Effect of modelling parameters on calculated PWR spent fuel observables

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Modelling uncertainties

- Modelling, computational, numerical?
- Uncertainties, biases, errors?
- Types of modelling uncertainties?

Modelling uncertainties: Monte Carlo vs. deterministic

Monte Carlo n. transport

- Continuous energy
- Continuous direction
- Continuous time (e.g. for n. kinetics)
- Space continuum (particle tracking)
- Counting statistics from n. history

Deterministic n. transport

- Energy intervals (multi-group)
- Solid angle discretization (S_n) or polynomial expansion (P_n)
- Discretization of the time variable
- Discretization of the spatial variables
- „Exact“ solution (except round-off)

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- **Apart from counting statistics, are there any other souces of numerical error in continuous enegy MC particle transport codes?**
- **YES:**
  - **Discretization of thermal scattering data (e.g. Serpent 2.1.29 → fixed in 2.1.32)**
  - **Ignoring Doppler Broadening Rejection Correction (DBRC) (e.g. MCNP)**
  - **Energy release per fission proportional to atomic mass (e.g. Serpent before v. 2.1.31)**
  - **etc.**

Modelling uncertainties: depletion vs. n. transport

MC neutron transport

- Continuous energy
- Continuous direction
- Continuous time (e.g. for n. kinetics)
- Space continuum (particle tracking)
- Counting statistics from n. history

Material depletion by n. irradiation

- Reaction rates from continous *E*
- Not needed for depletion (4π int.)
- Depletion time steps
- Depletion geometric zones
- Counting statistics from n. history

Additional modelling uncertainties:

- Model simplifications (e.g. 2D)
- Physical approximations (e.g. no DBRC)
- Energy deposition model (fission; all n reactions; n+γ)

Types of modelling uncertainties

- Counting statistics
- **Discretization**
  - **Independent variables**
  - **Conditions (e.g. temperature, density)**
- Physical approximations
- Simplifications (e.g. 3D→2D, boundary conditions)
- Round-off (negligible in double precision for well-conditioned problems)

Discretization parameters

Independent variables:

- Irradiation time steps:
  - Depletion solver (i.e. mathematical method used to solve Bateman equations)
  - Implicit/explicit
  - Interpolation/extrapolation scheme
  - Substeps
- Depletion geometrical zones:
  - Radial zones within pin (to model „rim effect“)
  - Pins grouped in separate zones (to account for asymmetry, e.g. due to boundary conditions)
  - Axial zones (in 3D model or 2D slices with different irradiation conditions)
  - Azimuthal regions within pin (not studied, probably negligible effect?)

Conditions:

- Fuel temperature profiles: radial, axial (negligible)
- Moderator axial density and temperature profiles

SNF observables

Main studied observables:

- Decay heat rate : H
- Neutron emission rate : S_n
- γ-ray emission rate : S_γ

Possible to measure, but different difficulties...

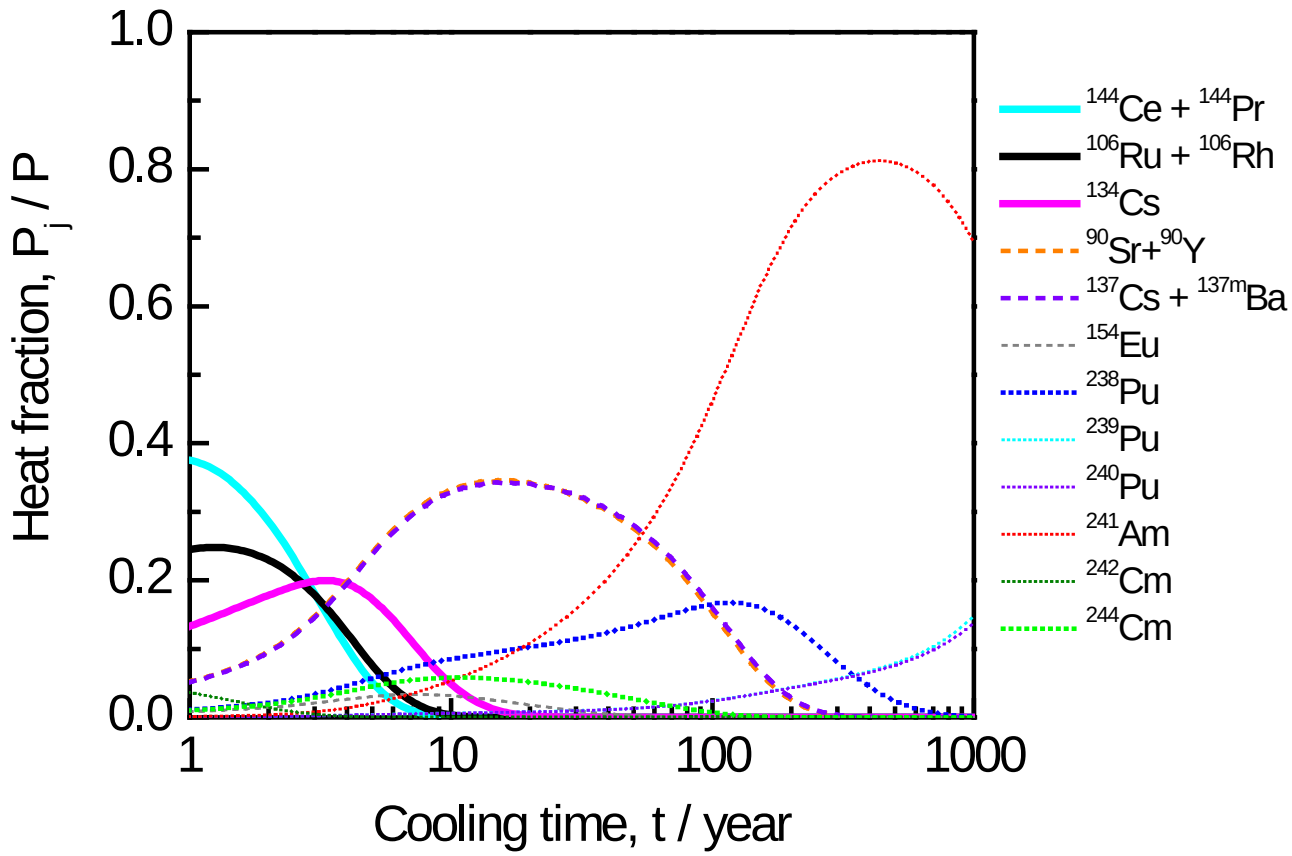
$\Rightarrow$ Determined/estimated by **theoretical calculations**

$\Rightarrow$ Summation formula starting from **nuclide vector**

Decay heat of SNF: main contributing nuclides

Decay heat rate: $H(t) = \sum_j H_j(t)$

- 1 a ≤ t_c ≤ 10 a
  - **^{144}Ce / ^{144}Pr**
  - **^{106}Ru / ^{106}Rh**
  - **^{134}Cs**
  - ^{90}Sr / ^{90}Y & ^{137}Cs / ^{137m}Ba
- 10 a ≤ t_c ≤ 100 a
  - **^{90}Sr / ^{90}Y & ^{137}Cs / ^{137m}Ba**
  - ^{238}Pu
  - ^{241}Am
  - ^{244}Cm
- 100 a ≤ t_c ≤ 1000 a
  - **^{241}Am**
  - ^{238}Pu
  - ^{239,241}Pu



