf} at zero burnup with JEFF2.2 data

LEU	SERPENT (S)	MCNP4B (M)	Δk (M-S)·10^5
S2	1.17987 ± 8.9E-05	1.1800 ± 6E-05	13
S3	1.19365 ± 8.6E-05	1.1925 ± 6E-05	-115
S4	1.25387 ± 8.5E-05	1.2531 ± 7E-05	-77
S5	1.32394 ± 7.6E-05	1.3235 ± 6E-05	-44
MOX	**SERPENT (S)**	**MCNP4B (M)**	**Δk (M-S)·10^5**
S2	1.19258 ± 8.6E-05	1.1922 ± 7E-05	-38
S3	1.20919 ± 8.4E-05	1.2091 ± 6E-05	-9
S4	1.24408 ± 8.5E-05	1.2430 ± 6E-05	-108
S5	1.32487 ± 7.6E-05	1.3256 ± 7E-05	73

- Objective: **assess the validity of our model through comparison with the reference MCNP4B solutions**
  - Overall good agreement
  - Small deviations due to different data (ENDF/B.V) for ^{16}O, ^{152}Gd, ^{nat}Zr and ^{1}H in the MCNP4B results and different statistics

Monte-carlo and deterministic solutions - k_{inf}

Karlsruhe Institute of Technology

SERPENT and SCALE results for k_{inf} at zero burnup with different NDLs

LEU	SERPENT (SJ) [JEFF3.1]	SERPENT (SE) [ENDF/B-VII]	SCALE (SCE) [ENDF/B-VII]	Δk (SE-SJ)·10^5	Δk (SE-SCE)·10^5
S2	1.17399 ± 8.9E-05	1.17587 ± 8.8E-05	1.17068	188	519
S3	1.18787 ± 8.7E-05	1.18996 ± 8.6E-05	1.18557	209	439
S4	1.24808 ± 8.5E-05	1.24993 ± 8.7E-05	1.24538	185	455
S5	1.32088 ± 7.6E-05	1.32305 ± 7.7E-05	1.31770	217	535
MOX	**SERPENT (SJ) [JEFF3.1]**	**SERPENT (SE) [ENDF/B-VII]**	**SCALE (SCE) [ENDF/B-VII]**	**Δk (SE-SJ)·10^5**	**Δk (SE-SCE)·10^5**
S2	1.19596 ± 8.5E-05	1.19762 ± 8.6E-05	1.19178	166	584
S3	1.21259 ± 8.4E-05	1.21419 ± 8.4E-05	1.21005	160	414
S4	1.24765 ± 8.4E-05	1.24923 ± 8.4E-05	1.24491	158	432
S5	1.32908 ± 7.6E-05	1.33013 ± 7.6E-05	1.32652	105	361

- Systematic under-prediction of JEFF3.1 with respect to JEFF2.2 (LEU)
- Systematic over-prediction of JEFF3.1 with respect to JEFF2.2 (MOX)
- ENDF/B-VII-k_{inf} larger with respect to JEFF3.1-k_{inf} by ~100-200 pcm
- SCALE results are systematically higher than SERPENT ones due to the multi-group and spatial approximations

