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PE/TR/003

Depletion Benchmark of an OpenMC Model of the Molten Salt Reactor Experiment (MSRE)

U-235 operation: code-to-code comparison with TRITON and MCNP-ADDER, and comparison with measured fuel-salt activities

KEYWORDS

Molten Salt Reactor Experiment, MSRE, OpenMC, DAGMC, OpenMSR, fuel depletion, burnup, fission products, ADDER, TRITON, benchmark validation, PolyEnergetics

Abstract

A transport-coupled depletion model of the Molten Salt Reactor Experiment (MSRE) has been built in OpenMC 0.16 on the OpenMSR project's three-dimensional CAD geometry, coupled through DAGMC, and benchmarked against the U-235 fuel-depletion benchmark reported by Argonne National Laboratory in ANL/NSE-22/48 [1]. Two cases from that benchmark are reproduced.

In the code-to-code case (8 MW for 375 effective full-power days, with continuous removal of noble gases and noble metals), the U-235 inventory agrees with the ORNL TRITON calculation to within 0.2 %. Eight of the nine fission products compared deviate from TRITON by +1.7 % to +6.8 %, and Sm-149 by +12.4 %. Tritium, produced mainly from lithium in the salt rather than by fission, is 16.8 % below TRITON. The median deviation from TRITON across 14 nuclides is 3.6 %, against 5.0 % for the benchmark's own MCNP-ADDER calculation. OpenMC predicts 19.3–44.1 % more U-239, Pu-239 and Pu-238 than TRITON, consistent with a harder salt-averaged neutron spectrum in the full three-dimensional model.

In the experimental case, the MSRE U-235 power history (91 depletion steps over 791 days, 65,159 MWh) is replayed and compared with radiochemical analyses of pump-bowl fuel-salt samples reported in ORNL-4865 [2]. Using the ORNL-calculated values from 1975 as a common reference, OpenMC and MCNP-ADDER differ from each other by −1.3 % to +4.9 % on all 13 nuclides compared. Against the measurements, OpenMC deviates by −24.1 % (Ce-144) to +52.0 % (Cs-137), similar to MCNP-ADDER (−25.6 % to +54.0 %). The largest overpredictions by OpenMC relative to measurements – for Cs-137 and the iodine isotopes (+35–+52%) – are consistent with removal of these elements or their precursors from the salt; neither code models this, and ADDER also overpredicts in a similar range.

RESULTS AT A GLANCE

Table 1. Headline results.

0.2 %	3.6 %	+2.1 %
Deviation of the calculated U-235 inventory from TRITON at 375 EFPD (Case A)	Median deviation from TRITON over 14 nuclides at 375 EFPD; MCNP-ADDER: 5.0 % (Case A)	Mean deviation of OpenMC from MCNP-ADDER over 13 measured fission products, range −1.3 % to +4.9 % (Case B)

READER'S NOTE

A depletion calculation follows how the composition of a reactor's fuel changes as it operates: fissile material is consumed, fission products build up and decay, and heavier actinides such as plutonium are bred. Validating one means comparing its predicted inventories either with other codes or with measured samples. The MSRE, operated at Oak Ridge National Laboratory from 1965 to 1969, is the only molten salt reactor for which such measurements exist. In this paper, EFPD is effective full-power days; dpm/g is radioactive disintegrations per minute per gram of salt; and a positive deviation means the calculation is higher than the reference.

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Appendix A. Abbreviations and nomenclature

1. Introduction

Molten salt reactors carry their fuel dissolved in a circulating salt. The fuel composition therefore evolves continuously and is shaped by processes a solid-fuel reactor does not have: fuel spends most of its time outside the core, gaseous fission products are stripped into an off-gas system, insoluble noble metals plate out on surfaces, and fresh fuel can be added while the reactor runs. Depletion codes used to design and license these reactors need validating against data from a real circulating-fuel system, and the only such data come from the MSRE.