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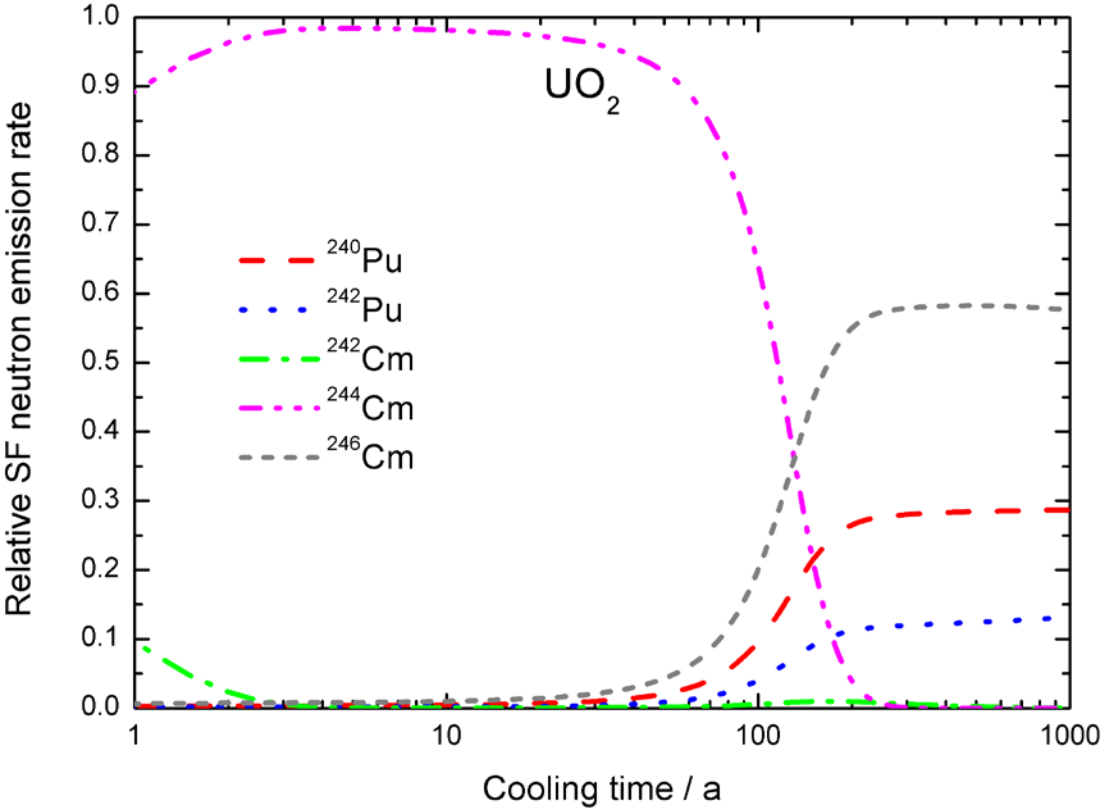
Neutron emission of SNF: main contributing nuclides

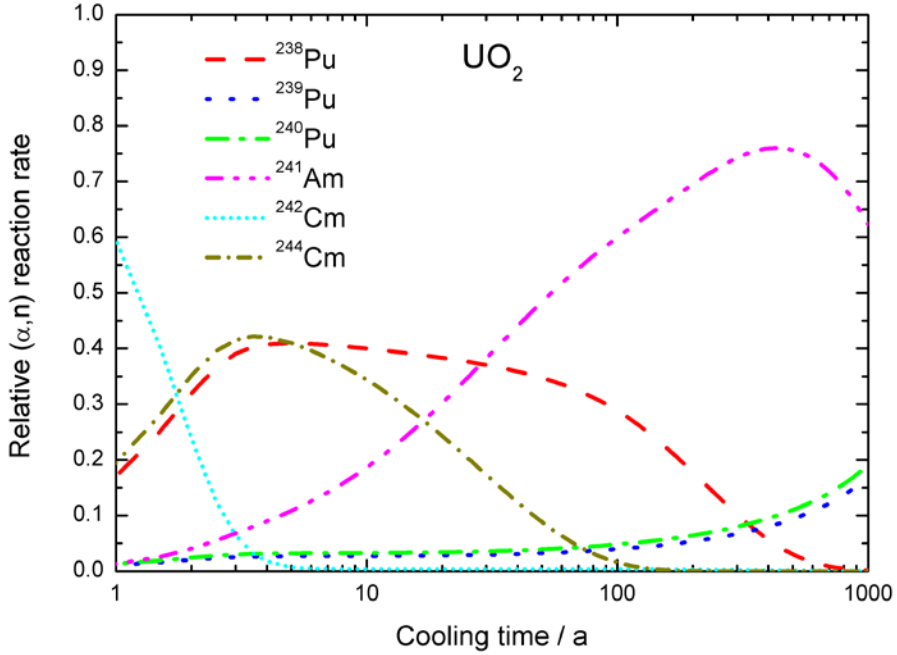
Neutron emission rate:

$$S_n(t) = \sum_j S_{n,j}(t)$$

Contribution from SF dominating!

- for cooling time < 100 a, **(α,n) rate** at least 10× lower than SF n. emission rate





$S_n(t) \Rightarrow$ **sensitive to ^{244}Cm production**

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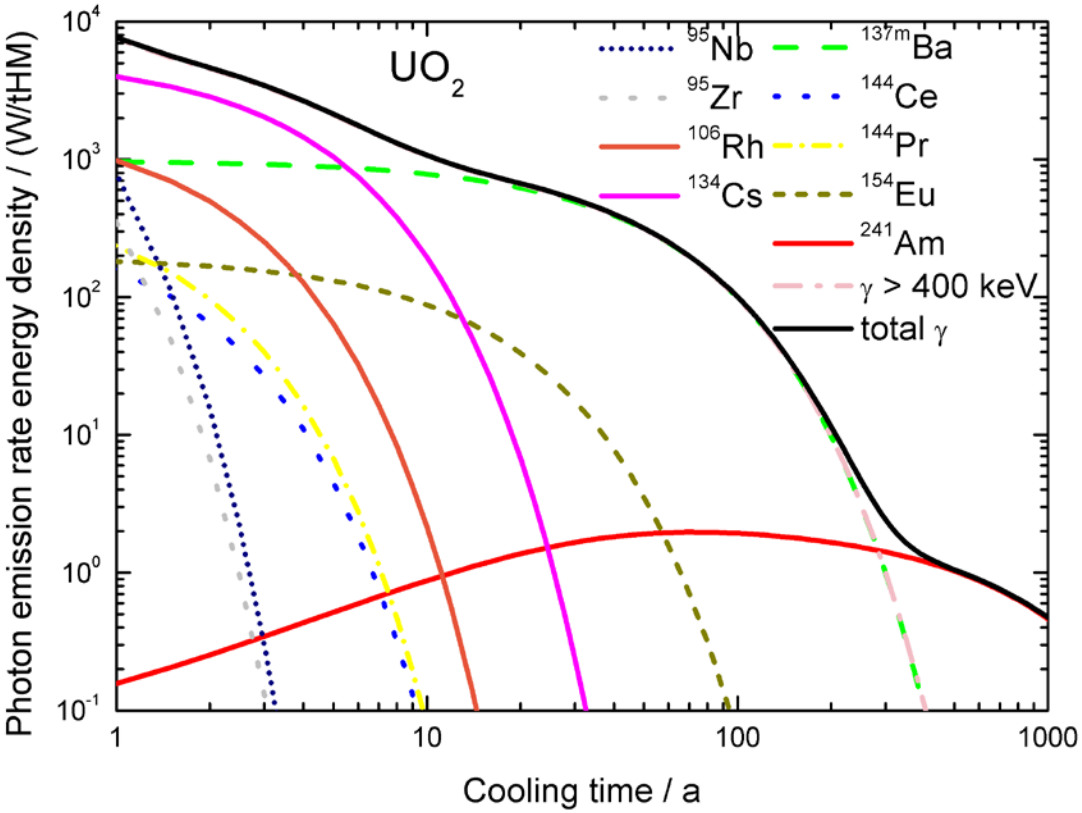
γ-ray emission by SNF: main contributing nuclides

Photon emission rate energy density:

$$H_\gamma(t) = \sum_j H_{\gamma,j}(t) = \sum_j N_j(t)\,\lambda_j E_{\gamma,j}$$

= Contribution of γ-rays to decay heat

- 1 a ≤ t_c ≤ 10 a
  - **^{134}Cs**
  - ^{137}Cs / **^{137m}Ba**
  - ^{106}Ru / **^{106}Rh**
- 10 a ≤ t_c ≤ 300 a
  - ^{137}Cs / **^{137m}Ba**
  - **^{154}Eu**
  - ^{241}Am
- 300 a ≤ t_c ≤ 1000
  - **^{241}Am**
  - ^{137}Cs / ^{137m}Ba



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Definition of the study case

2D PWR 17×17, Zircaloy-4, 4% enriched UO_2 fuel, 4 × 300 d fuel cycles, cooling periods 30 d. Fuel radius 4.095 mm, clad inner/outer radii 4.18/4.75 mm, rod pitch 12.6 mm.

