

UNIVERSITY OF OSLO

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 critically 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 Orion 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

Main Objective

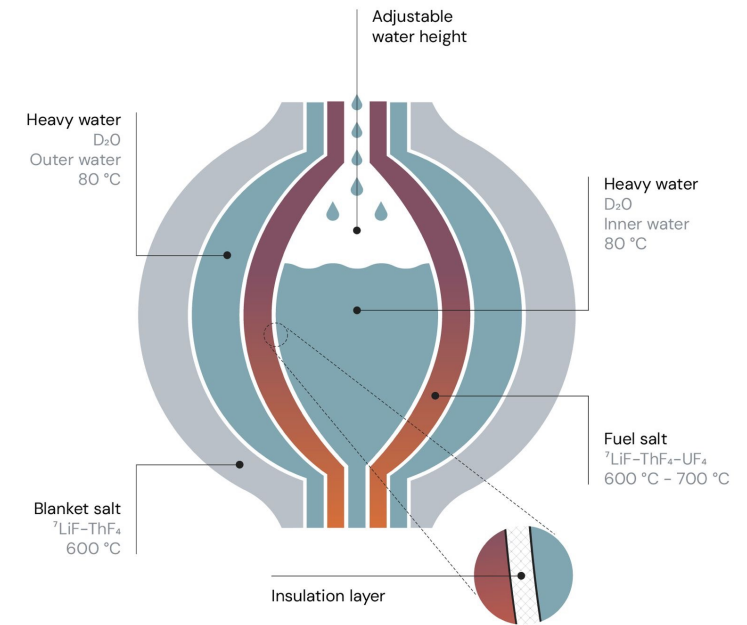
Source term calculation by simulating CA-MSR inventory under normal operation and accident conditions

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

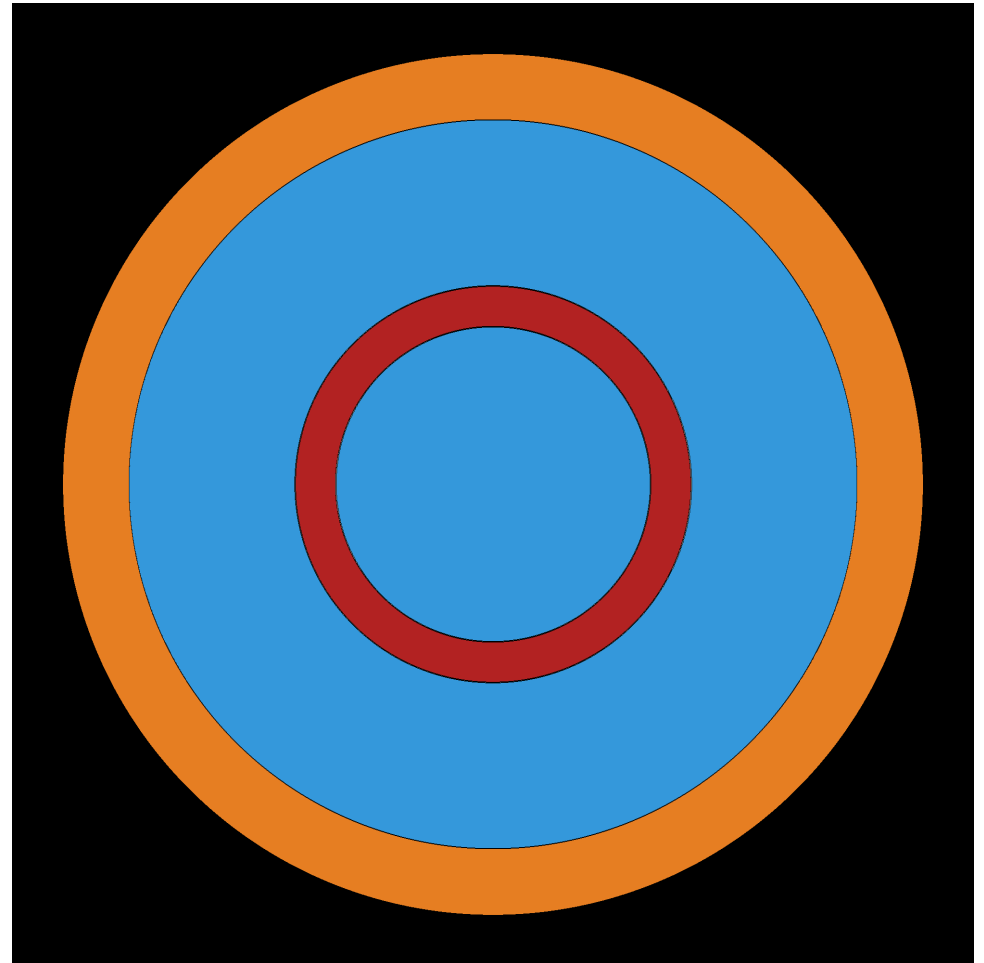
We have benchmarks but not the model. The approach is to reverse engineer a simple core model.

