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CA-MSR Inventory Simulations

Using OpenMC and Serpent

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Multi-step verification of the Copenhagen atomics molten salt experiment radioactive inventory at the Paul Scherrer Institute using OpenMC, Serpent, and EQL0D

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The molten salt experiment (MSE) is a 30-day 1 MW (thermal) molten salt criticality experiment designed by Copenhagen Atomics that will be conducted at the Paul Scherrer Institute (PSI) Swiss research center. A detailed analysis of the radioactive inventory available during the operation and after shutdown has been carried out for future estimates of potential source term release in case of undesired accidents using the Monte Carlo transport and depletion code OpenMC. To benchmark the radioactive inventory obtained through the OpenMC burn-up calculation (version 0.15.2), code-to-code comparison with the Serpent Monte Carlo and depletion code (v2.2.1), as well as with Serpent coupled to the EQL0D depletion module developed at PSI, were performed. All of the utilized codes support neutron transport on CAD-based geometries and allow continuous material reprocessing during depletion. This feature is essential for modeling the MSE concept, where gaseous fission products are continuously extracted from the circulating fuel salt. For the present verification study, three models of increasing geometric and physical detail were developed: (1) a nested hollow sphere model in constructive solid geometry (CSG), with the scope of aligning basic settings beyond geometry; (2) a geometrically simplified CAD model of the Copenhagen Atomics Onion Core, mainly utilized for testing the integration of CAD models within the above depletion codes; (3) the same simplified CAD model but with the implementation of reactor fluid flows from the inner active core to the outer inactive region, mainly to account for the effect of out-of-core decay. The results were compared to benchmark the original OpenMC model. Particular attention was given to the end-of-cycle (EOC) isotopic inventory, with detailed comparisons for key radionuclides and total radiotoxicity.

KEYWORDS
Monte Carlo neutron transport, burnup calculations, molten salt reactor, OpenMC, Serpent, EQL0D, CAD, CSG

NERIS

PIANOFORTE
EUROPEAN PARTNERSHIP FOR RADIATION PROTECTION RESEARCH

NMBU Norges miljø- og biovitenskapelige universitet

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Main Objective

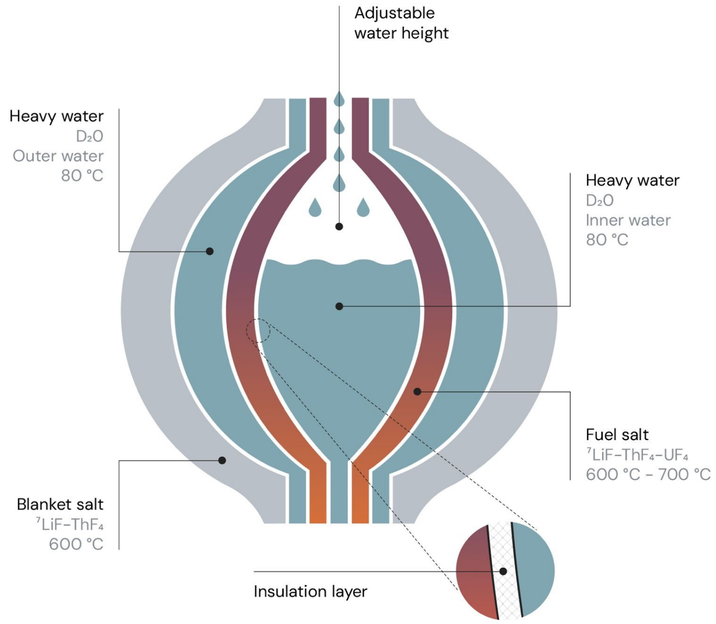
Source term calculation by simulating CA-MSR inventory under normal operation and accident conditions

Introduction

Onion Core

Concept Reactor

- Compact molten salt reactor
  - Liquid (dissolved) fuel
  - Breedable blanket
- Small, can fit in a container
- LEU fuel
- Possibility for fuel processing
  - E.g. Off-gas system
- Scheduled to be tested 2026—2027



Background

What the reference literature includes:

- Material definitions
- Total volumes
- Scripts
- Total mass of FP, synthetic ac+, ogs
- Depletion settings
- k_{eff}

What the reference literature does not include:

- No geometry file provided
  - Free parameters: Spherical radii, cladding thicknesses
- No exact quantities of FP, actinides, ogs isotopes

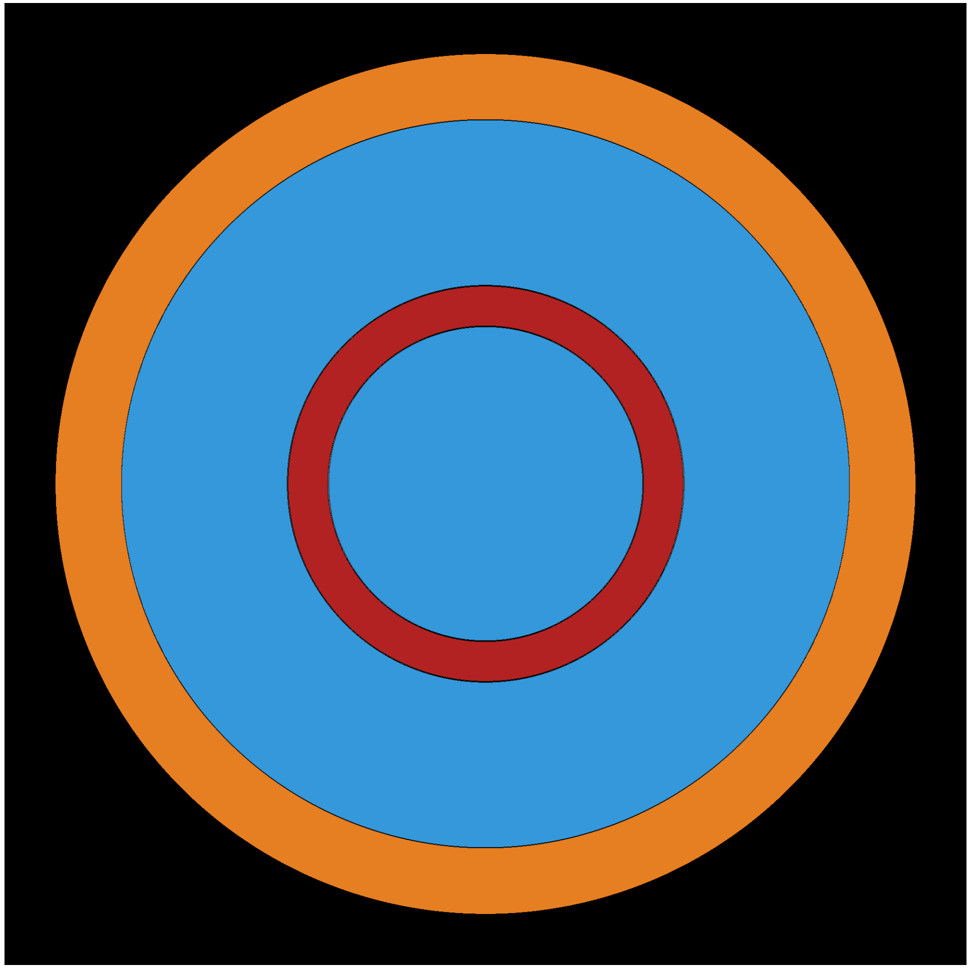
We have benchmarks but not the model. The approach is to reverse engineer a simple core model.