Simplified operating conditions:

- Power levels 50, 50, 40 and 30 MW/tHM during each cycle.
- Coolant density 0.655 kg/cm^3, constant boron level 800 ppm.
- Fuel density (95% theoretical density): 10.4 g/cm^3.
- Constant *T*: fuel and gap: 900 K; coolant and cladding: 600 K.

Numerical approximations (ref. model):

- 4 equi-volume radial depletion zones
- Time steps per cycle: 1 d, 10 d, 14 d, 3 × 25 d, 2 × 50 d
- reflective boundary conditions

Code: Serpent (v2.1.29/30)

Nuclear data library: ENDF/B-VII.1

Counting statistics: nuclide vector at cooling time 5 a

No. of neutron histories: 2.5×10^6 (5000 n. in 500 active cycles)

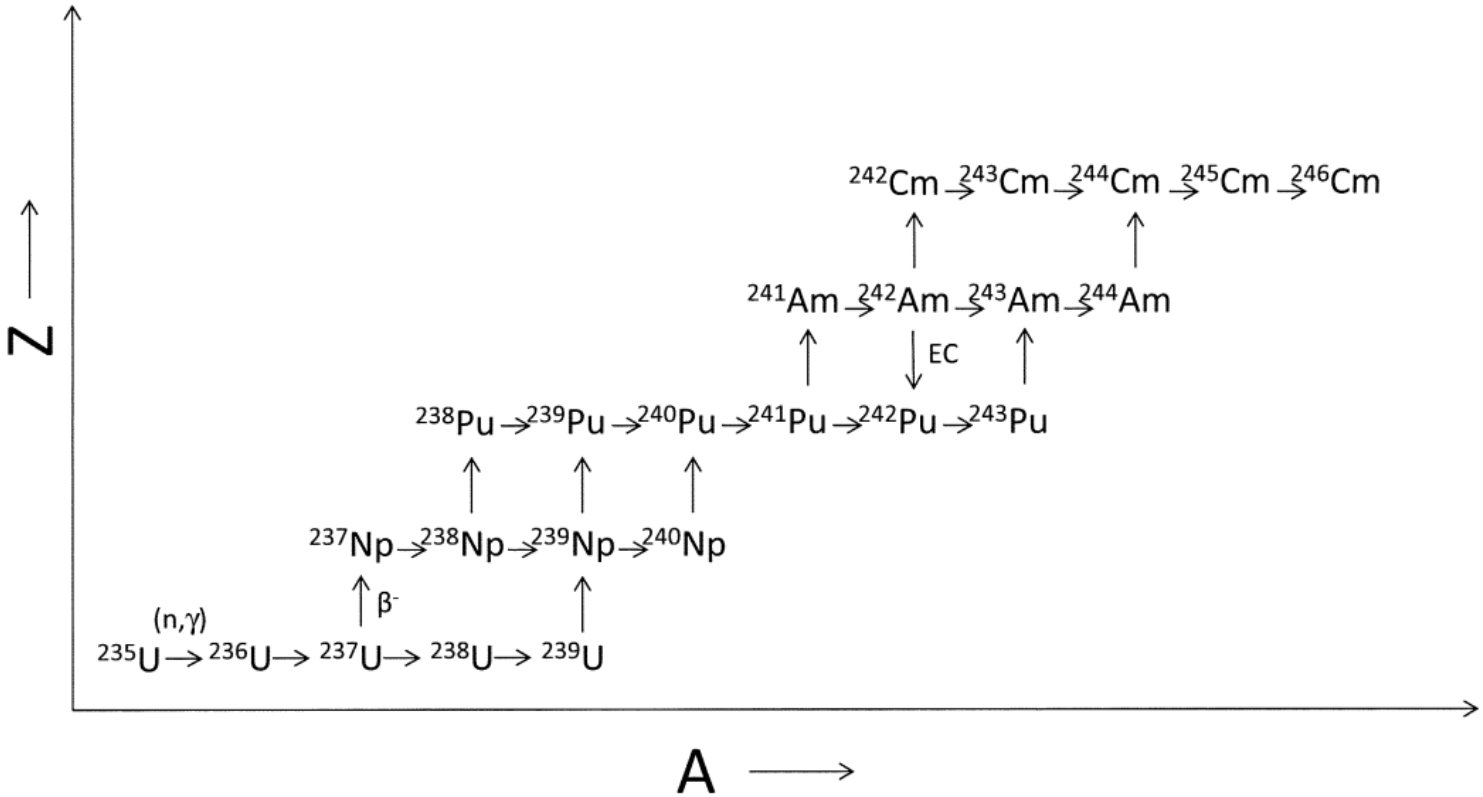
Count. stat. unc.: estimated from **50 runs** with different random seeds

Nuclide	c_0 /(g/tHM)	σ_c/c_0	Nuclide	c_0 /(g/tHM)	σ_c/c_0
^{90}Sr	678.56 (2)	0.003%	^{238}Pu	426.44 (18)	0.04%
^{133}Cs	1621.7 (1)	0.01%	^{239}Pu	6747.4 (18)	0.03%
^{134}Cs	43.86 (2)	0.04%	^{240}Pu	3065.2 (13)	0.04%
^{137}Cs	1638.0 (0)	0.001%	^{241}Pu	1556.7 (6)	0.04%
^{148}Nd	567.92 (6)	0.01%	^{242}Pu	970.92 (30)	0.03%
^{235}U	7109.9 (14)	0.02%	^{241}Am	499.66 (17)	0.03%
^{238}U	920116 (4)	0.0004%	^{244}Cm	109.38 (8)	0.08%

Actinide production chains

Actinide production processes: $R_j = \sum_i \phi\, \sigma_{fi} \gamma_{ij}$

- Radioactive decay
  - **β-decay**
  - Isomeric transition
  - α-decay
- Nuclear reactions:
  - **Neutron capture**
  - Other reactions:
    - (n,2n)
    - (n,α)
    - (n,p)
    - etc.



Irradiation time discretization

Reference model:

- Time steps per cycle: 1 d, 10 d, 14 d, 3 × 25 d, 4 × 50 d
- Depletion solver: CRAM order 14
- Predictor/corrector: linear extrapolation/linear interpolation
- Substeps: 10/10

Time step with longest time steps within 0.2% for ^{244}Cm:

- 1 d, 10 d, 14 d, 25 d, 50 d, 2 × 100 d

The optimal time step scheme is problem dependent. The findings are only valid for specific fuel type and power density range (only valid for PWR UO_2 fuel and not valid e.g. for MOX fuel!).