Setup

Determining Geometry

- Geometry radii not given in the paper
- Constraints: k_{eff} and material volumes
- 2 free parameters*:
 - R_1 : Inner radius
 - t : Cladding thickness

**Other radii expressed in terms of R_1 and t , constrained by total volume*

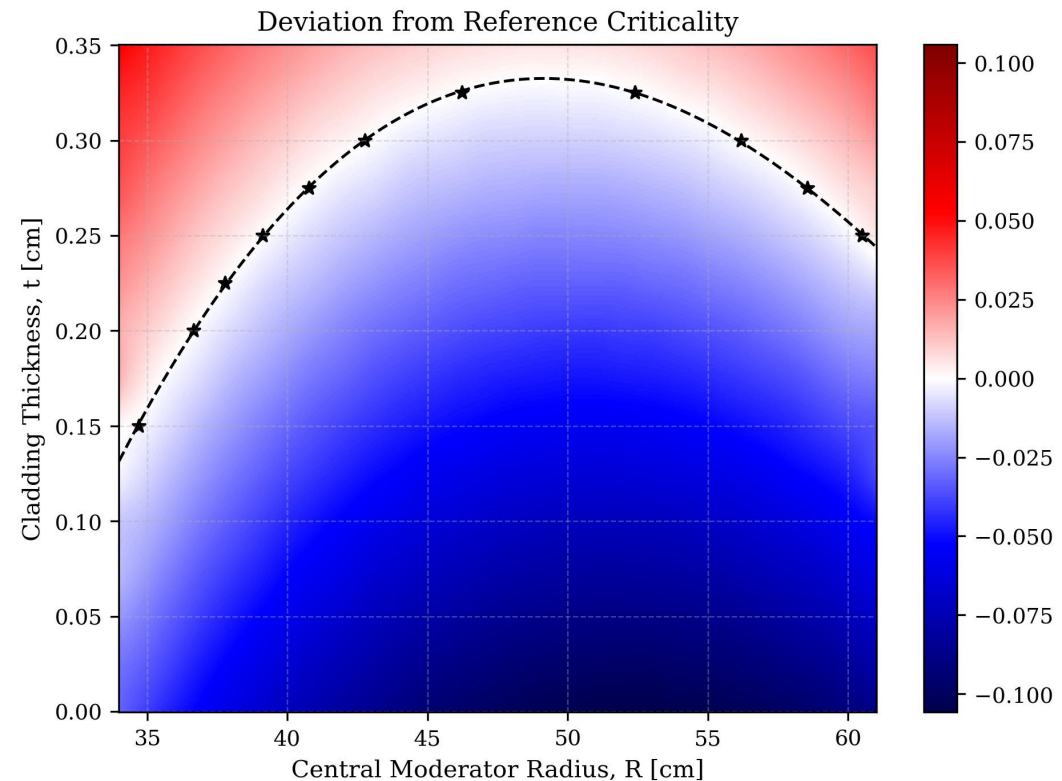


Methodology

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

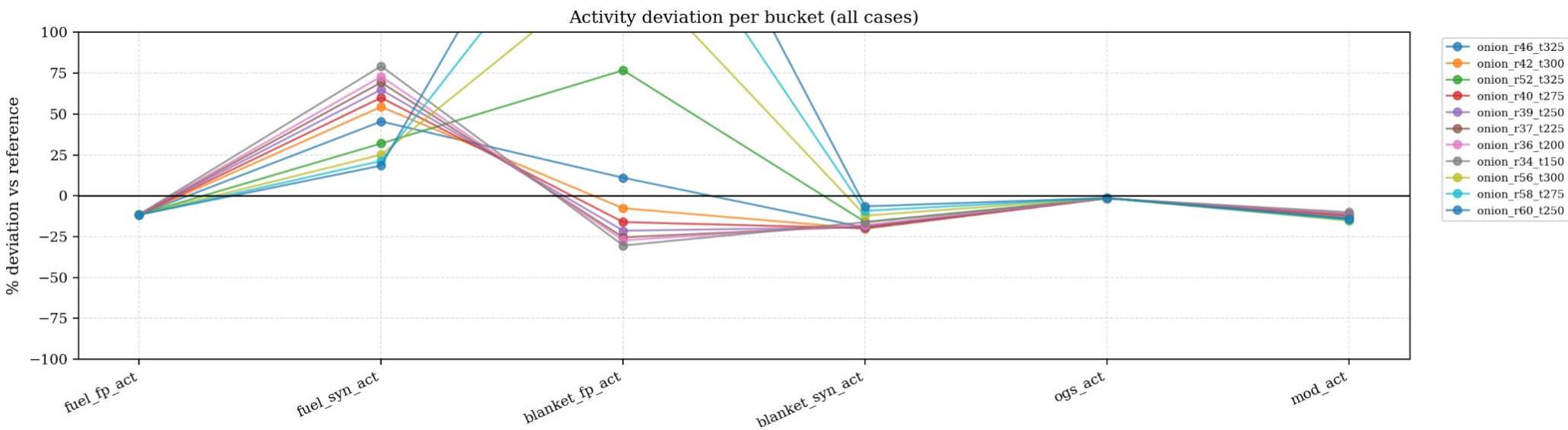
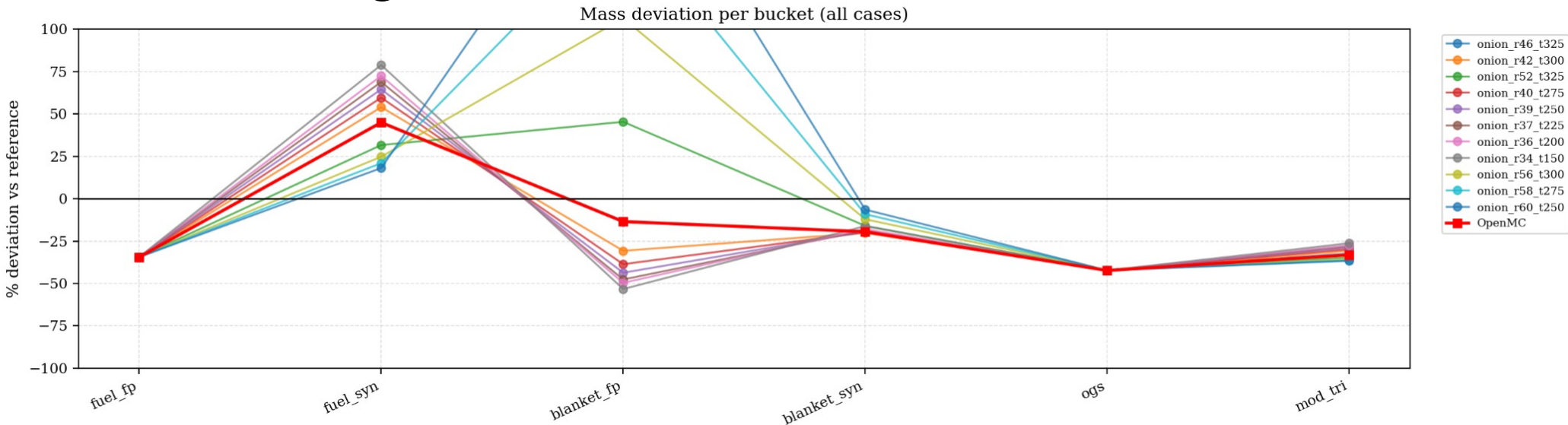
- We categorized nuclides in Wheeler* groups, according to molten-salt behavior
 - Gaseous: 100% RF
 - Always soluble 0% RF
 - Sometimes soluble 10% RF
 - Insoluble 0% RF
 - Actinides 10% RF