Reactivity effects

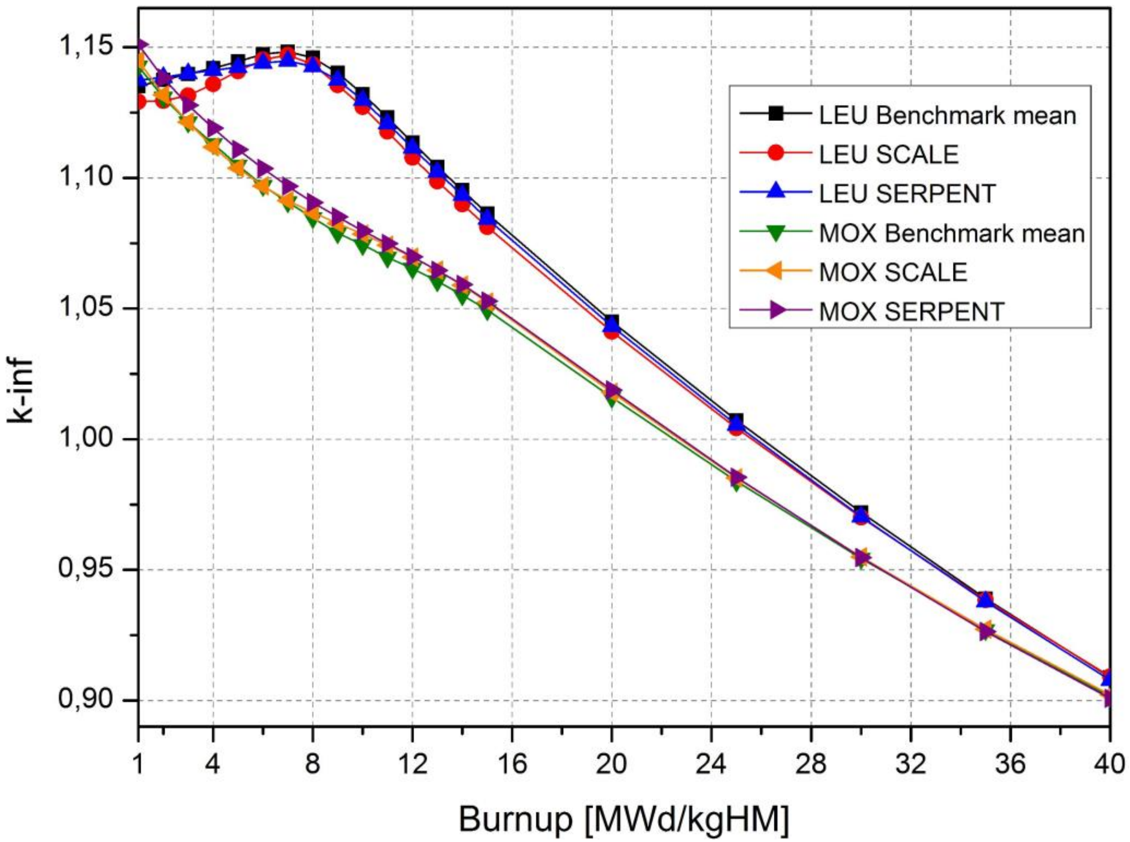
LEU and MOX assemblies: 100 x ($k_{init.} – k_{fin.}$)

Initial state	Final state	Burnup (MWd/KgHM)	LEU SERPENT	LEU SCALE	LEU Mean	MOX SERPENT	MOX SCALE	MOX Mean
S1	S2	0	-3.58	-*	-4.03	-2.63	-	-3.33
		20	-2.91	-	-3.96	-2.44	-	-3.44
		40	-2.37	-	-3.29	-2.16	-	-3.08
S2	S3	0	-1.41	-1.48	-1.36	-1.66	-1.83	-1.74
		20	-1.48	-	-1.52	-1.48	-	-1.55
		40	-1.35	-	-1.40	-1.33	-	-1.40
S3	S4	0	-6.00	-5.98	-5.99	-3.50	-3.49	-3.46
		20	-5.40	-	-5.48	-3.76	-	-3.83
		40	-4.81	-	-4.91	-3.86	-	-3.98
S4	S5	0	-7.28	-6.98	-6.90	-8.09	-8.16	-7.93
		20	-6.87	-	-6.72	-6.98	-	-7.03
		40	-4.35	-	-5.33	-5.49	-	-5.41