Depletion zone discretization: pin level, radial

- Burn card: equi-volume
- Div card: equi-thickness
- Manual: 2 zones to study the ring effect

No. of radial zones	1	2	4 (ref.)	6	8	10	1+1 (ring)
^{244}Cm / ref.	0.984	0.994	1	0.999	1.002	1.002	0.997
^{241}Am / ref.	1.002	1.000	1	1.000	1.000	1.000	1.001
^{239}Pu / ref.	1.005	1.002	1	1.000	0.999	1.000	1.001

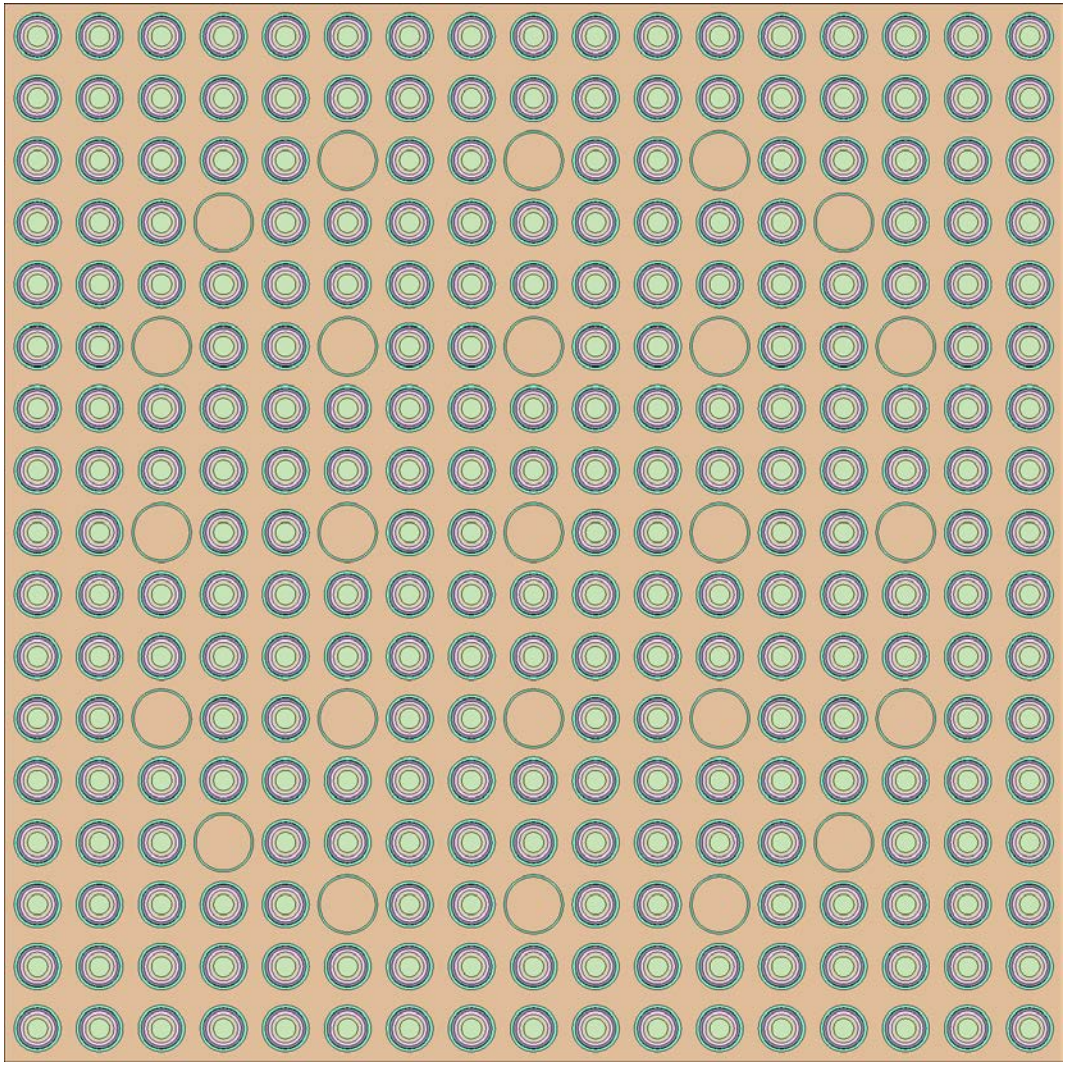
Depletion zone discretization: assembly level; boundary conditions

Reference model:

- 17 × 17 pins
  - 264 equal fuel pins
  - 25 empty positions (for CR)
- All pins grouped in a single depletion zone
- 4 radial (equi-volume) zones
- Reflective boundary conditions

Separate pin treatment study:

- As a function of boundary conditions (1-group albedo)
- Optimal pin grouping?
- Effect on observables



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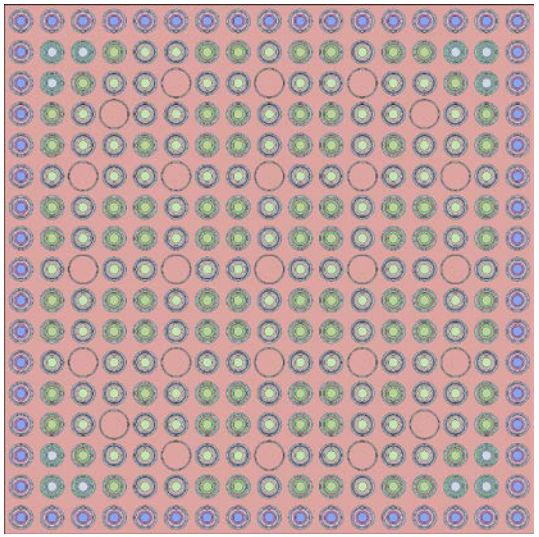
Pin grouping: by „feeling“

4



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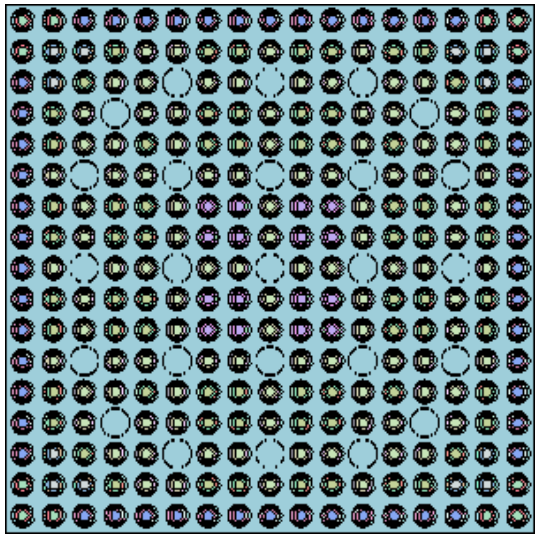

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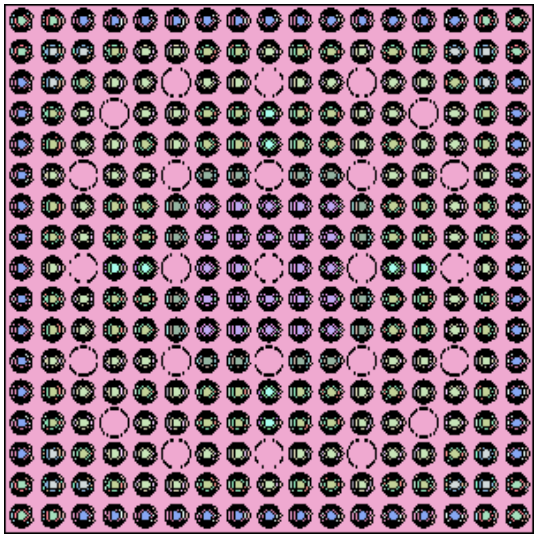

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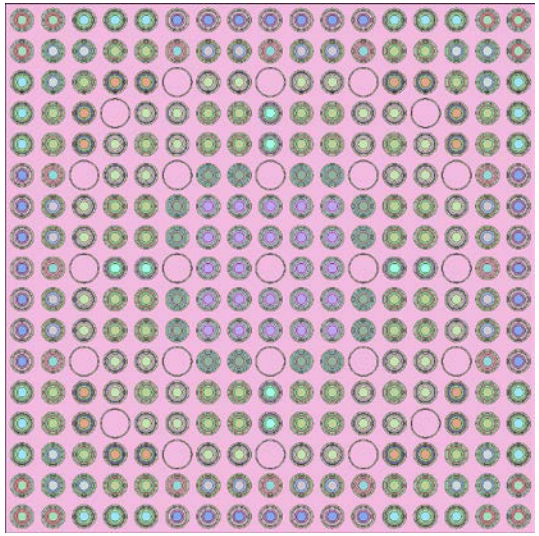