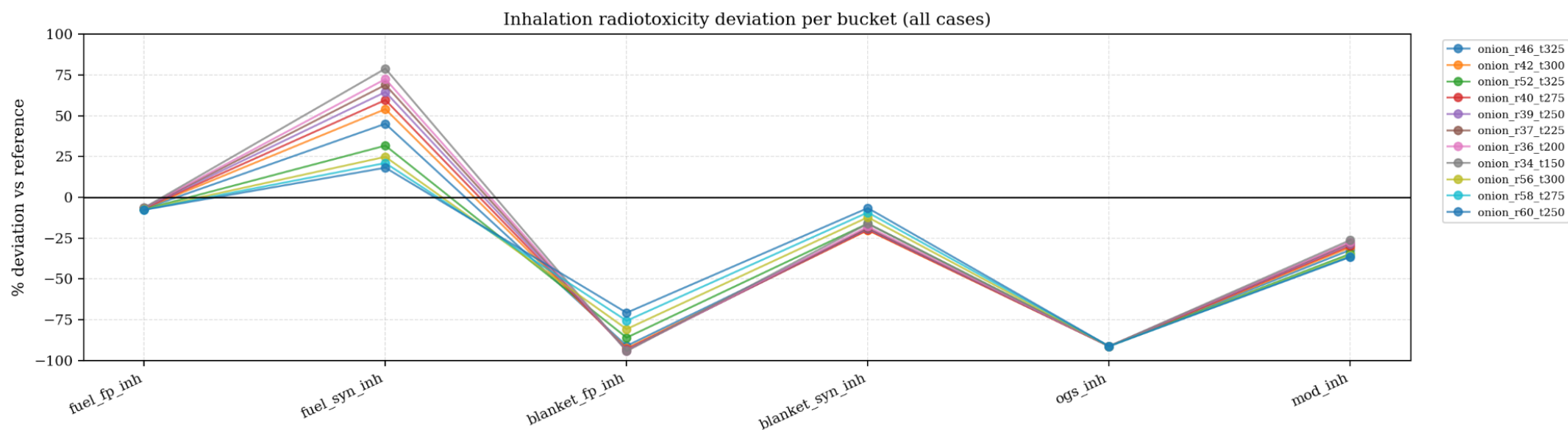
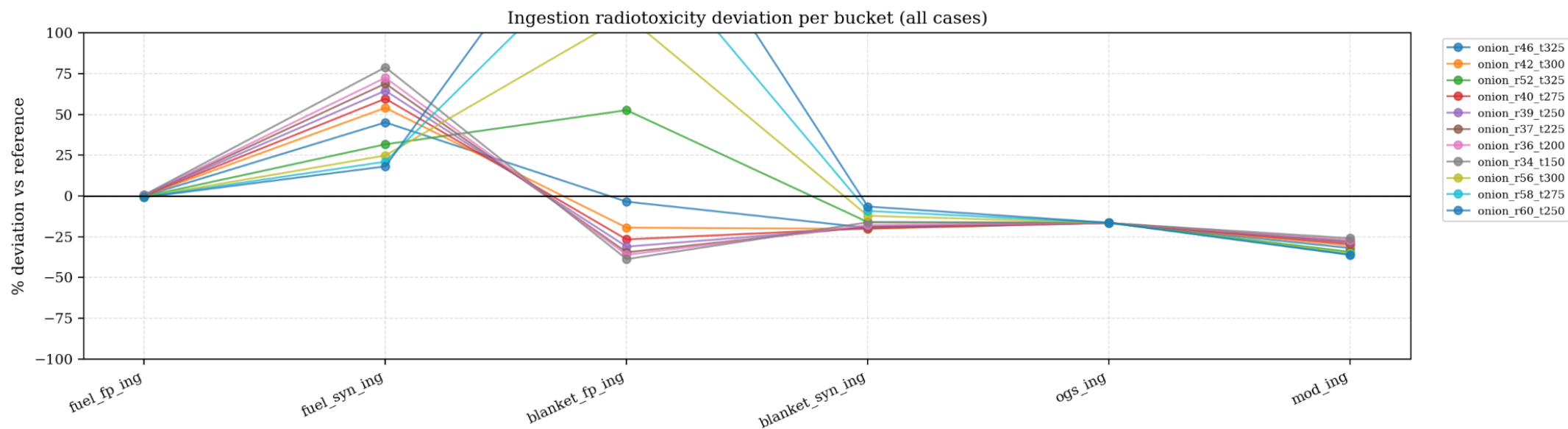
1 H Hydrogen 1.008																	2 He Helium 4.003																																																											
3 Li Lithium 6.941	4 Be Beryllium 9.012																	5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180																																																					
11 Na Sodium 22.990	12 Mg Magnesium 24.305																	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948																																																					
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.796																																																											
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.906	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.905	46 Pd Palladium 106.367	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.294																																																											
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71		72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.225	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [209]	85 At Astatine [210]	86 Rn Radon [222]																																																										
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103		104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [277]	109 Mt Meitnerium [278]	110 Ds Darmstadtium [281]	111 Rg Roentgenium [282]	112 Cn Copernicium [285]	113 Nh Nihonium [286]	114 Fl Flerovium [289]	115 Mc Moscovium [289]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]																																																										
Gaseous Always soluble Sometimes soluble Insoluble <table><tr><td colspan="14">Lanthanide Series</td><td>57 La Lanthanum 138.905</td><td>58 Ce Cerium 140.12</td><td>59 Pr Praseodymium 140.908</td><td>60 Nd Neodymium 144.24</td><td>61 Pm Promethium [145]</td><td>62 Sm Samarium 150.36</td><td>63 Eu Europium 151.964</td><td>64 Gd Gadolinium 157.25</td><td>65 Tb Terbium 158.925</td><td>66 Dy Dysprosium 162.50</td><td>67 Ho Holmium 164.930</td><td>68 Er Erbium 167.259</td><td>69 Tm Thulium 168.934</td><td>70 Yb Ytterbium 173.054</td><td>71 Lu Lutetium 174.967</td></tr><tr><td colspan="14">Actinide Series</td><td>89 Ac Actinium 227.028</td><td>90 Th Thorium 232.038</td><td>91 Pa Protactinium 231.036</td><td>92 U Uranium 238.029</td><td>93 Np Neptunium 237.048</td><td>94 Pu Plutonium 244.064</td><td>95 Am Americium 243.061</td><td>96 Cm Curium 247.070</td><td>97 Bk Berkelium 247.070</td><td>98 Cf Californium 251.080</td><td>99 Es Einsteinium [252]</td><td>100 Fm Fermium [257]</td><td>101 Md Mendelevium [258]</td><td>102 No Nobelium [259]</td><td>103 Lr Lawrencium [262]</td></tr></table>																			Lanthanide Series														57 La Lanthanum 138.905	58 Ce Cerium 140.12	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium [145]	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.967	Actinide Series														89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [252]	100 Fm Fermium [257]	101 Md Mendelevium [258]	102 No Nobelium [259]	103 Lr Lawrencium [262]
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*Wheeler, A. M., Singh, V., Miller, L. F., & Chvala, O. (2021). Initial calculations for source term of Molten Salt Reactors. Progress in Nuclear Energy, 132, 103616.