Setup

Determining Geometry

- Geometry radii not given in the paper
- Constraints: k_eff and material volumes
- 2 free parameters*:
  - R1: Inner radius
  - t: Cladding thickness

**Other radii expressed in terms of R1 and t, constrained by total volume*

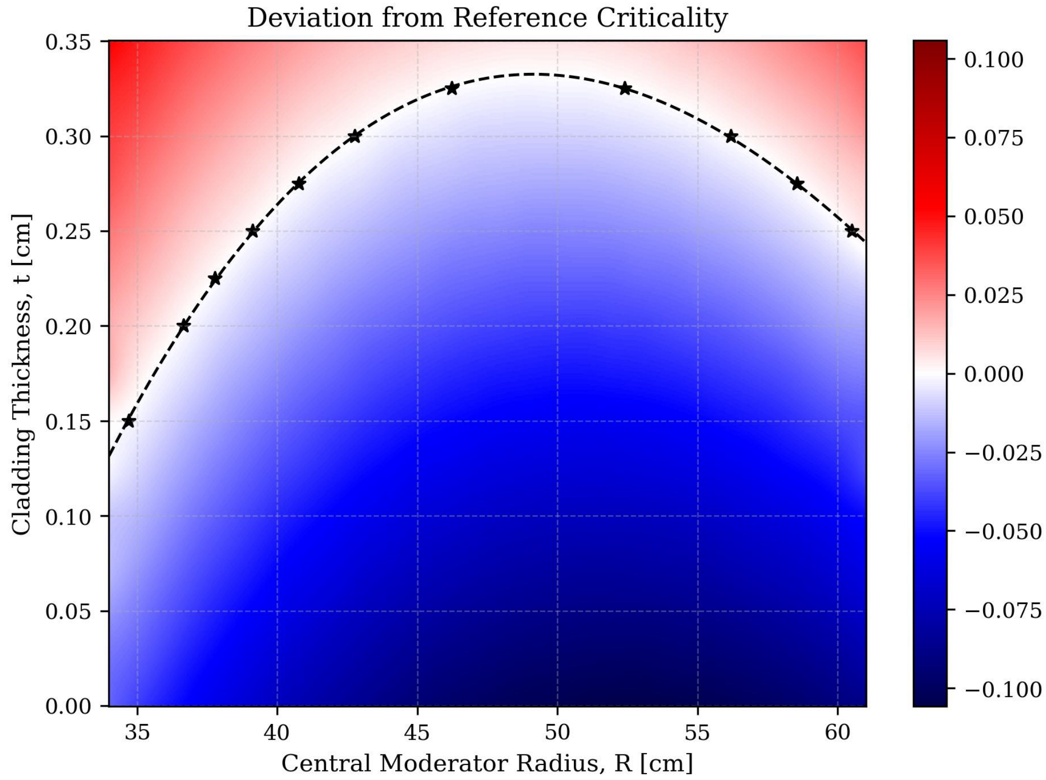


Methodology

Methodology

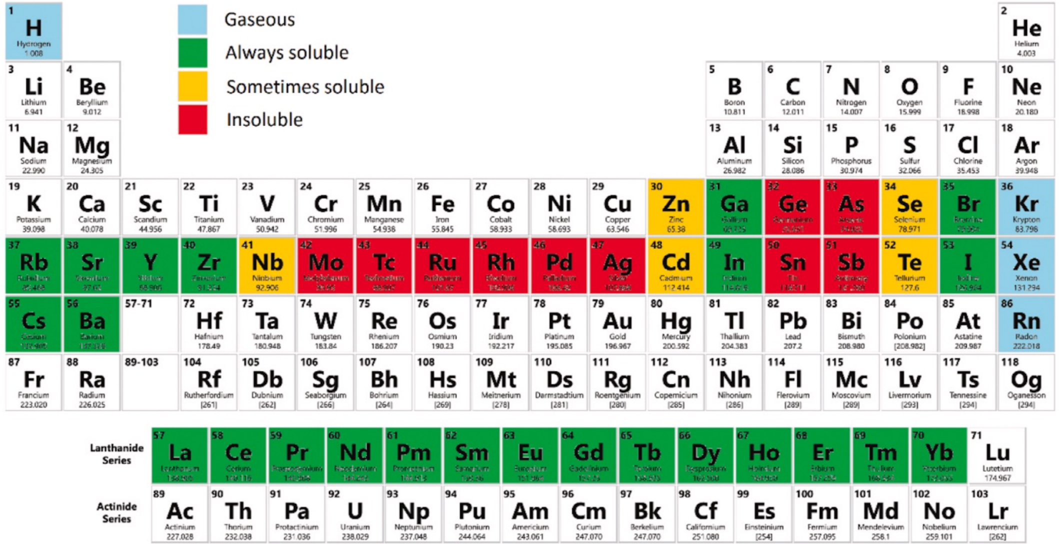
GOAL: Replicate the keff of the paper AND the inventory