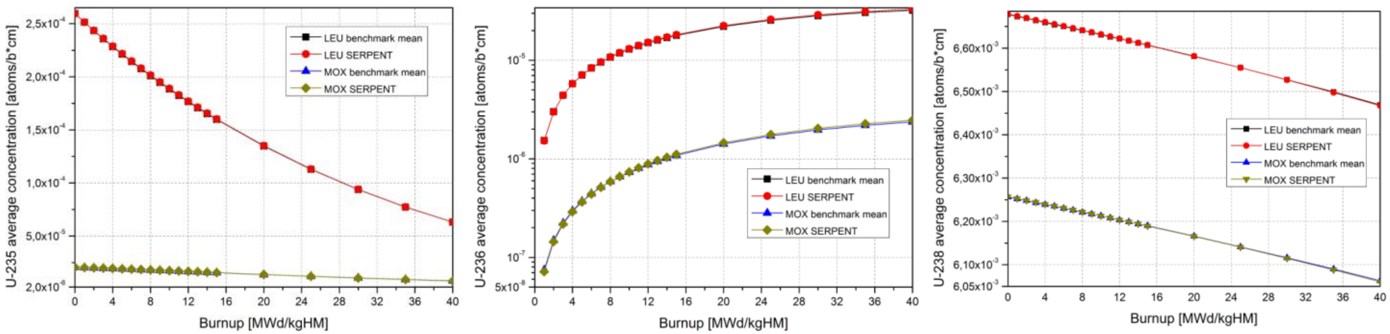
- Due to the harder neutron spectrum of the MOX assembly:
  - Xenon effect lower in MOX, the difference becoming less important with the increasing of burnup
  - Boron worth reduced in MOX. Difference: ~71% (BOC) - ~24% (EOC)
- Doppler coefficient slightly more negative for the MOX at BOC and almost equals at EOC
- Moderator temperature coefficient more negative in the case of MOX

Burn-up calculations - kinf

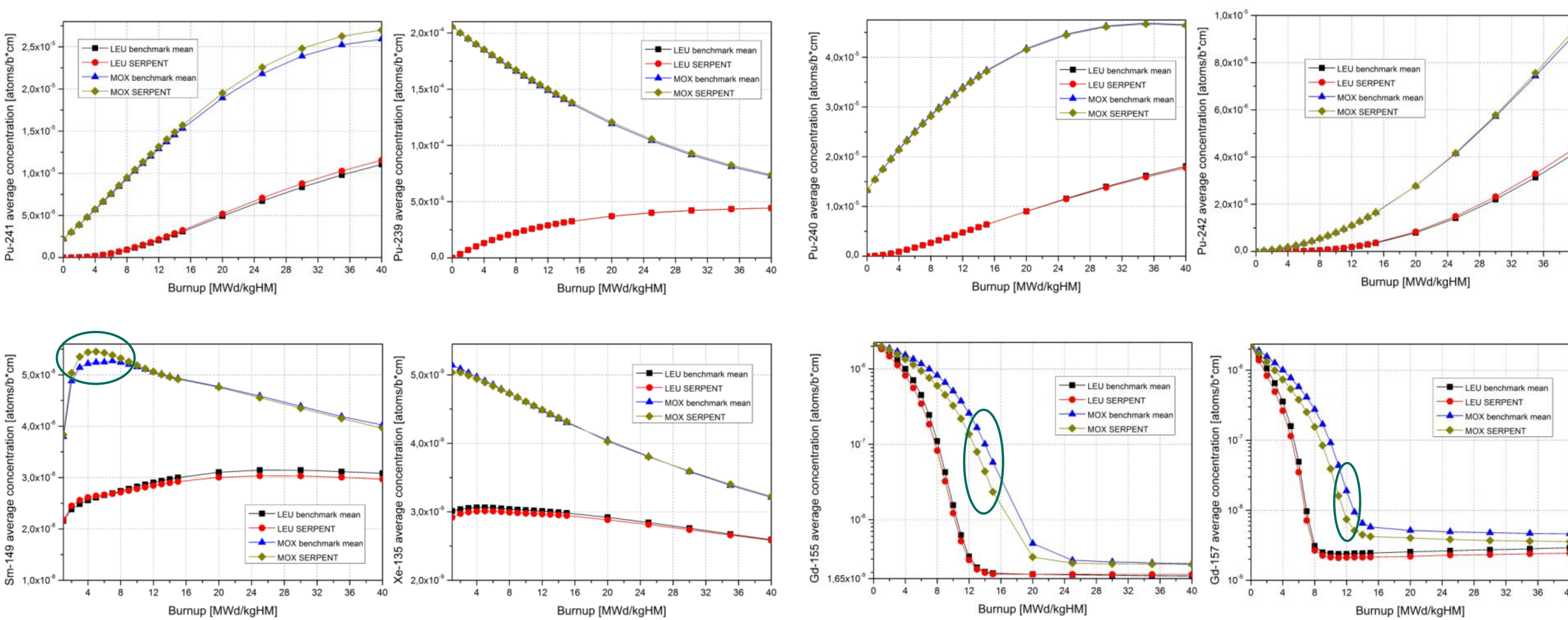
- The decrease of k_{inf} is slower for MOX
- Different shapes of the burn-up swings due to different spectra
- SERPENT- k_{inf} systematically higher than SCALE- k_{inf}
- The agreement in between SERPENT/SCALE stands within ±0.39% (LEU) and ±0.33% (MOX)