Results

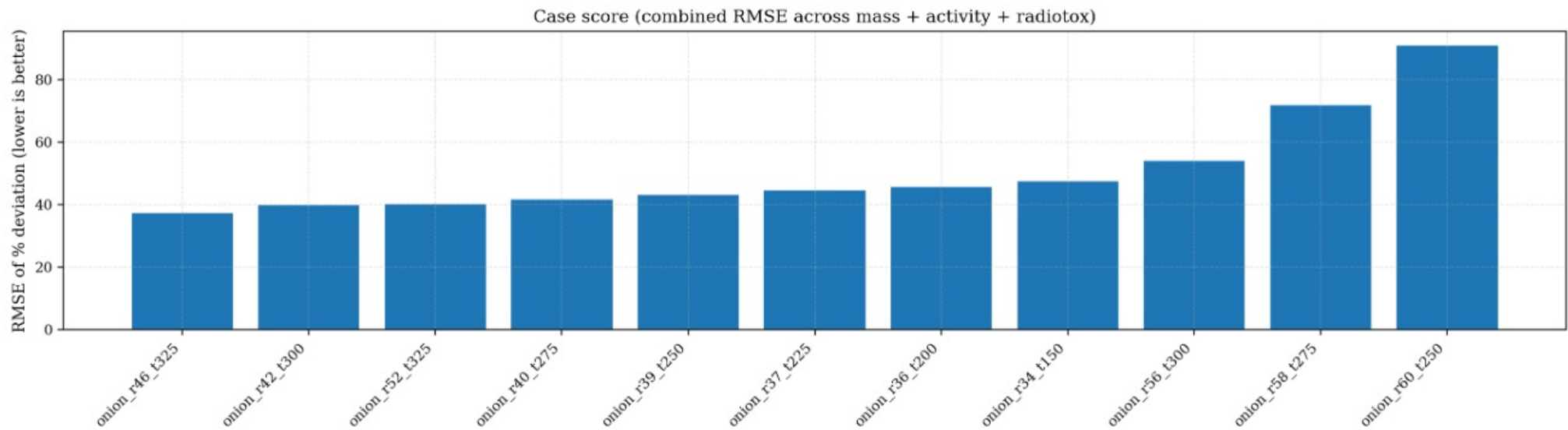
Best Matching Candidate Search





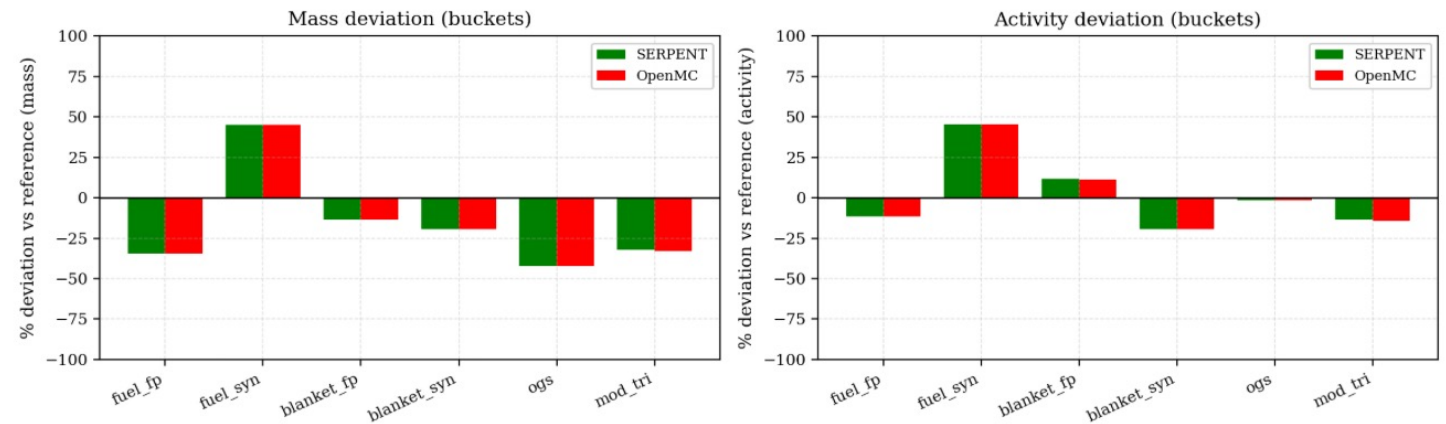
Best Matching Candidate

- Inner Radius: 46 cm
- Cladding: 3.25 mm