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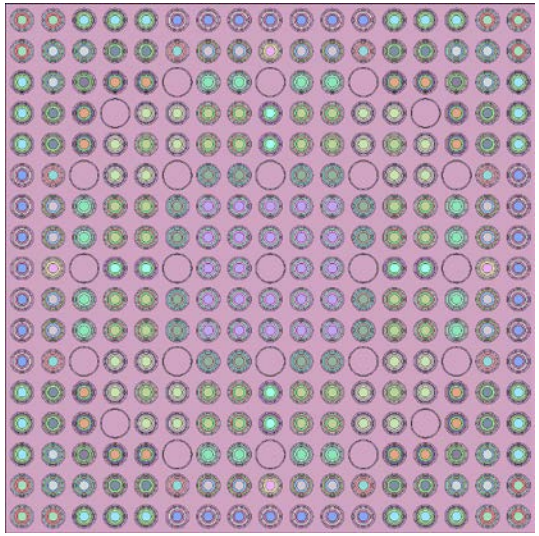

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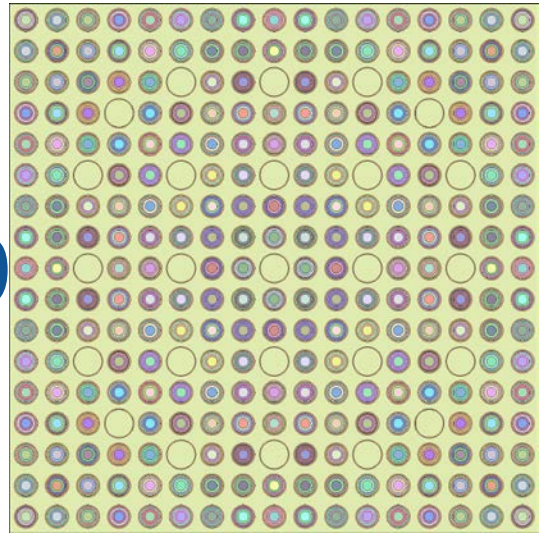

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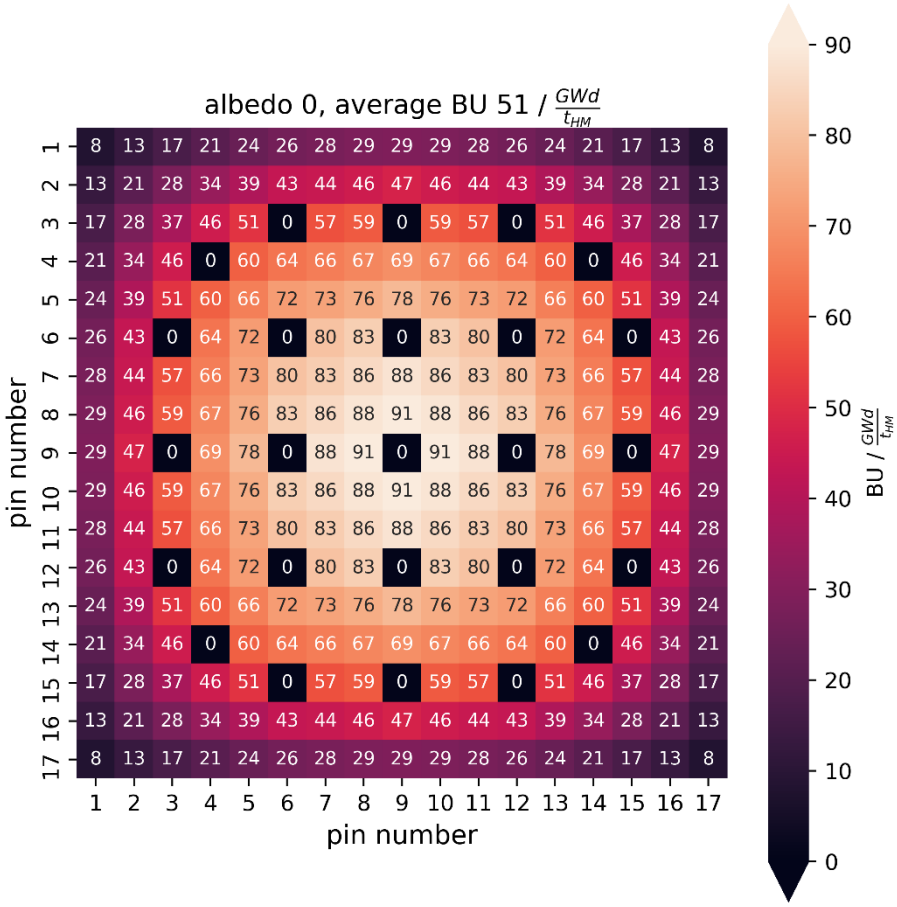
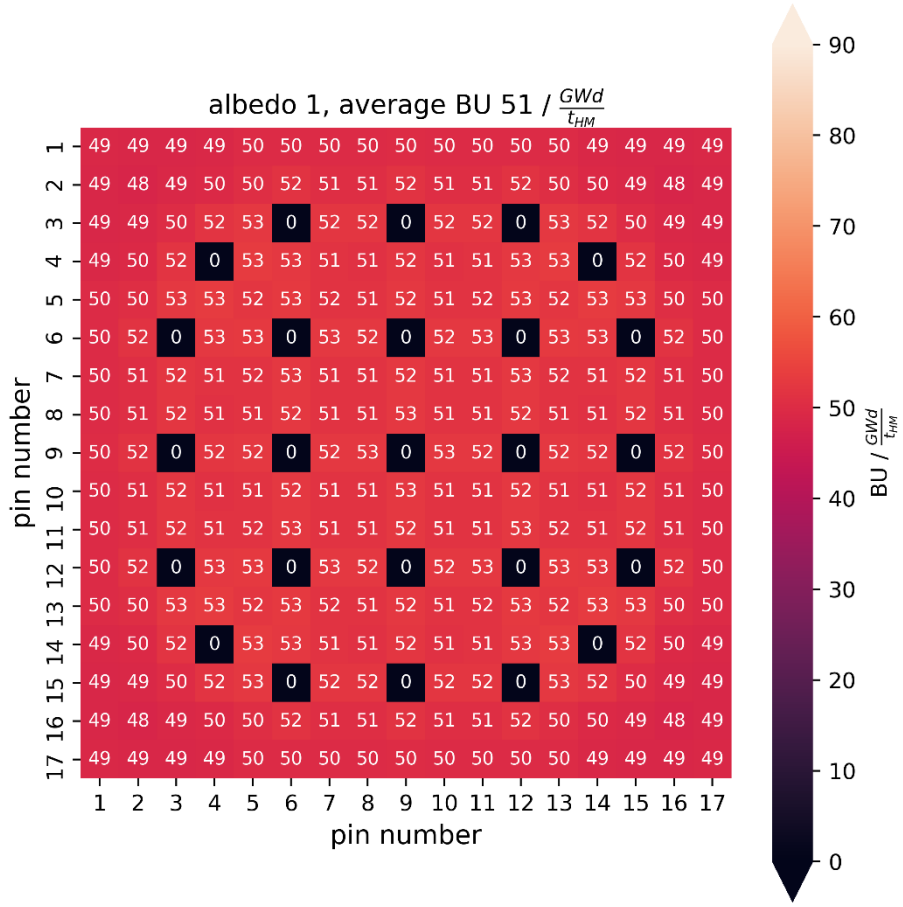
Pin burnup distributions