1. Test different geometric configurations
2. Select candidate cases that fulfil criteria
3. Deplete and benchmark against reference mass and activity
4. Select best-matching case geometry
5. Scale up to 100 MWth
6. Calculate inventory after 30 days



Source Term calculation

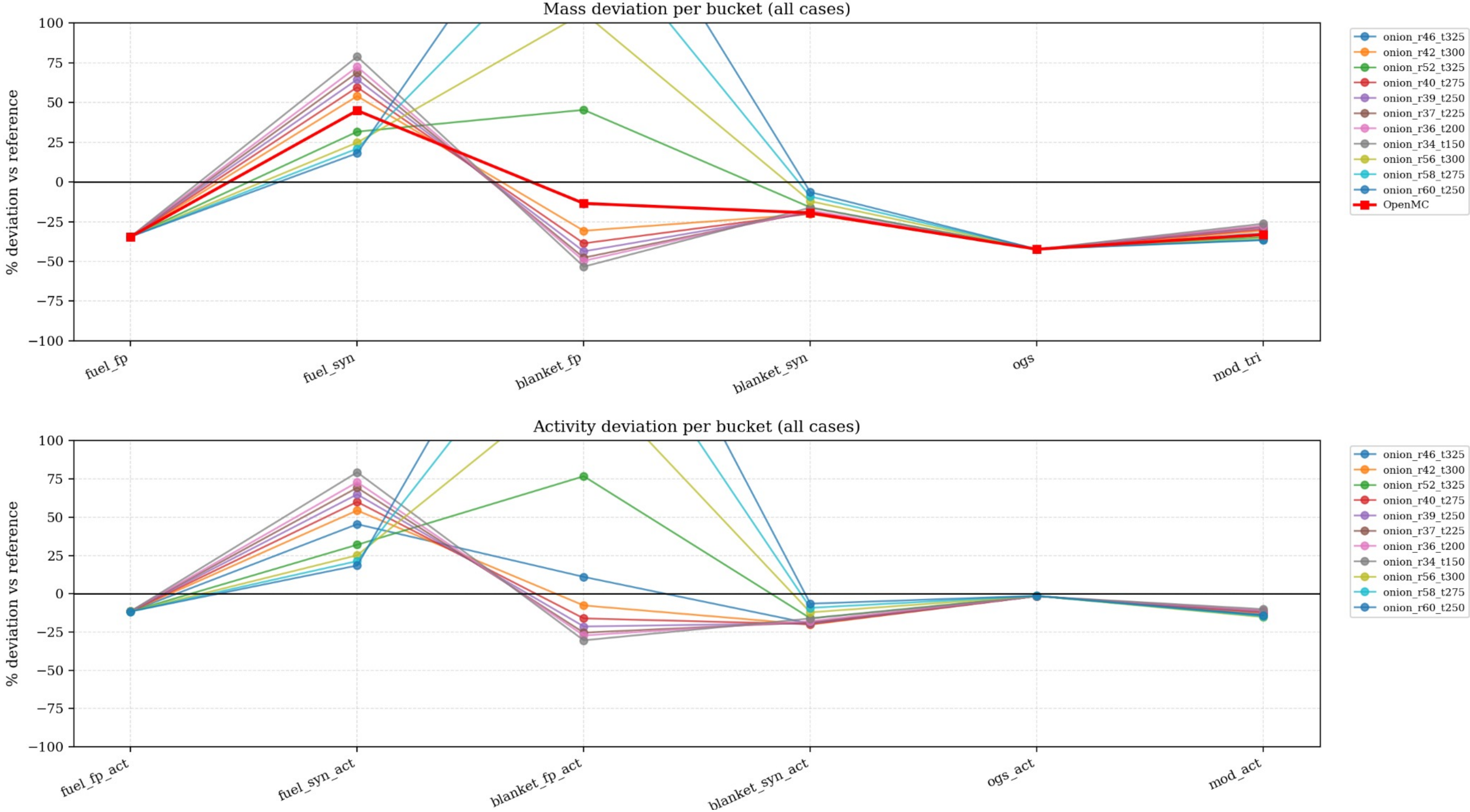
- We categorized nuclides in Wheeler* groups, according to molten-salt behavior
  - Gaseous: 100% RF
  - Always soluble 0% RF
  - Sometimes soluble 10% RF
  - Insoluble 0% RF
  - Actinides 10% RF