Our earlier white paper validated an OpenMC model of the MSRE against three of the 1965 zero-power benchmark experiments: initial criticality, regulating-rod worth and the U-235 reactivity coefficient [8]. That model used the CAD geometry released by the OpenMSR project [5], coupled to OpenMC through DAGMC. This paper extends the same model from static criticality to fuel depletion over the reactor's U-235 operating period (January 1966 to March 1968).

The reference is the MSRE fuel-depletion benchmark developed by Argonne National Laboratory under the NEAMS programme and reported in ANL/NSE-22/48 [1]. That report builds a depletion benchmark using MCNP coupled to the ADDER depletion driver, which can model flowing fuel. It checks ADDER first against an ORNL TRITON calculation (a code-to-code comparison) and then against radiochemical measurements of fuel-salt samples drawn from the MSRE pump bowl during U-235 operation and tabulated in ORNL-4865 [2]. We reproduce both comparisons:

- **Case A, code-to-code:** 8 MW for 375 days with continuous removal of noble gases and noble metals; compared with the TRITON and MCNP-ADDER inventories (Section 4.1).
- **Case B, power history:** the digitised MSRE U-235 power history with no removal; compared with the measured activities and ORNL-calculated values from 1975 (Section 4.2).

To our knowledge, this is the first OpenMC depletion calculation on the full three-dimensional CAD model of the MSRE to be compared with both the ANL/NSE-22/48 code-to-code results and the ORNL-4865 salt-sample measurements.

Related work includes the OpenMSR project's OpenMC depletion notebook for the MSRE [10], which uses the same CAD model with continuous removal of noble gases and noble metals but does not compare the resulting inventories with a benchmark loop nor with measurements, and Elhareef and Wu [9], who couple OpenMC to the ONIX depletion code in a multi-point model of the primary loop to validate it against MSRE data.

2. Input data used

The depletion model starts from the first-criticality configuration of our earlier white paper [8]: the same salt, materials, geometry and control-rod positions. Table 2 gives the fuel-salt specification, Table 3 the structural and absorber materials, and Table 4 the computational configuration.

2.1 Fuel salt composition

Table 2. Fuel-salt specification of the OpenMC model.

PARAMETER	VALUE
Salt type	LiF–BeF_2–ZrF_4–UF_4 (IRPhEP MSRE benchmark composition [7], as used by OpenMSR [5])
Molar composition	LiF 64.88, BeF_2 29.27, ZrF_4 5.06, UF_4 0.79 mol %
Temperature	911.15 K (638 °C), uniform
Density	2.3278 g/cm³ at 911.15 K (thermally expanded, as in [8])
Loop inventory used for depletion	4,590 kg (as used by MCNP-ADDER [1]); salt volume 1.9718×10^6 cm³
Initial U-235 atom density	8.408×10^{19} atoms/cm³ (benchmark: 8.40×10^{19})
U-235 / heavy metal in loop	64.71 kg / 206.38 kg
Specific power	38.8 MW/MTiHM at 8 MW; 35.6 MW/MTiHM at 7.34 MW (TRITON: 36.7 MW/MTiHM at 8 MW)

2.2 Other materials

Table 3. Structural and absorber materials (densities and temperatures as in the first-criticality model [8]).

MATERIAL	DENSITY [G/CM³]	TEMPERATURE	NOTES
Graphite moderator	1.8494	911.15 K	Trace impurities including boron; c_Graphite S(α,β)
INOR-8 (Hastelloy N)	8.7786	911.15 K	Vessel and internals
Inconel-600	8.47	338.75 K	Control-rod thimble and cable
Gd_2O_3–Al_2O_3 bushing	5.873	338.75 K	70/30 wt % absorber
Thermal shield, concrete, insulation, steel, sand–water	Nominal	No setting	Outside the vessel, as in OpenMSR [5]

2.3 Nuclear data, depletion chain and OpenMC configuration

The depletion runs use ENDF/B-VIII.0 [6], with the matching ENDF/B-VIII.0 depletion chain. The stock ENDF/B-VIII.0 thermal depletion chain does not track the Li-6(n,t) reaction; it was added explicitly, because without it the salt would breed essentially no tritium. A first-order predictor algorithm was used for depletion.