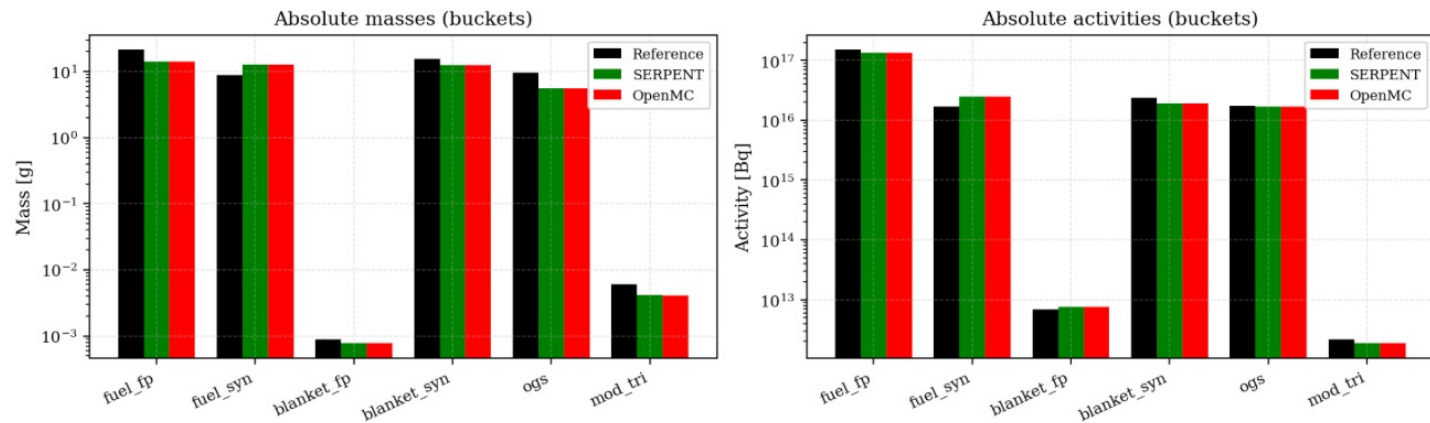


Reference Case Activity and Mass Comparison

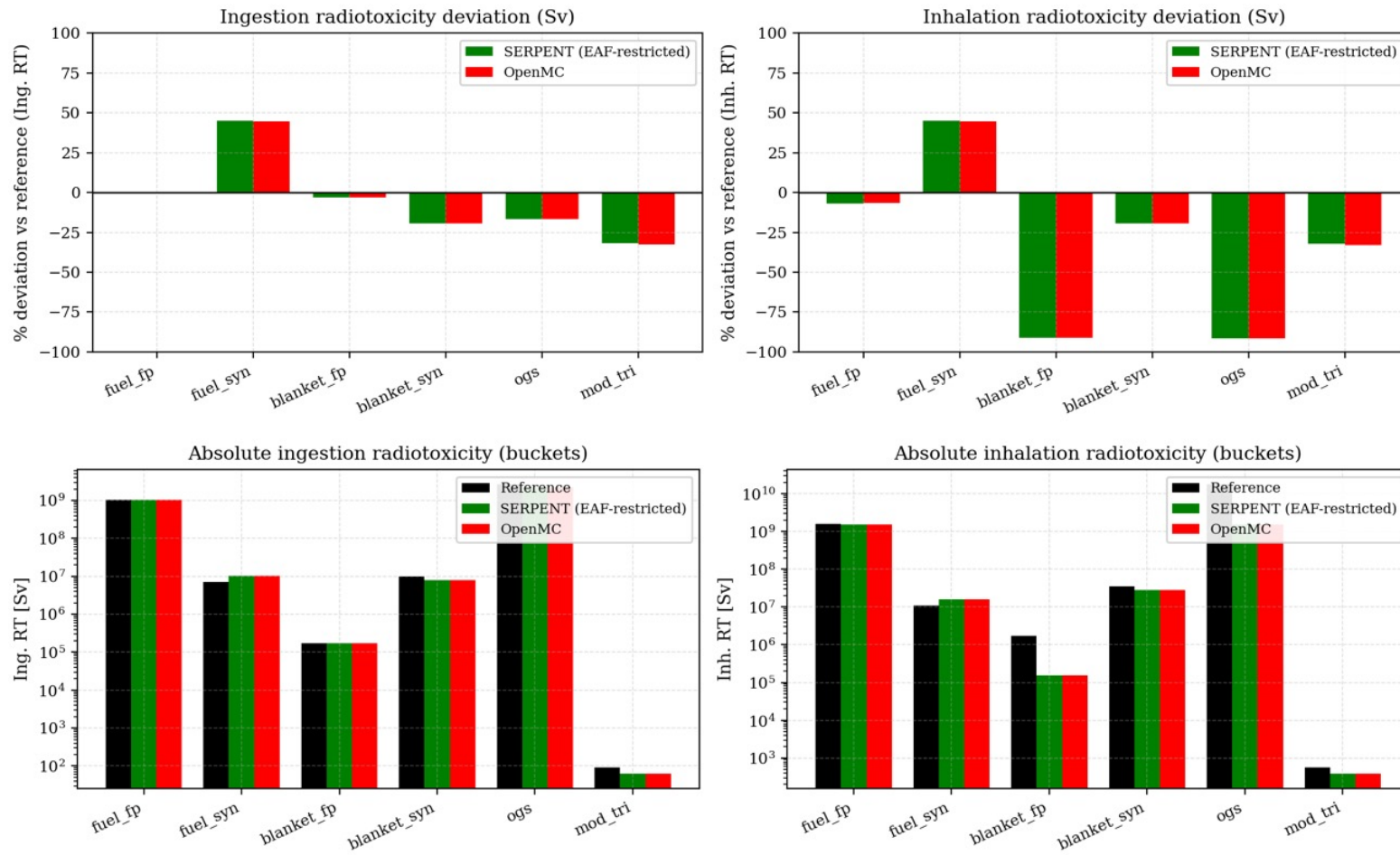
- Excellent agreement between SERPENT and OpenMC