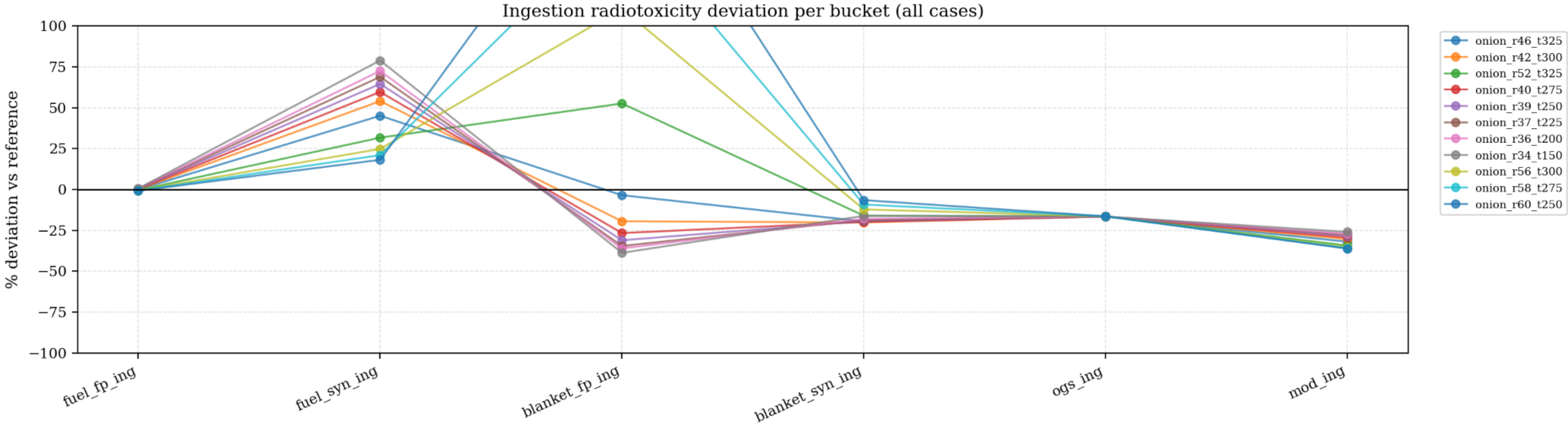


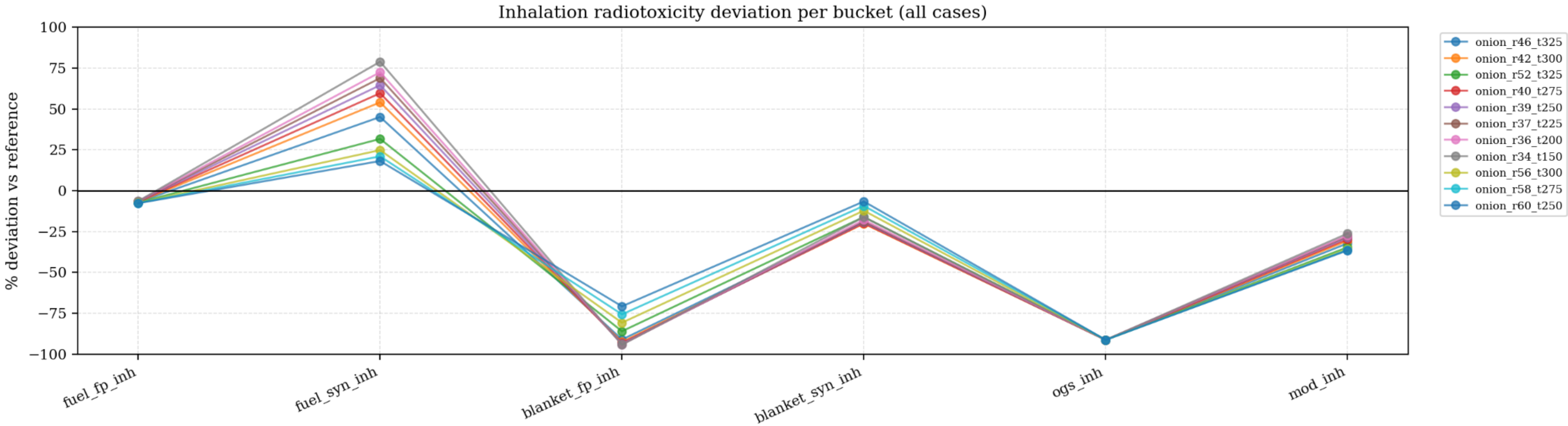
*Wheeler, A. M., Singh, V., Miller, L. F., & Chvála, O. (2021). Initial calculations for source term of Molten Salt Reactors. Progress in Nuclear Energy, 132, 103616.

Results

Best Matching Candidate Search

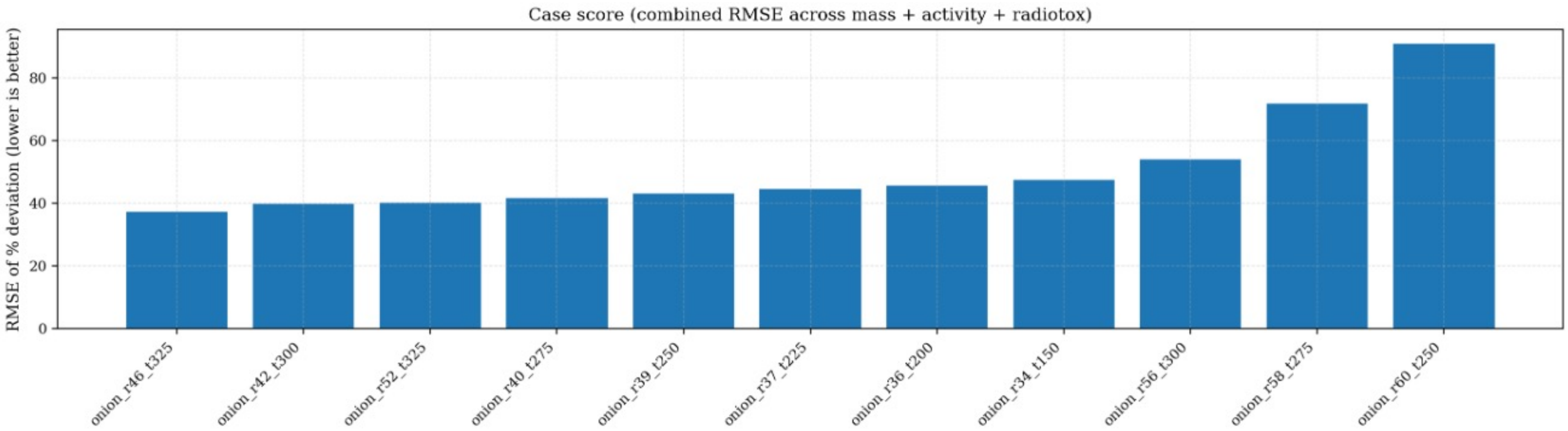



Ingestion radiotoxicity deviation per bucket (all cases)
% deviation vs reference
100
75
50
25
0
−25
−50
−75
−100
fuel_fp_ing
fuel_syn_ing
blanket_fp_ing
blanket_syn_ing
ogs_ing
mod_ing
onion_r46_t325
onion_r42_t300
onion_r52_t325
onion_r40_t275
onion_r39_t250
onion_r37_t225
onion_r36_t200
onion_r34_t150
onion_r56_t300
onion_r58_t275
onion_r60_t250


Inhalation radiotoxicity deviation per bucket (all cases)
% deviation vs reference
100
75
50
25
0
−25
−50
−75
−100
fuel_fp_inh
fuel_syn_inh
blanket_fp_inh
blanket_syn_inh
ogs_inh
mod_inh
onion_r46_t325
onion_r42_t300
onion_r52_t325
onion_r40_t275
onion_r39_t250
onion_r37_t225
onion_r36_t200
onion_r34_t150
onion_r56_t300
onion_r58_t275
onion_r60_t250