Table 4. Computational configuration.

PARAMETER	VALUE
Monte Carlo code	OpenMC 0.16.0 [3], DAGMC geometry [4]
Cross sections	ENDF/B-VIII.0 [6], graphite S(α,β); temperature interpolation between library points
Depletion chain	ENDF/B-VIII.0 thermal (PWR) chain, 3,820 nuclides, with Li-6(n,t) added
Power normalisation	Fission-Q, using 201.7 MeV per U-235 fission as per benchmark [1]

2.4 Treatment of the circulating fuel

OpenMC has no model of fuel flowing around a loop, so the salt is treated as stationary. The benchmark describes two ways of making a stationary model represent circulating fuel [1, §2.2.2]: (a) spread the power over the whole loop inventory during the burn, or (b) burn only the in-core salt at full power and scale the resulting concentrations by the in-core fraction of 0.267 (the fraction of the primary-loop salt that is inside the core). We use method (a), as TRITON did: the depletable salt volume is set to the entire 4,590 kg loop inventory.

Method (a) is exact for any nuclide whose half-life is long compared with the loop transit time of about 30 s. Such a nuclide is spread evenly inside the loop, and its time-averaged production and destruction rates equal the rates at the loop-averaged flux. The benchmark's own flowing-fuel tests show deviations only for nuclides having half-lives of seconds (Kr-90, Kr-91, Sr-96) and the deviations are below 1 % (within plot reading error, as raw data is not available) for nuclides having half-lives upwards of a few minutes [1]. In Case A, these shorter-lived nuclides are compared code-to-code only, with all codes treating the fuel as stationary. Every nuclide compared with measurement in Case B has a half-life of at least 2.7 hours (Sr-92), so flow has less impact on the results.

3. Geometry

The geometry is the OpenMSR CAD model of the MSRE [5], meshed to DAGMC surface-mesh files: one for the vessel, core, shielding and surroundings, and one for a single control rod, which is replicated at the three thimble positions. Rod 1 is 46.6 in withdrawn and rods 2 and 3 are fully withdrawn (51 in), the first-criticality positions; rods are held there throughout depletion. The modelled geometry extends to the concrete and thermal shield, so neutrons escaping the core are absorbed before reaching the outer boundary. Figure 1 shows side and plan views of the model.