Burn-up calculations – assembly averaged nuclide concentrations (SERPENT/Benchmark mean)

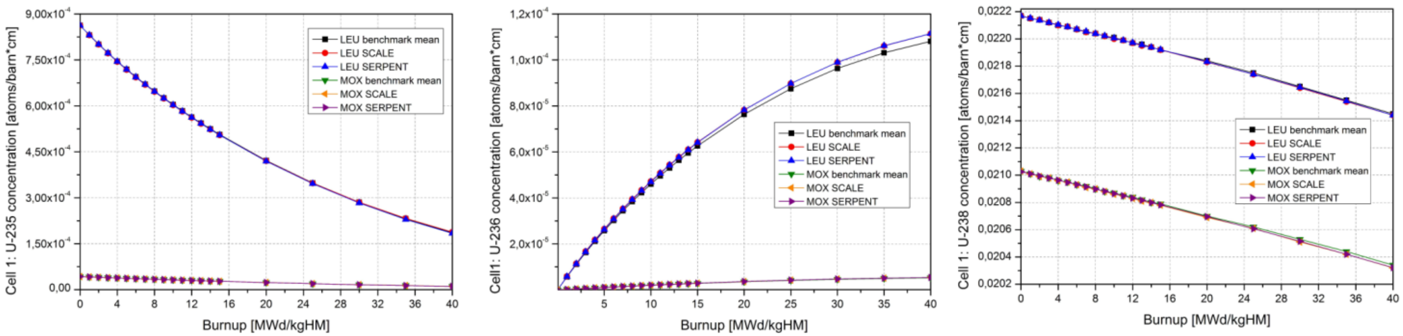


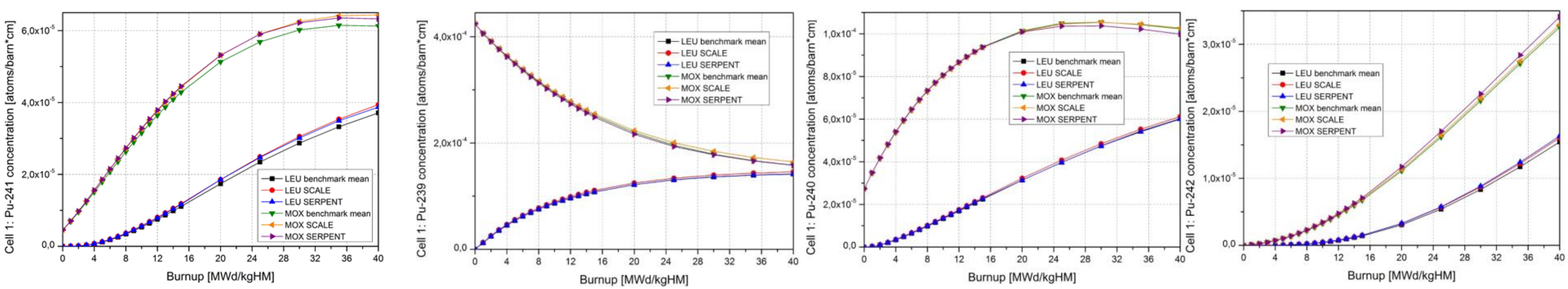
- Excellent agreement for U
- Good agreement for Pu
- Slight discrepancies for Sm-149, Gd-155 and Gd-157 in the MOX case