- Less agreement with benchmark



Reference Case Radiotoxicity Results

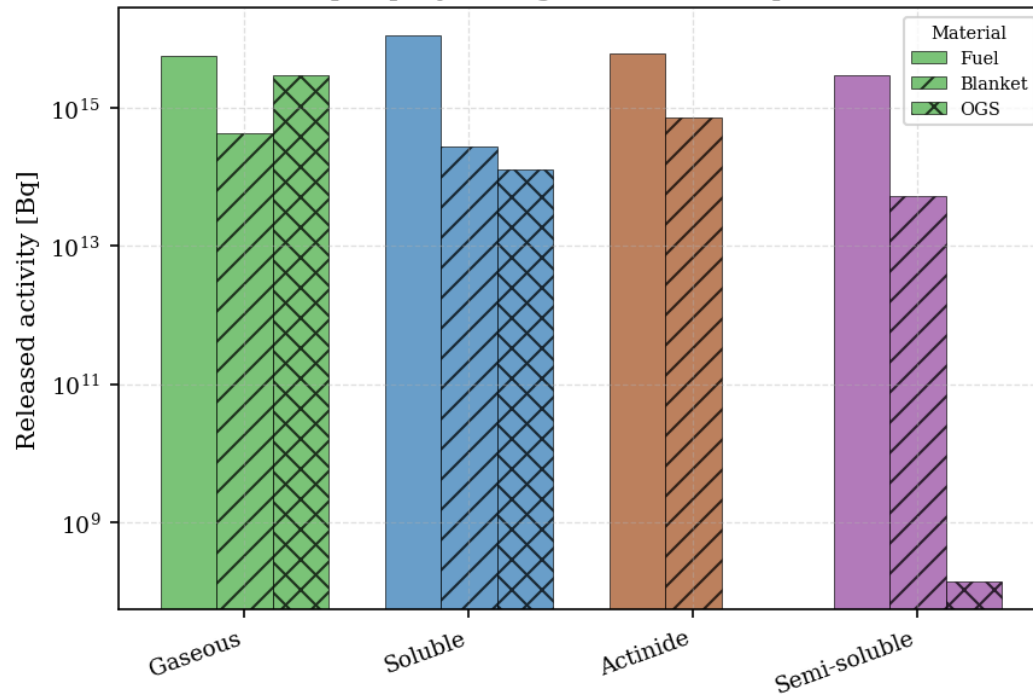


After scaling the reactor and depleting best case to 485 days

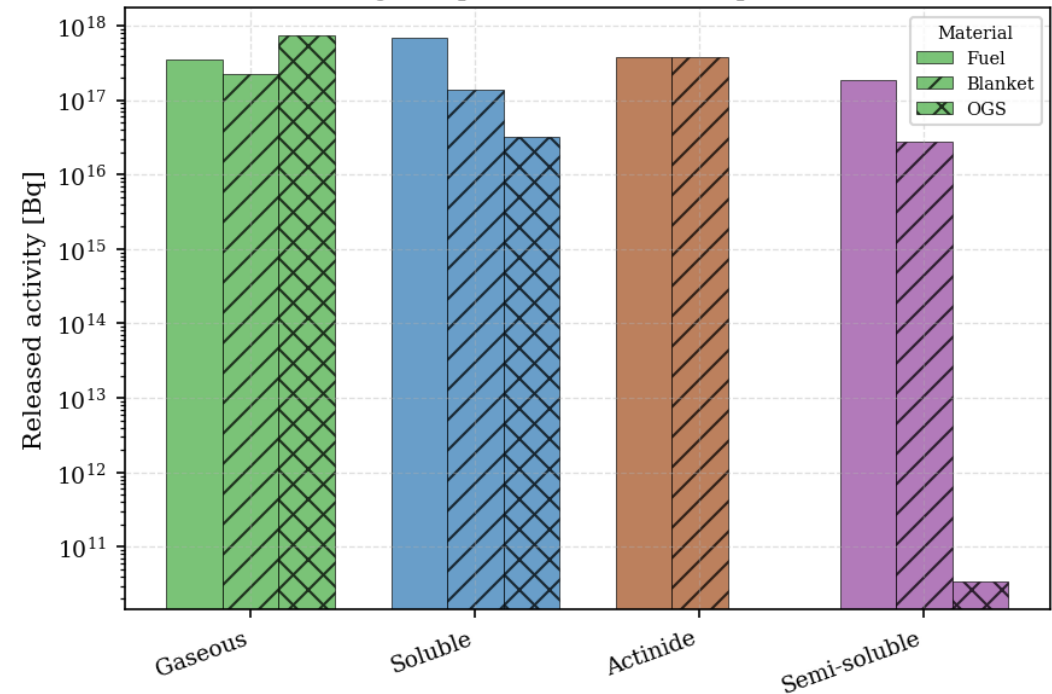
2 Accident scenarios: 4L Drip/spray

Major Rupture: Full Release

Drip / spray leakage, material comparison

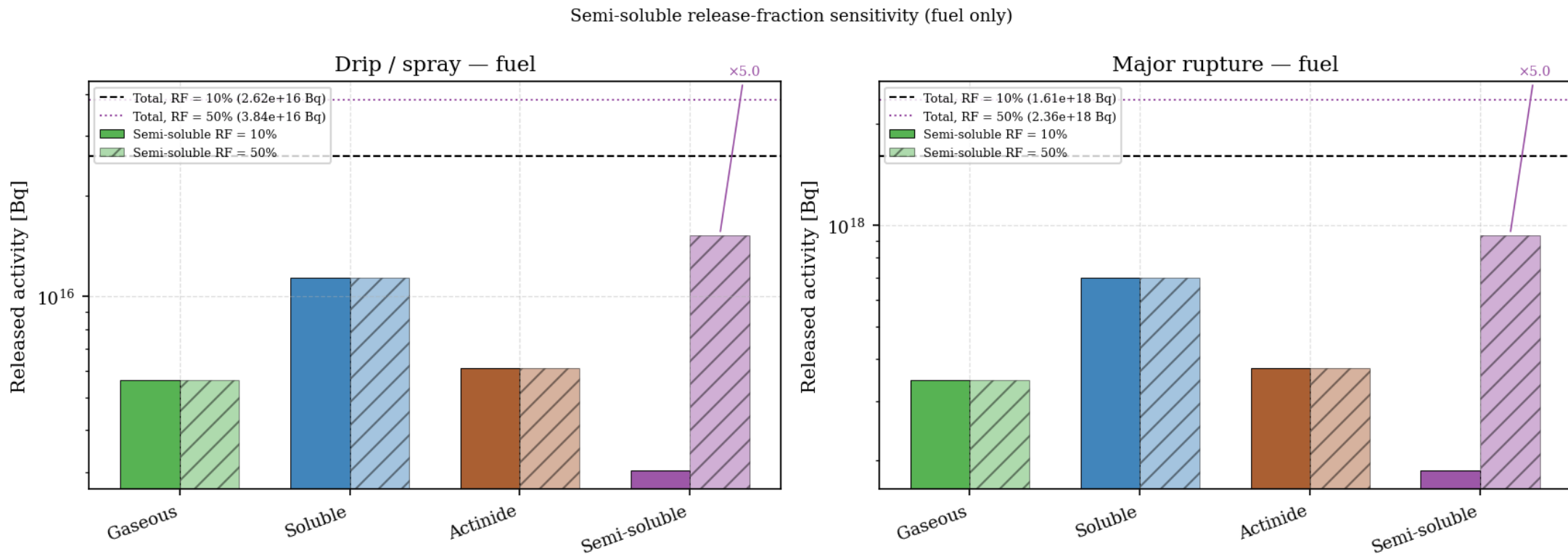


Major rupture, material comparison



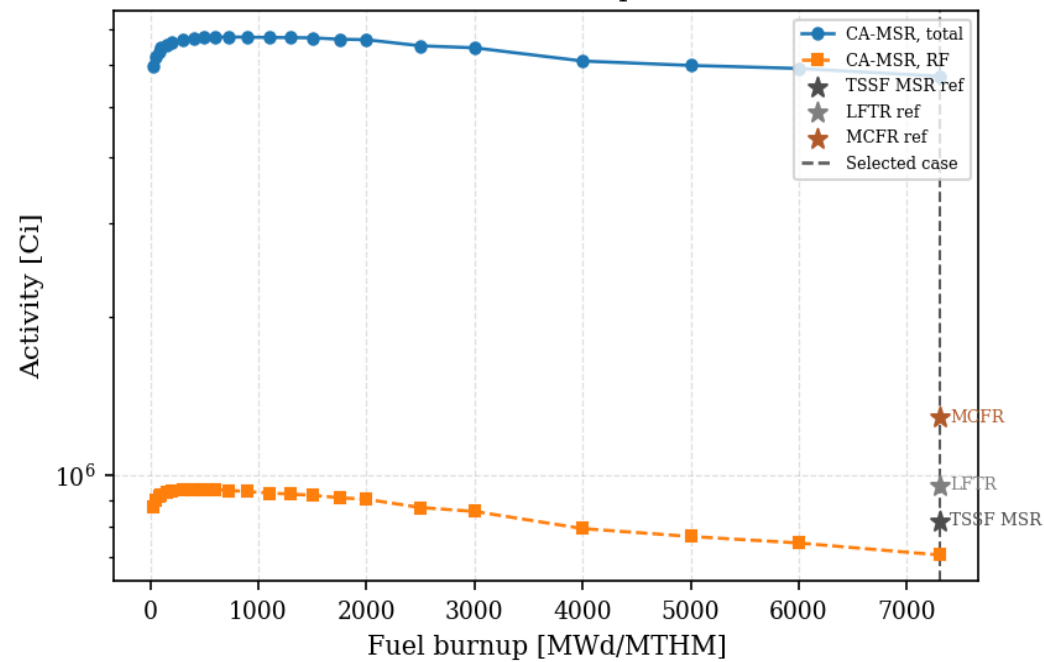
Little Sensitivity Comparison