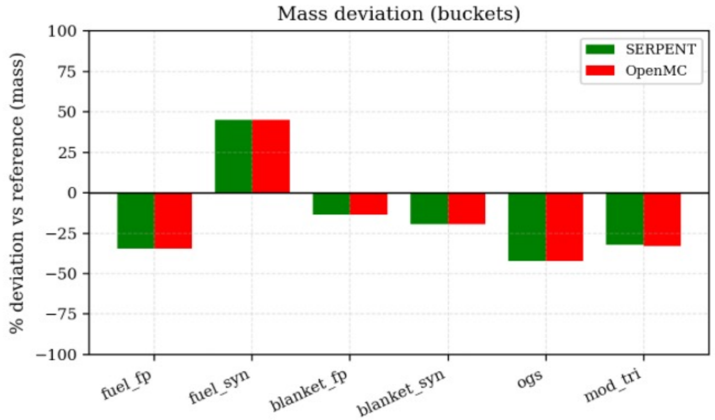
Best Matching Candidate

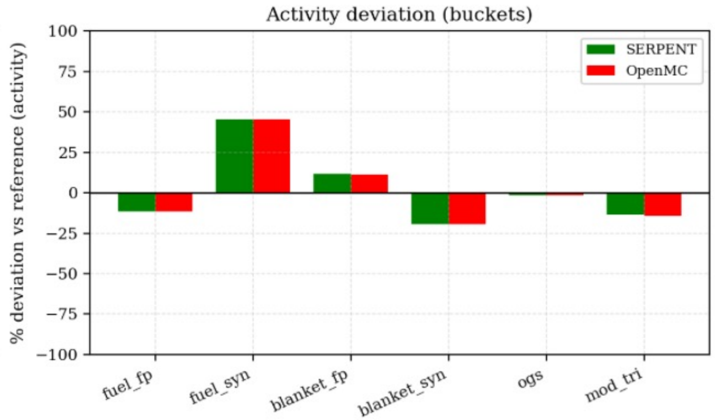
- Inner Radius: 46 cm
- Cladding: 3.25 mm



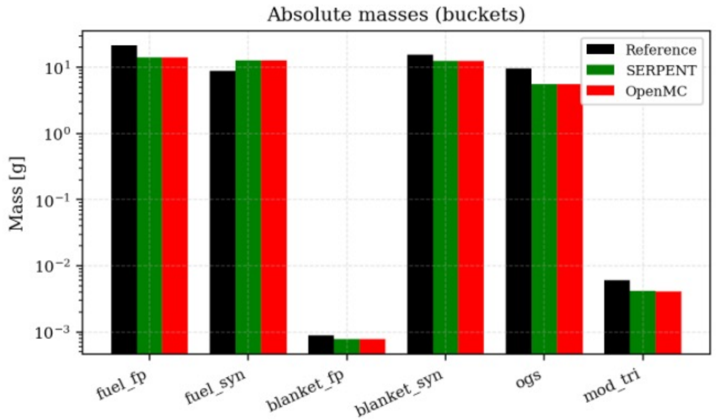
Reference Case Activity and Mass Comparison

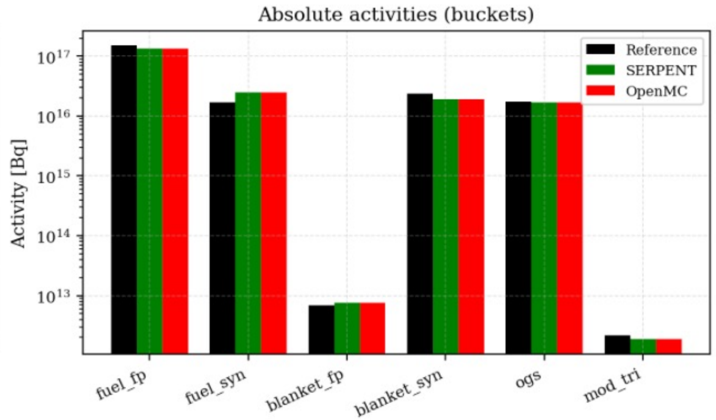
- Excellent agreement between SERPENT and OpenMC