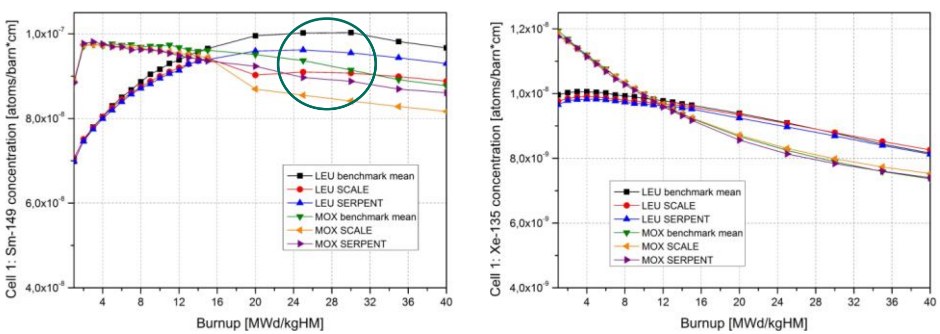


Burn-up calculations – Cell 1: nuclide concentrations (SERPENT/SCALE/Benchmark mean)

Karlsruhe Institute of Technology

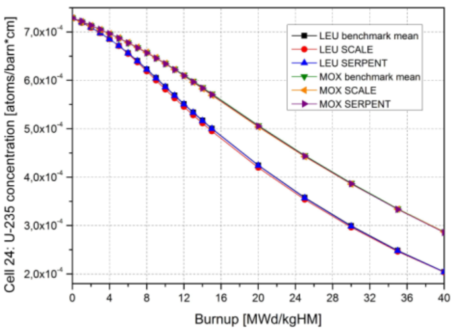


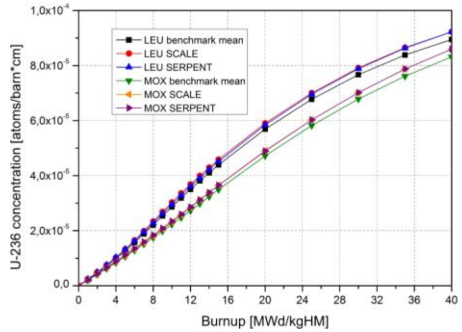


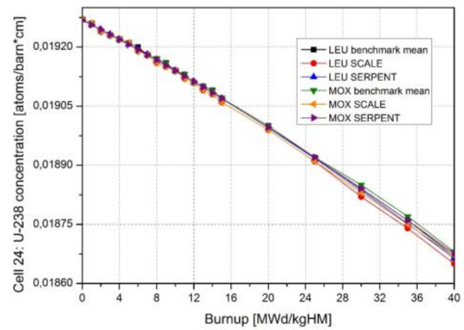


- **Excellent/good agreement for U and Pu isotopes**
- **Discrepancies for Sm-149 at high burn-up levels**

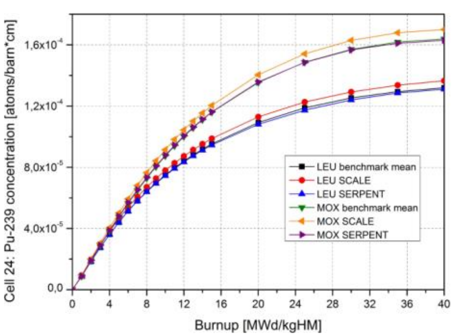
Burn-up calculations – Cell 24: nuclide concentrations (SERPENT/SCALE/Benchmark mean)