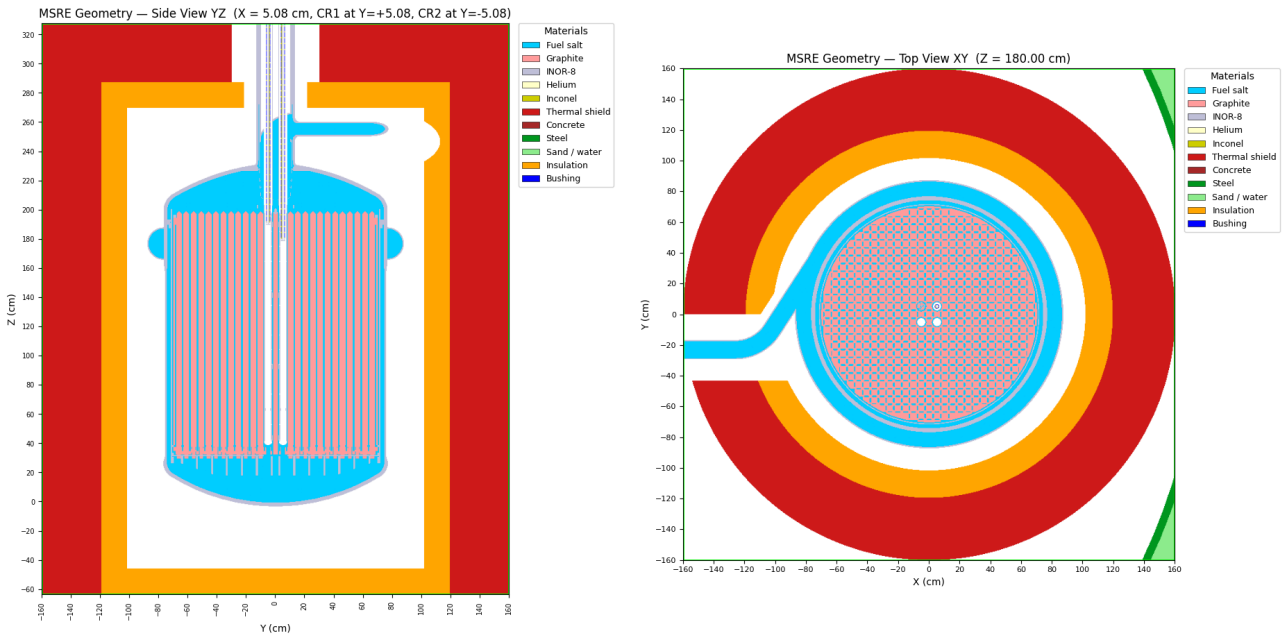

Figure 1. OpenMC model of the MSRE from the OpenMSR CAD geometry [5, 8]: (left) side view through the control-rod thimbles; (right) plan view at z = 180 cm. Rod 1 is shown at its 46.6 in withdrawn first-criticality position.

Unlike the reference calculations, which model a slice of the core (TRITON) or a single fuel channel and graphite stringer with reflective boundaries (MCNP-ADDER), this model contains the whole vessel, including the lower and upper plenums and the downcomer, where salt sees little graphite. This has implications for the neutron spectrum and hence the predictions, that are discussed in Section 5.1.

4. Results

The results are presented in the following subsections. Section 4.1 presents the code-to-code comparison with TRITON and MCNP-ADDER for Case A. Section 4.2 presents the MSRE power-history calculation and its comparison with the measured salt-sample activities for Case B. For each case we describe the benchmark, the inputs, our results, and the comparison.

4.1 Case A: code-to-code comparison with TRITON

4.1.1 Benchmark description

Case A is an idealised test, not a reconstruction of MSRE operation: the reactor runs at constant 8 MW for 375 days, about 72,000 MWh. This is about the energy of the whole MSRE U-235 history on the same 8 MW basis (about 71,000 MWh), and 10 % more than the 65,159 MWh of the 7.34 MW history used in Case B. No measurements exist for it; it can only be compared between codes. In the benchmark, an ORNL TRITON model of a slice through the core centre is the reference, and MCNP-ADDER copies its compositions, boundaries and removal rates, runs without fuel flow, and normalises power over the whole loop inventory [1].

4.1.2 Inputs

Table 5 lists the input data used for the Case A depletion analysis.

Table 5. Input data used for Case A [1].

PARAMETER	VALUE
Power	8 MW, constant
Duration	375 EFPD
Time points	0, 5, 10, 40, 70, 100, 280, 375 days (7 depletion steps)
Removal, Xe and Kr	4.067×10^{-5} s^{-1}
Removal, Se, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Sb, Te	8.777×10^{-3} s^{-1}

4.1.3 Comparison with TRITON and MCNP-ADDER

Depletion analysis has been performed with OpenMC, and the inventories of actinides and fission products have been computed as a function of time. The results have been compared with the benchmark analysis [1] for Case A. The benchmark gives Case A inventories only as plots [1], so the TRITON and MCNP-ADDER values were digitised from them. Reading accuracy is about ±3 %, worse for the smallest curves, so differences of a few percent are not significant. Figures 2(a), 2(b) and 2(c) compare the inventories computed by OpenMC, TRITON and MCNP-ADDER as a function of time. Table 6 gives the OpenMC inventories after 375 EFPD (atoms/cm^3), together with the TRITON and MCNP-ADDER values from the benchmark [1] and the deviations between them. Figure 3 shows the same comparison as a bar chart, and Table 7 summarises the level of agreement for the 14 nuclides studied.