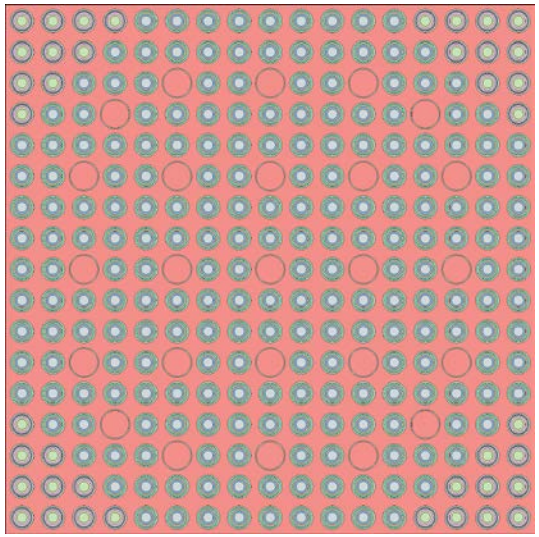
pin number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	8	13	17	21	24	26	28	29	29	29	28	26	24	21	17	13	8
2	13	21	28	34	39	43	44	46	47	46	44	43	39	34	28	21	13
3	17	28	37	46	51	0	57	59	0	59	57	0	51	46	37	28	17
4	21	34	46	0	60	64	66	67	69	67	66	64	60	0	46	34	21
5	24	39	51	60	66	72	73	76	78	76	73	72	66	60	51	39	24
6	26	43	0	64	72	0	80	83	0	83	80	0	72	64	0	43	26
7	28	44	57	66	73	80	83	86	88	86	83	80	73	66	57	44	28
8	29	46	59	67	76	83	86	88	91	88	86	83	76	67	59	46	29
9	29	47	0	69	78	0	88	91	0	91	88	0	78	69	0	47	29
10	29	46	59	67	76	83	86	88	91	88	86	83	76	67	59	46	29
11	28	44	57	66	73	80	83	86	88	86	83	80	73	66	57	44	28
12	26	43	0	64	72	0	80	83	0	83	80	0	72	64	0	43	26
13	24	39	51	60	66	72	73	76	78	76	73	72	66	60	51	39	24
14	21	34	46	0	60	64	66	67	69	67	66	64	60	0	46	34	21
15	17	28	37	46	51	0	57	59	0	59	57	0	51	46	37	28	17
16	13	21	28	34	39	43	44	46	47	46	44	43	39	34	28	21	13
17	8	13	17	21	24	26	28	29	29	29	28	26	24	21	17	13	8



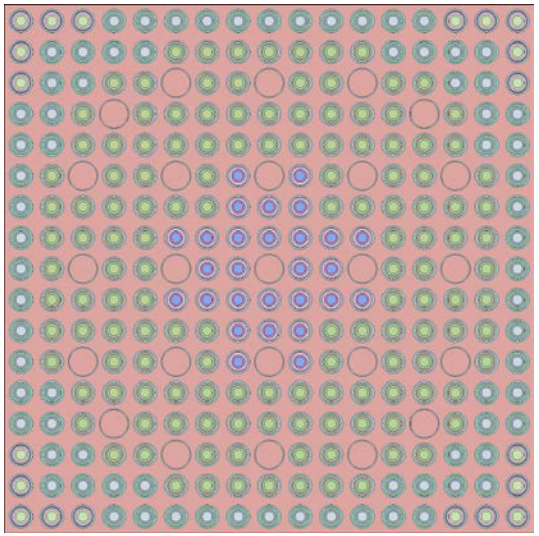
pin number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	49	49	49	49	50	50	50	50	50	50	50	50	50	49	49	49	49
2	49	48	49	50	50	52	51	51	52	51	51	52	50	50	49	48	49
3	49	49	50	52	53	0	52	52	0	52	52	0	53	52	50	49	49
4	49	50	52	0	53	53	51	51	52	51	51	53	53	0	52	50	49
5	50	50	53	53	52	53	52	51	52	51	52	53	52	53	53	50	50
6	50	52	0	53	53	0	53	52	0	52	53	0	53	53	0	52	50
7	50	51	52	51	52	53	51	51	52	51	51	53	52	51	52	51	50
8	50	51	52	51	51	52	51	51	53	51	51	52	51	51	52	51	50
9	50	52	0	52	52	0	52	53	0	53	52	0	52	52	0	52	50
10	50	51	52	51	51	52	51	51	53	51	51	52	51	51	52	51	50
11	50	51	52	51	52	53	51	51	52	51	51	53	52	51	52	51	50
12	50	52	0	53	53	0	53	52	0	52	53	0	53	53	0	52	50
13	50	50	53	53	52	53	52	51	52	51	52	53	52	53	53	50	50
14	49	50	52	0	53	53	51	51	52	51	51	53	53	0	52	50	49
15	49	49	50	52	53	0	52	52	0	52	52	0	53	52	50	49	49
16	49	48	49	50	50	52	51	51	52	51	51	52	50	50	49	48	49
17	49	49	49	49	50	50	50	50	50	50	50	50	50	49	49	49	49