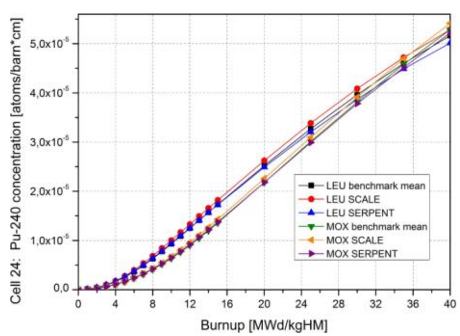


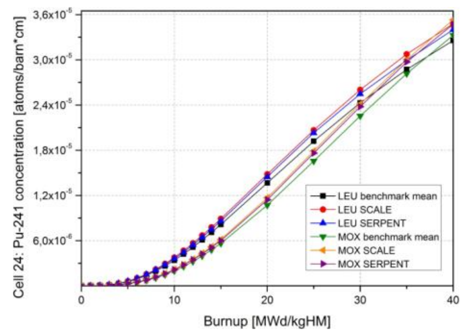


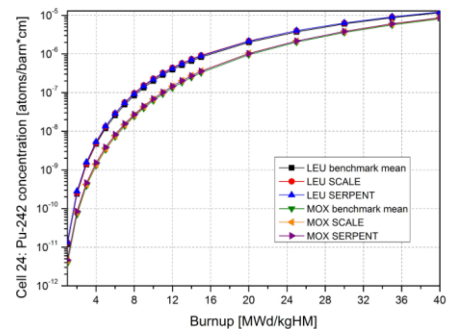


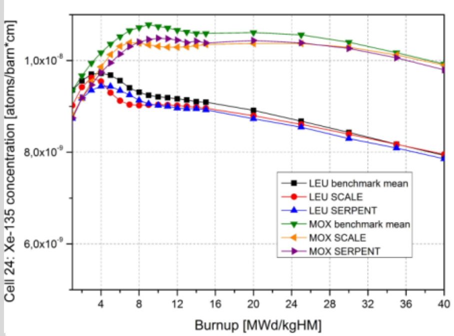
- Good agreement for U and Pu isotopes
- Discrepancies for Xe-135, Sm-149, Gd-155 and Gd-157