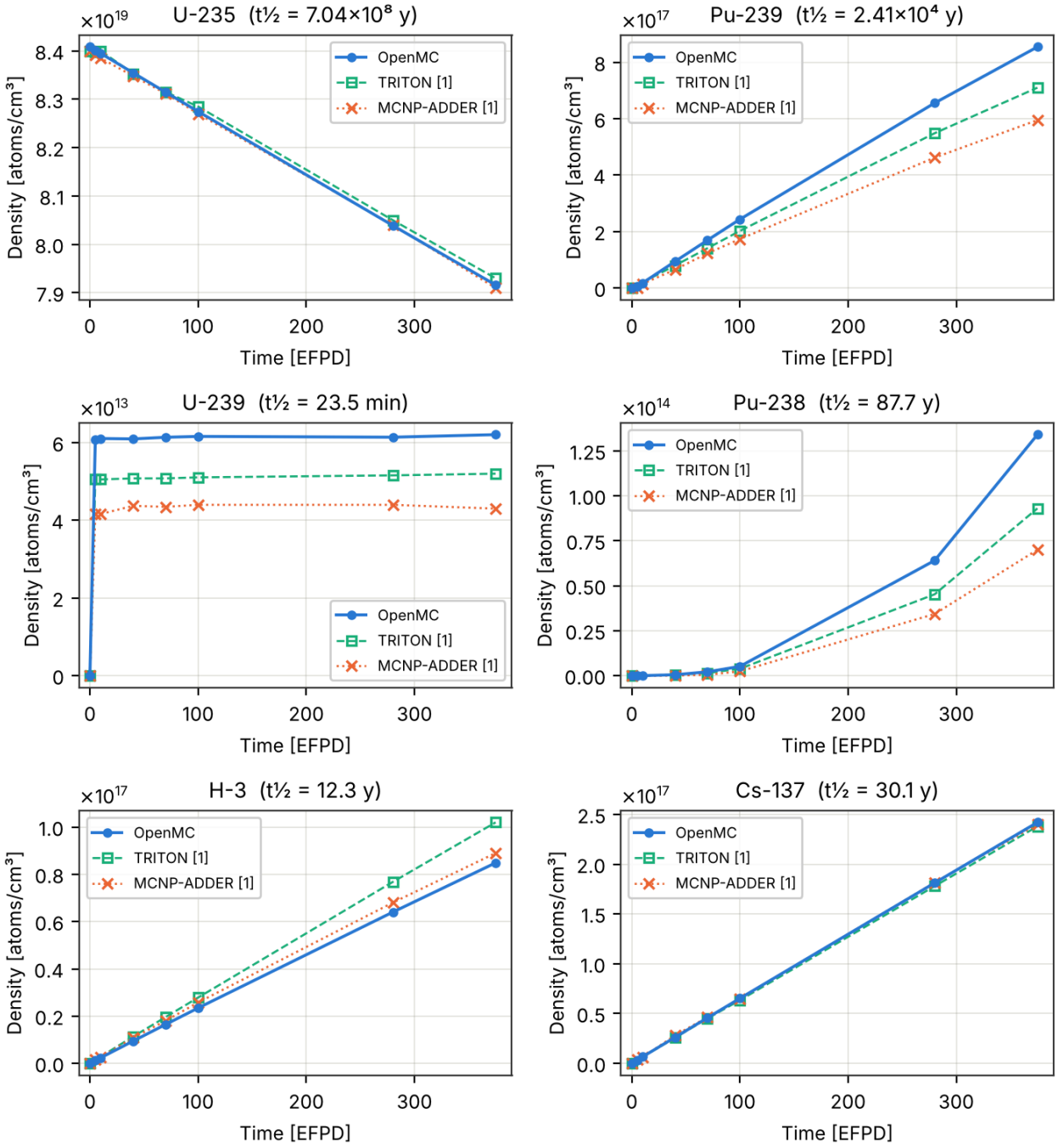

Figure 2(a). Comparison of calculated inventories as a function of time (U-235, Pu-239, U-239, Pu-238, H-3 and Cs-137) for Case A. TRITON and MCNP-ADDER values are digitised from [1].