Pin grouping: by burnup, separated by 10 GWd/tHM

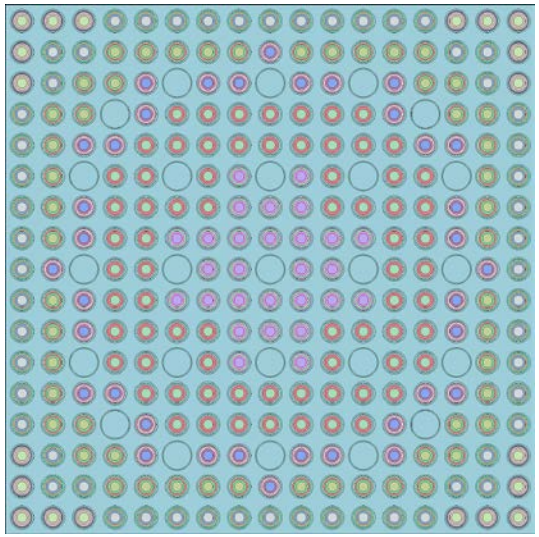
a=1
2 zones



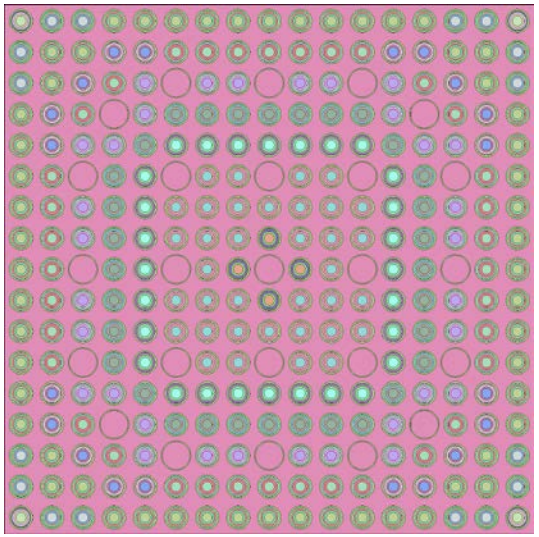
a=0.8
4 zones



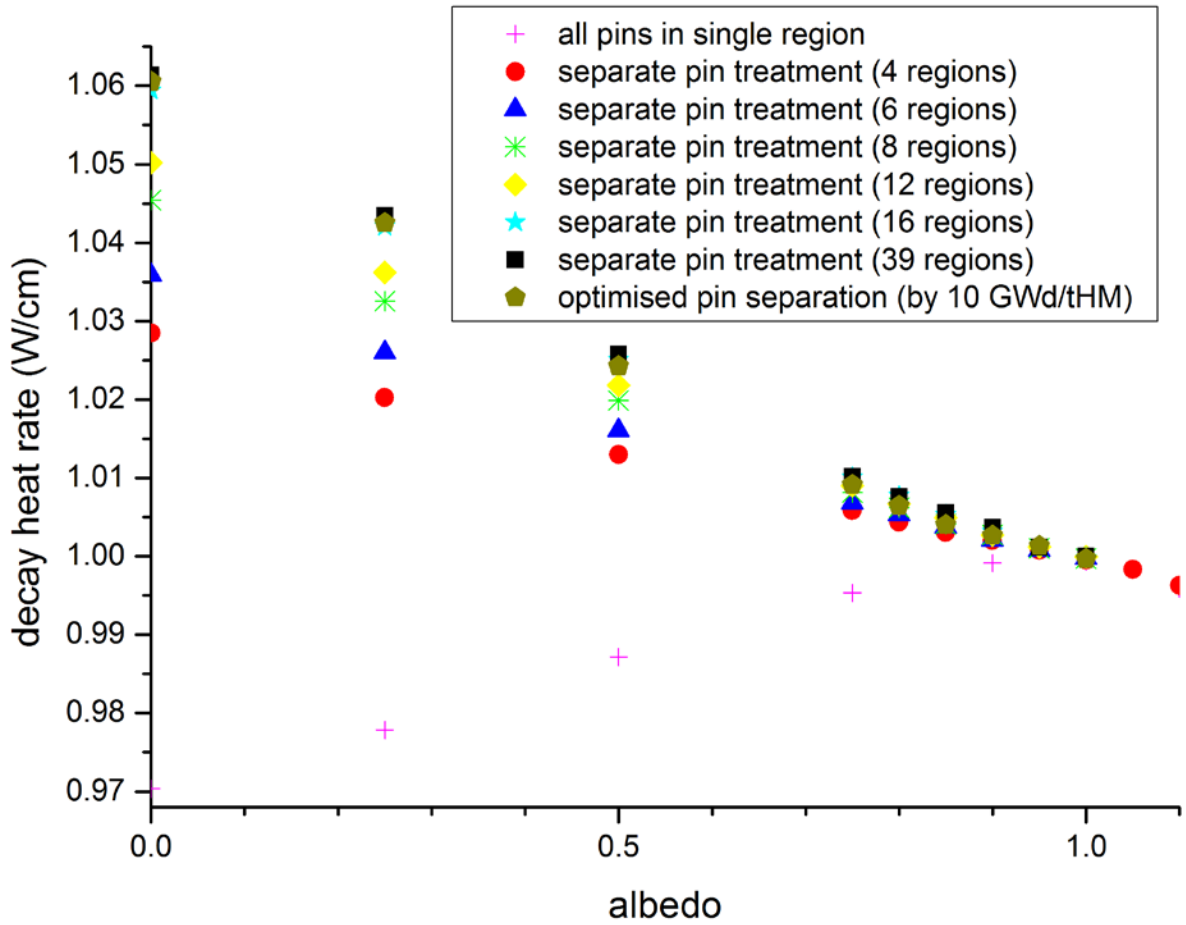
a=0.5
6 zones



a=0
10 zones



Separate pin treatment: results (decay heat rate at 5 a cooling)



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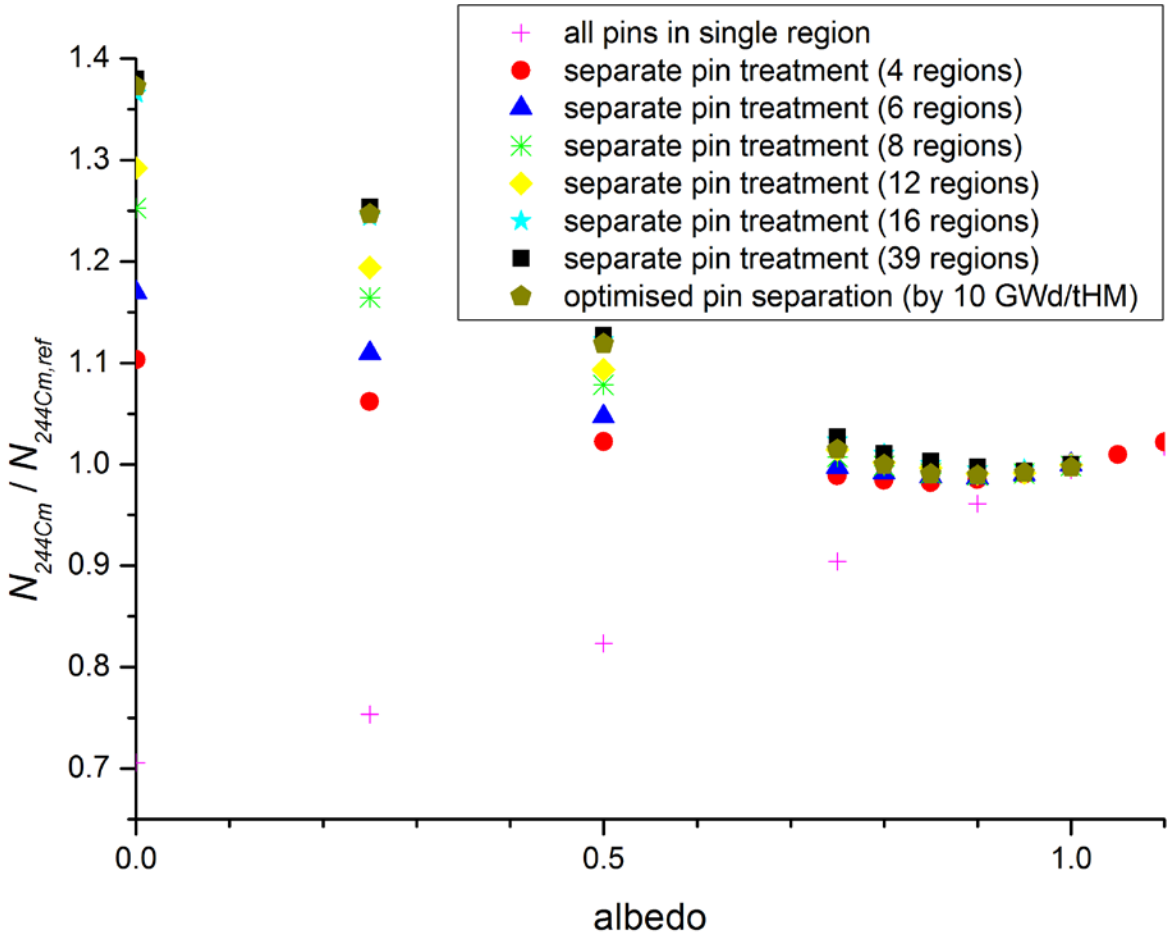
Separate pin treatment: results (^{244}Cm – n. emission)



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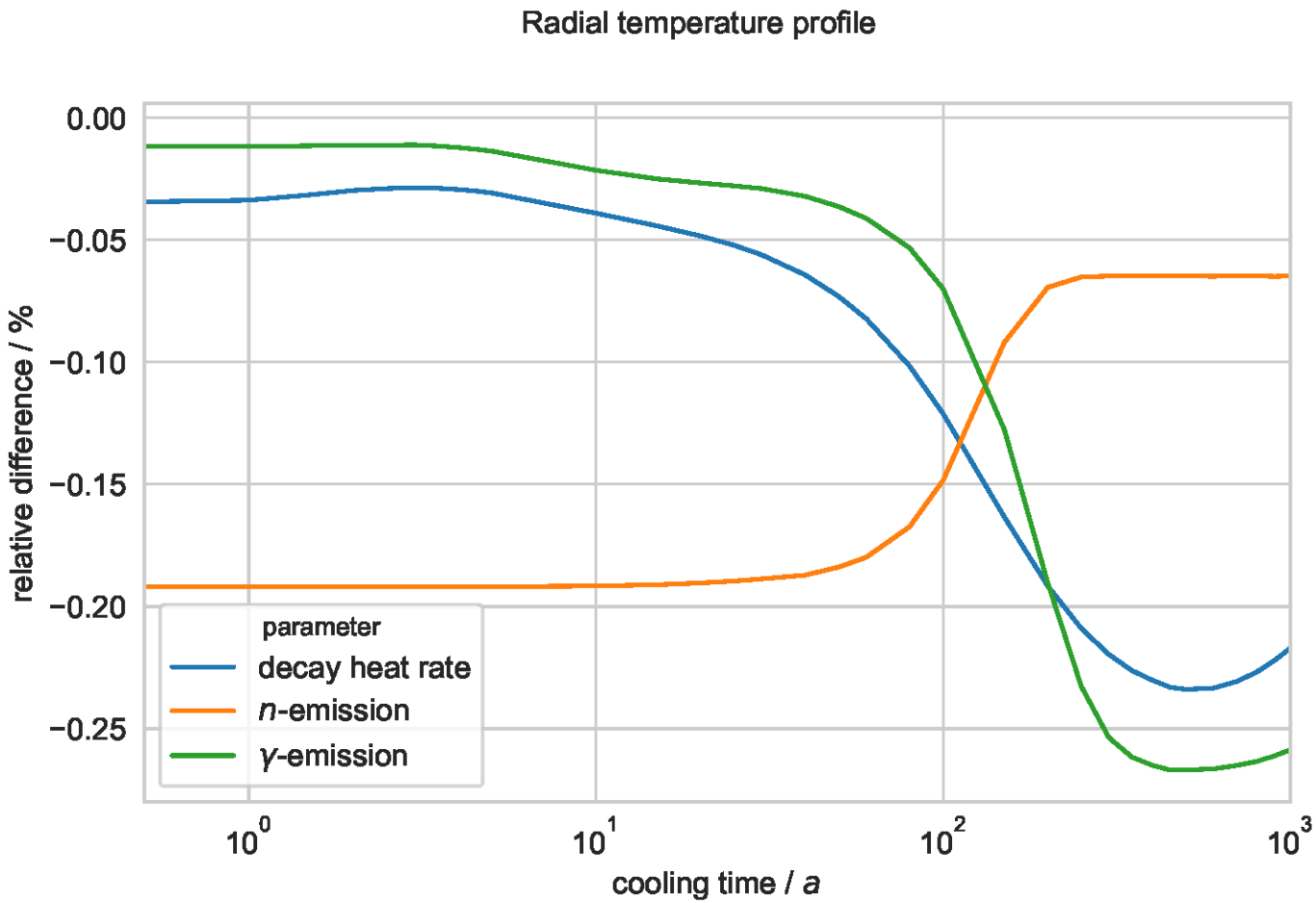
Irradiation conditions: fuel temperature profile