- What happens if we change our assumption of release fraction

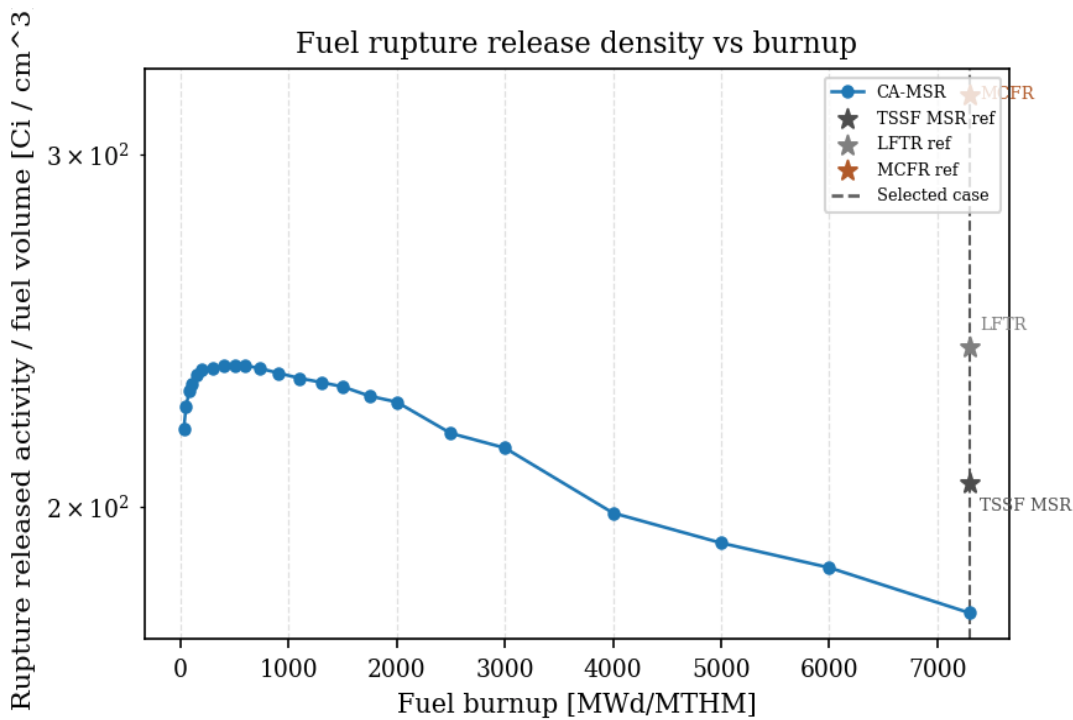


Comparison to literature

4L Fuel Drip



Fuel rupture release density vs burnup



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

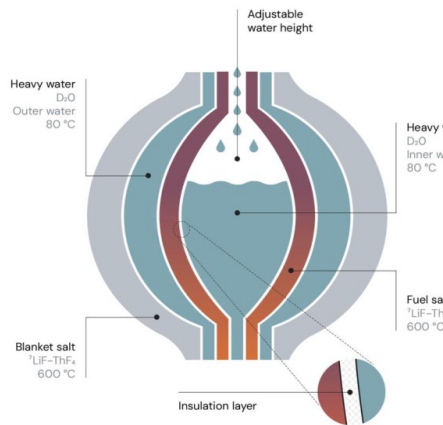
- We built a very simple model that can be used to learn about MSRs and built upon
- Our model achieves RMSE of 30--40
- We created a dataset of all contributing nuclides in both accident conditions and normal operation