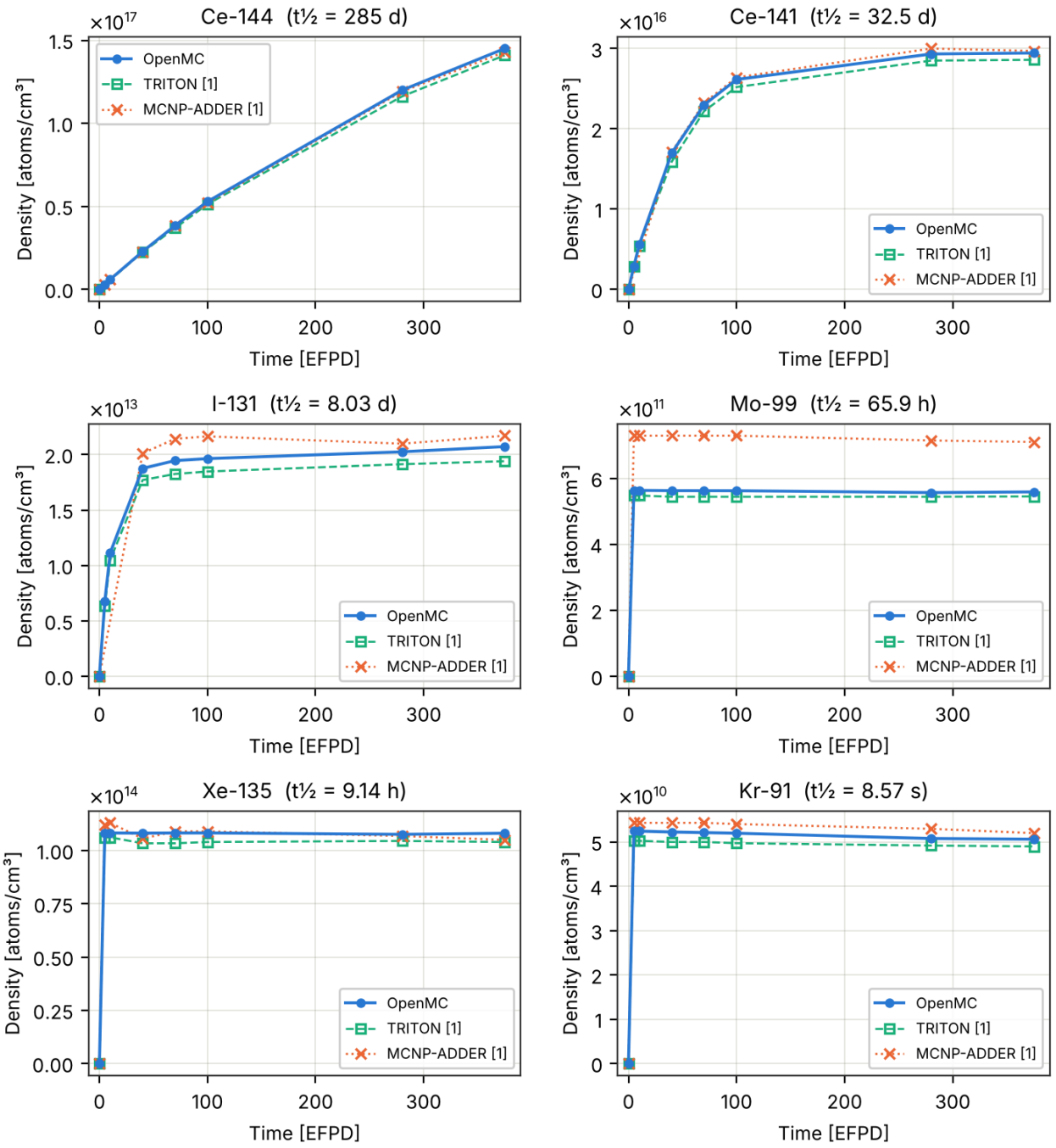

Figure 2(b). Comparison of calculated inventories as a function of time (Ce-144, Ce-141, I-131, Mo-99, Xe-135 and Kr-91) for Case A.