T_f: 4 equi-volume radial regions @ different T
Ref. case: T independent of radial position



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Irradiation conditions: moderator density and temperature

Moderator temperature profile in a typical PWR:

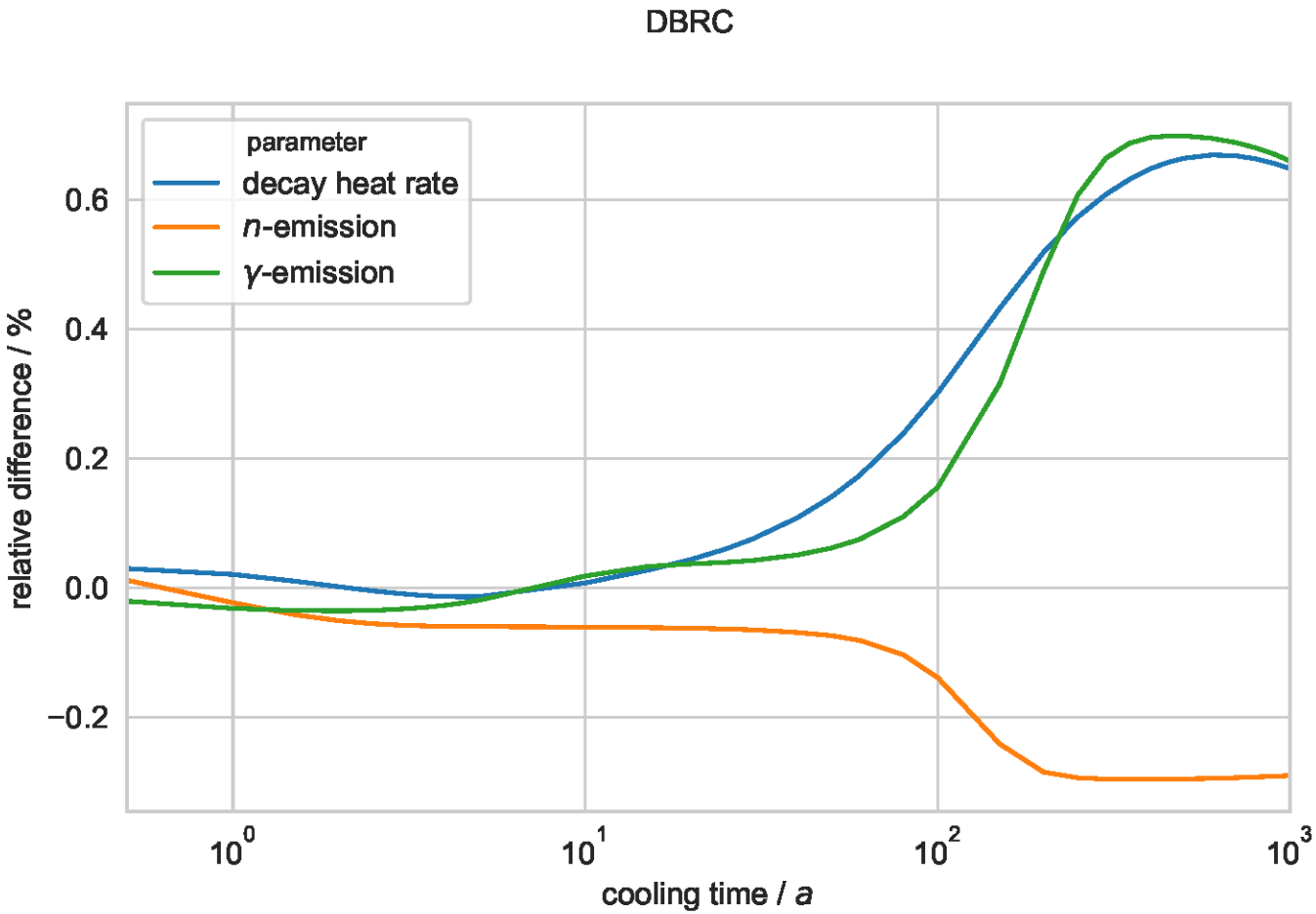
- Bottom: ~560 K (ρ = 0.752 g/cm^3 @ 15.5 MPa)
- Top: ~600 K (ρ = 0.661 g/cm^3 @ 15.5 MPa)
- 2D slices at different conditions: **T effect small, ρ effect large**

Nucl.	*c* (600 K) / *c* (580 K) - 1	*c* (560 K) / *c* (580 K) - 1	**Nucl.**	*c* (600 K) / *c* (580 K) - 1	*c* (560 K) / *c* (580 K) - 1
^{90}Sr	-0.73%	0.54%	^{238}Pu	3.21%	-2.51%
^{134}Cs	2.24%	-1.54%	^{239}Pu	**5.09%**	**-3.77%**
^{137}Cs	0.00%	0.00%	^{240}Pu	8.83%	-5.82%
^{148}Nd	-0.05%	0.04%	^{241}Pu	2.49%	-1.76%
^{149}Sm	8.33%	-5.28%	^{242}Pu	6.84%	-4.72%
^{235}U	6.53%	-4.80%	^{241}Am	7.18%	-4.94%

Physical approximations: DBRC (on/off)

DBRC: used for ^{238}U, $^{240,242}Pu$ and ^{241}Am

No DBRC: ref. case



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Summary and conclusions

Analysis of modelling uncertainties/biases – case study:

- Calculations: neutron transport (MC, det.) + depletion
- Case: simplified PWR assembly
- ND library: ENDF/B-VII.1
- Observed quantities: Nuclide vector, decay heat, neutron and γ-ray emission

Analysis of modelling uncertainties/biases – main results:

- Time discretization: optimal time step scheme is problem dependent.
- Spatial discretization of the depletion zones:
  - Optimal pin grouping depends on boundary conditions
  - For UO_2 fuel, 4 equi-volume radial depletion zones are sufficient (<0.1% bias for ^{244}Cm); 2 regions with optimized border are almost sufficient
- Operational conditions:
  - Axial moderator density important – non-linear effect (either 3D or 2D slices).
  - Radial fuel temperature: small differences, 1 radial zone almost sufficient.
- DBRC causes <1% difference in observables (has to be studied in more detail).

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Future work

- ⇒ Detailed sensitivity studies
  - ⇒ Nuclear data
  - ⇒ Operational history
  - ⇒ Geometry & materials
  - ⇒ Model parameters (depletion time steps, depletion zones, nuclide vector, etc.)
- ⇒ Experimental validation
  - ⇒ Decay heat measurements from from SNF (e.g. SKB-50, „Blind Test“)
  - ⇒ Neutron emission measurements from SNF (JRC/SCK)
  - ⇒ SFCOMPO database
  - ⇒ Nuclear data measurements (decay energies, actinide cross sections, etc.)