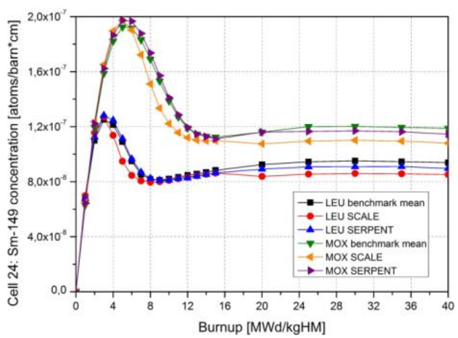


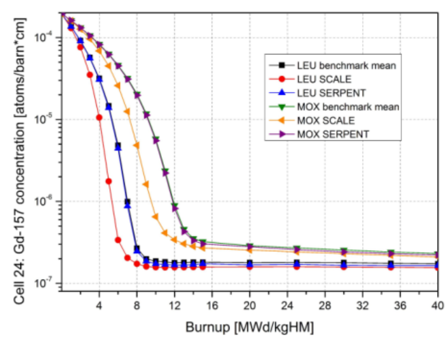


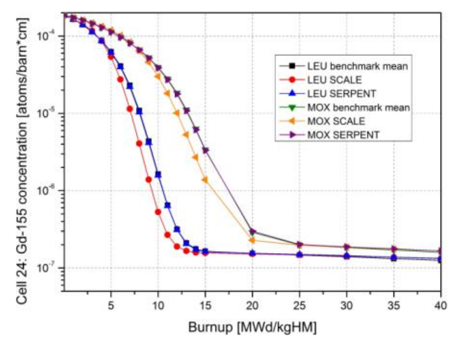












Pin-by-pin fission rates

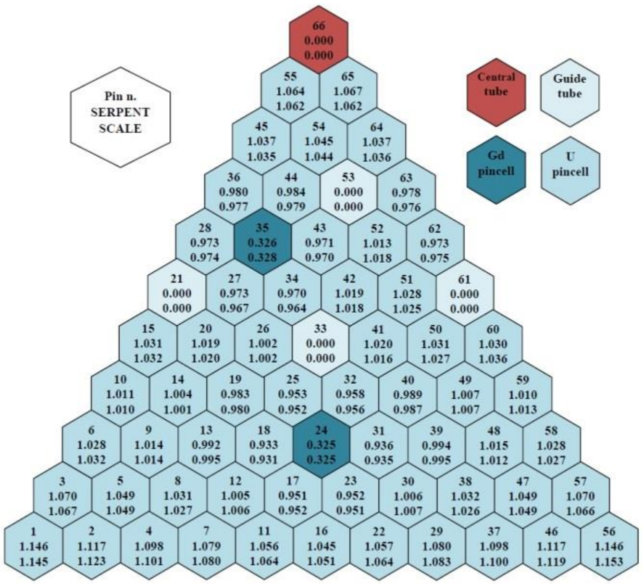
LEU Assembly	0 MWd/kgHM	20 MWd/kgHM	40 MWd/kgHM
Pin number	21	55	1
Max δ [%] (SCALE-SERPENT)	-0.78	2.14	3.22
Average δ [%] (SCALE-SERPENT)	0.25	0.69	1.45
MOX Assembly	**0 MWd/kgHM**	**20 MWd/kgHM**	**40 MWd/kgHM**
Pin number	10	4	46
Max δ [%] (SCALE-SERPENT)	-1.26	3.97	5.04
Average δ [%] (SCALE-SERPENT)	0.48	1.08	1.44

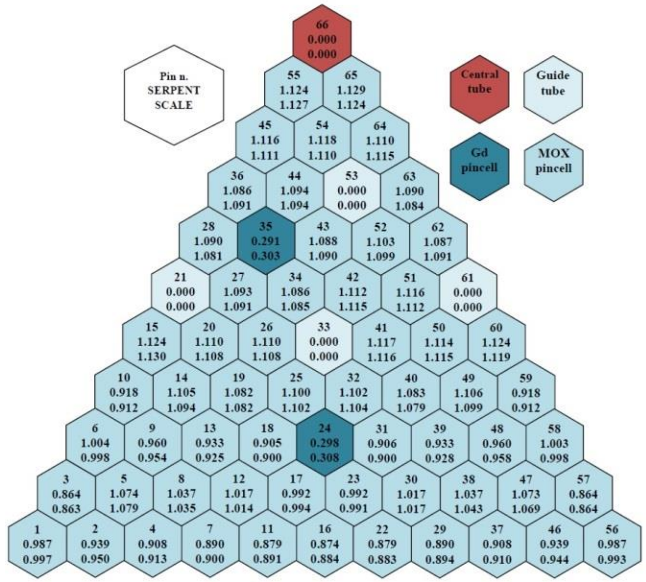
Good agreement SERPENT/SCALE

Maximum deviations:

LEU: -4.2% (pin 35)

MOX: -1.6% (pin 63)





Summary and conclusions

- **SERPENT and SCALE calculation schemes for VVER-1000 reactors have been tested on 2-D problems for fresh and depleted LEU and MOX fuel assemblies representative of the designs expected for the plutonium disposition mission**
- **Small deviations have been generally observed between the SCALE and SERPENT computed k_{inf}, nuclide concentrations and pin-by-pin fission rates.**
- **Very good agreement is found between SERPENT solutions and the corresponding previous MCNP4B results, making of this work also a new Monte Carlo reference solution for the *OECD VVER-1000 LEU and MOX Assemblies Burnup Computational Benchmark* with modern NDLs**