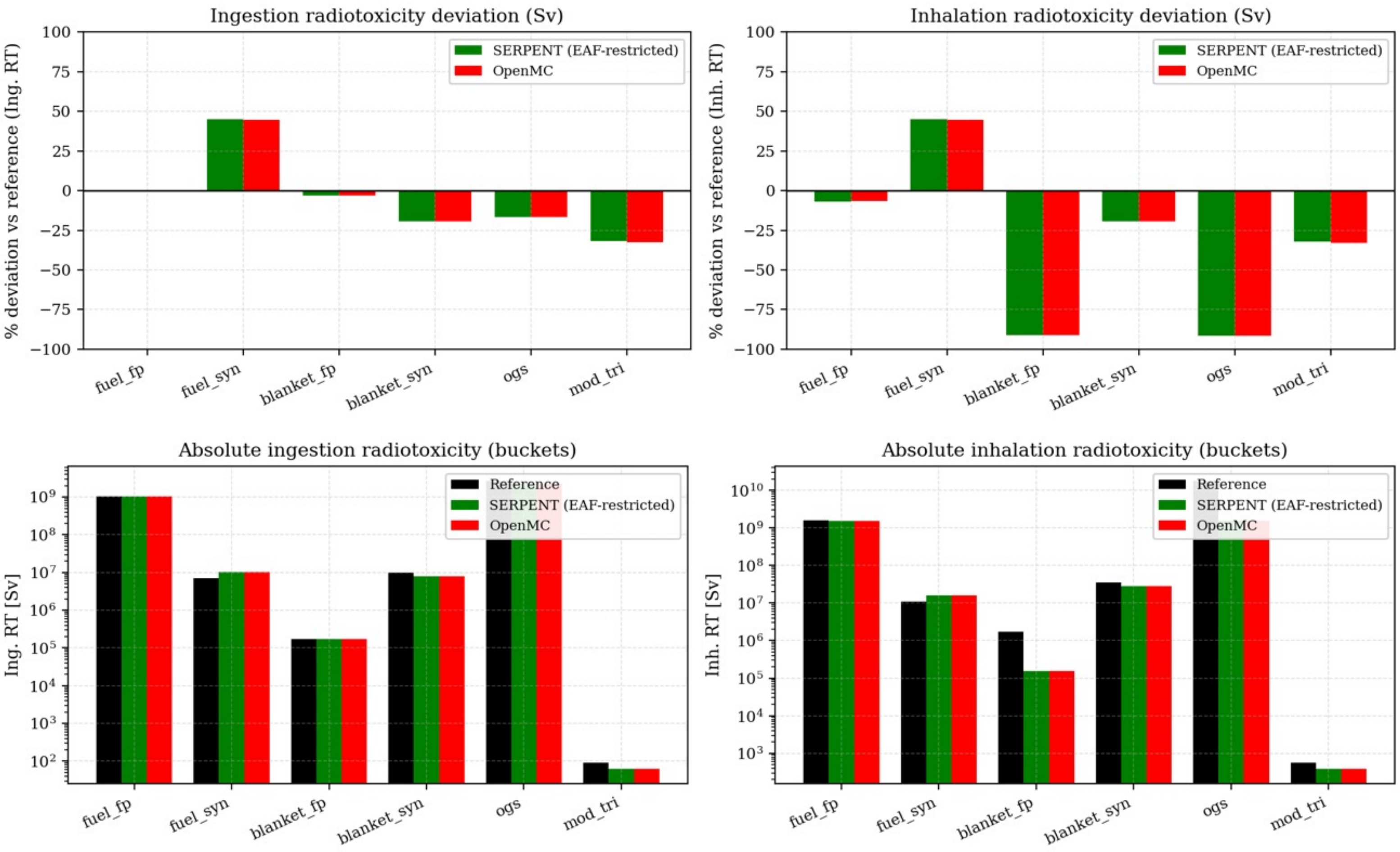


- Less agreement with benchmark





Reference Case Radiotoxicity Results



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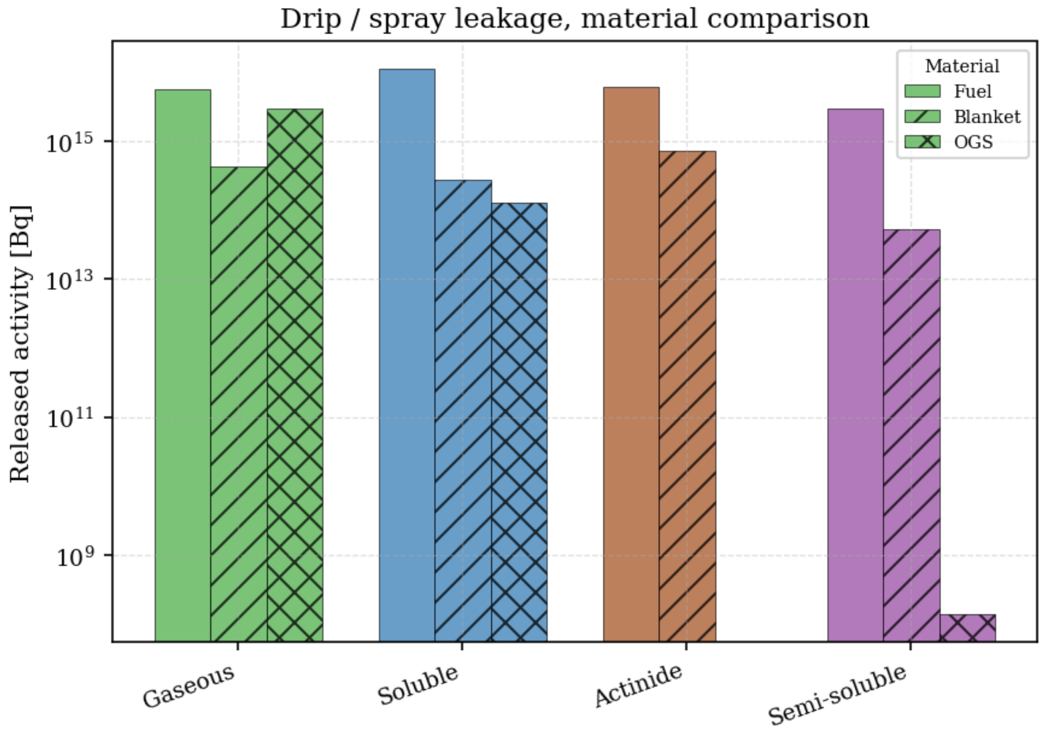
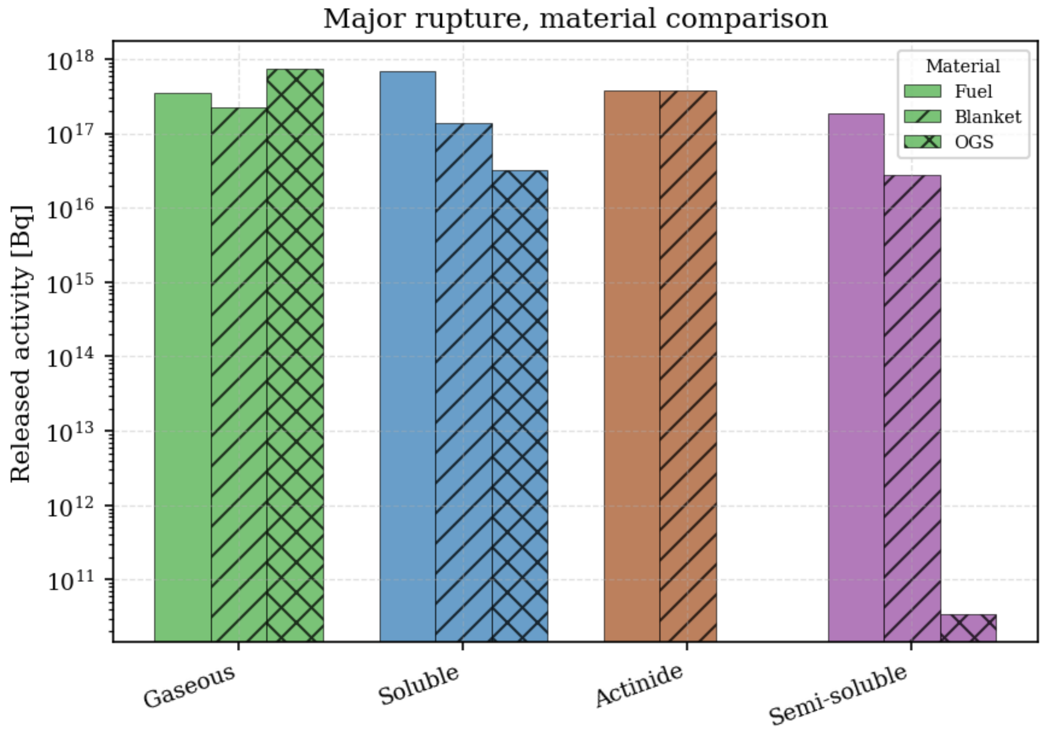
After scaling the reactor and depleting best case to 485 days