Thank you for your attention

CA-MSR source term modelling: reconstructed Onion Core benchmark

Josef Hisanawi, Baltasar Hemmerle

Onion Core concept

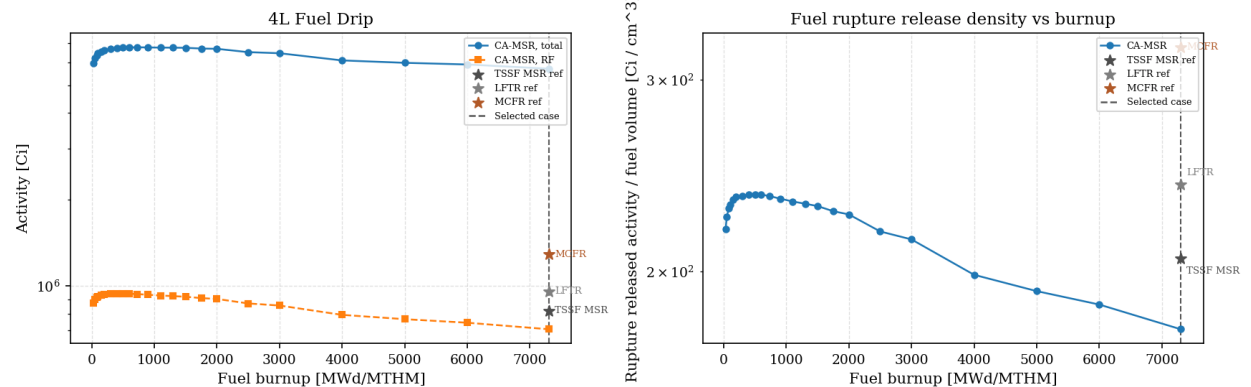


- Compact molten-salt reactor with liquid fuel and a breedable blanket
- LEU fuel concept with off-gas / fuel-processing relevance for source-term studies
- Container scale design used here as the benchmarked reference concept

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.