2 Accident scenarios: 4L Drip/spray

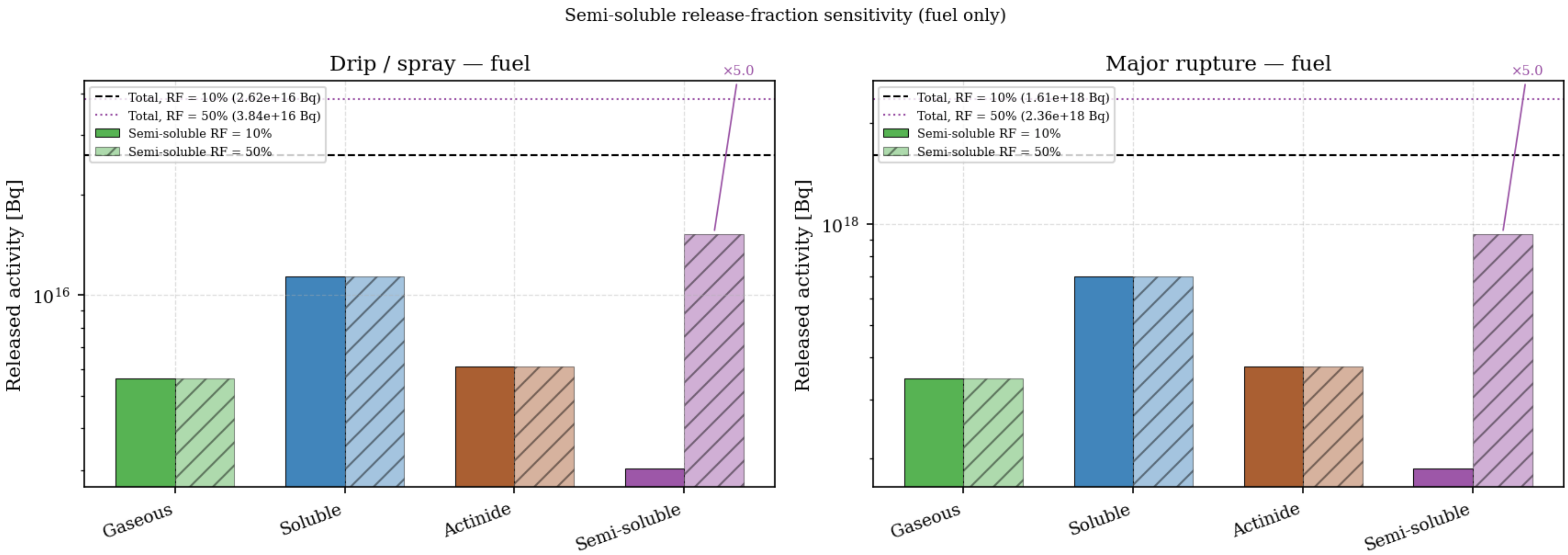
Major Rupture: Full Release



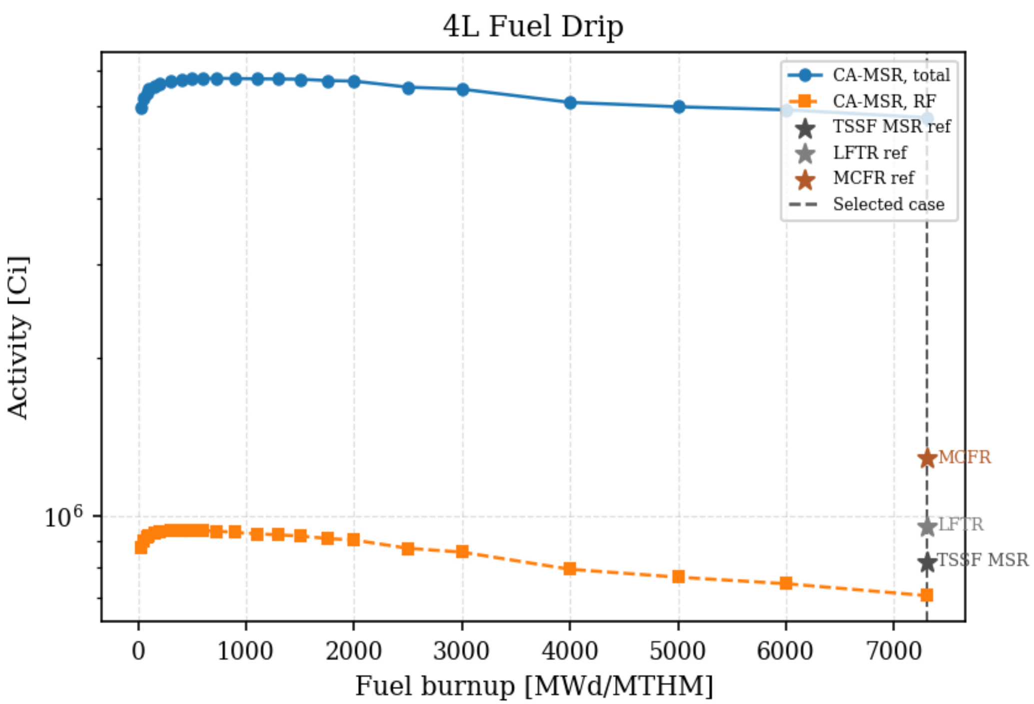


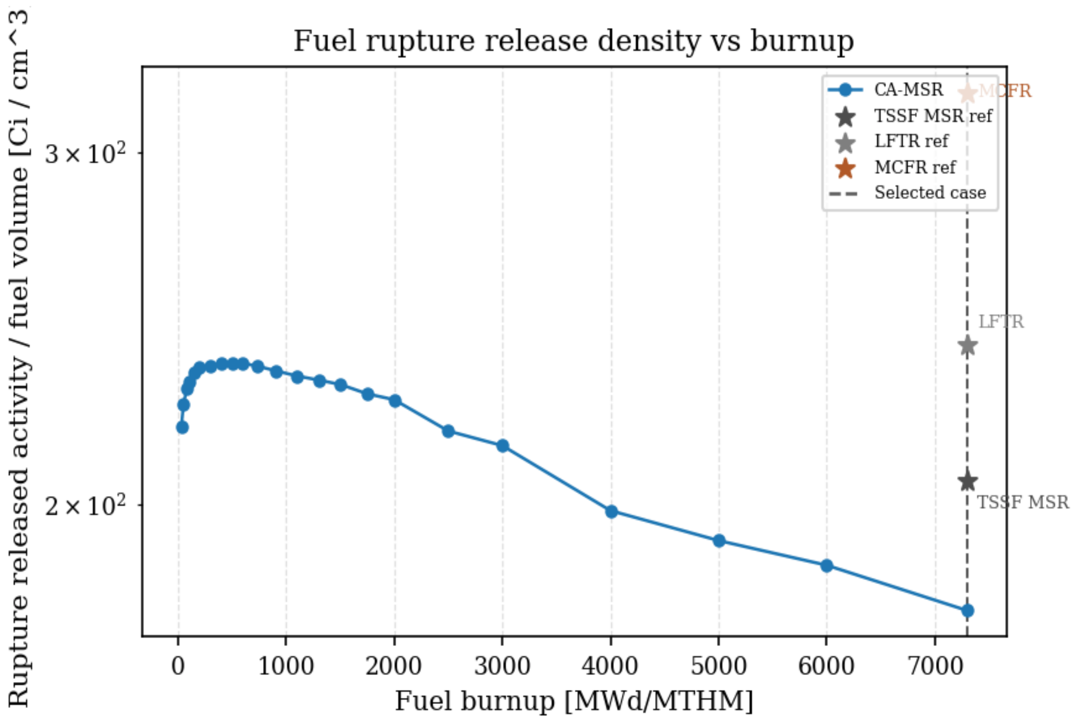
Little Sensitivity Comparison

- What happens if we change our assumption of release fraction



Comparison to literature





Discussion

Limitations and Scope

1. Ex-core salts were not modelled
2. Flow from in-core to ex-core and vice versa were not modelled
3. Inner radius and cladding thickness/composition are free parameters; not ground truths.
4. Lowest RMSE is 30 (40% if we include ing inh)
5. Unclear whether inhalation and ingestion coefficients used in this work match the ones used in the benchmark
6. Rigorous salt chemistry treatment is necessary to find more well-informed release fractions tailored to the CAMSR

Conclusion and Steps Forward

- We built a very simple model that can be used to learn about MSRs and built upon
- Our model achieves RMSE of 30--40
- We created a dataset of all contributing nuclides in both accident conditions and normal operation

Thank you for your attention

CA-MSR source term modelling: reconstructed Onion Core benchmark

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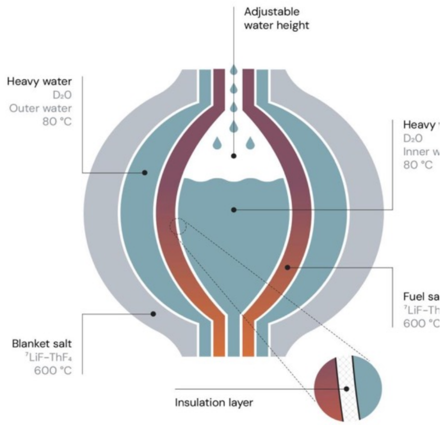
Onion Core concept

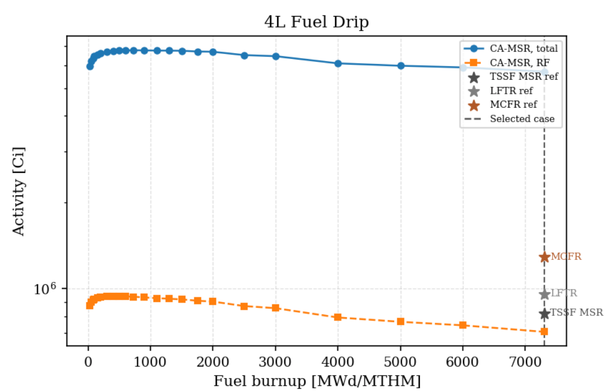


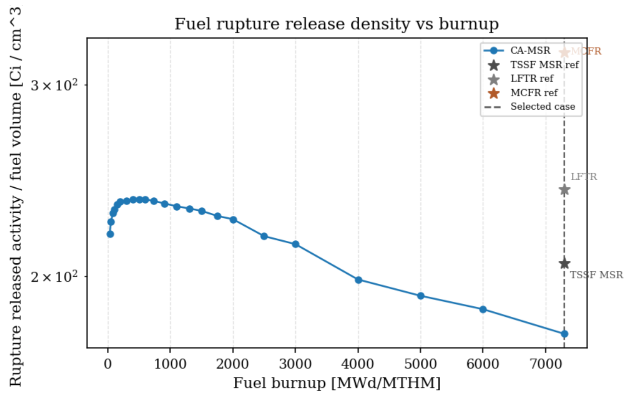
- Compact molten-salt reactor with liquid fuel and a breedable blanket
- LEU fuel concept with off-gas / fuel-processing relevance for source-term studies
- Container scale design used here as the benchmarked reference concept

Methodology: neutronics + depletion

Using published material definitions, total volumes, depletion settings and target k_eff — but no geometry file: we reverse engineered a simple spherical Onion Core model by sweeping inner radius and cladding thickness. Candidate geometries were screened with OpenMC and Serpent, benchmarked against reference mass and activity, and then used for source-term comparisons and accident calculations.

Comparison to literature





Cross-check against published MSR source term data (including TSSF-MSR, LFTR and MCFR) places the selected case in context since full design parameters were unavailable.