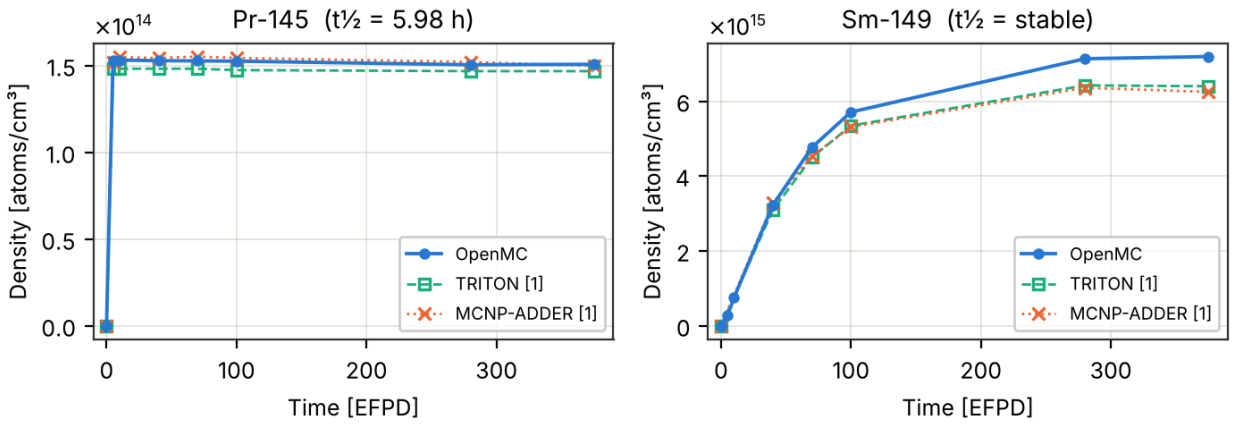

Figure 2(c). Comparison of calculated inventories as a function of time (Pr-145 and Sm-149) for Case A.

Table 6. Inventories at 375 EFPD (atoms/cm³) and deviations of OpenMC from each reference for Case A.

NUCLIDE	OPENMC	TRITON	MCNP-ADDER	OPENMC VS TRITON	OPENMC VS ADDER	ADDER VS TRITON
U-235	7.92E19	7.93E19	7.91E19	−0.2 %	+0.1 %	−0.3 %
Pu-239	8.54E17	7.10E17	5.95E17	+20.4 %	+43.6 %	−16.2 %
U-239	6.21E13	5.20E13	4.30E13	+19.3 %	+44.3 %	−17.3 %
Pu-238	1.34E14	9.30E13	7.00E13	+44.1 %	+91.4 %	−24.7 %
H-3	8.49E16	1.02E17	8.90E16	−16.8 %	−4.6 %	−12.7 %
Cs-137	2.42E17	2.38E17	2.40E17	+1.7 %	+0.8 %	+0.8 %
Ce-144	1.45E17	1.41E17	1.43E17	+2.9 %	+1.5 %	+1.4 %
Ce-141	2.94E16	2.86E16	2.97E16	+3.0 %	−0.8 %	+3.8 %
I-131	2.07E13	1.94E13	2.17E13	+6.8 %	−4.5 %	+11.9 %
Mo-99	5.59E11	5.45E11	7.10E11	+2.5 %	−21.3 %	+30.3 %
Xe-135	1.08E14	1.04E14	1.05E14	+3.9 %	+3.0 %	+1.0 %
Kr-91	5.06E10	4.90E10	5.20E10	+3.3 %	−2.6 %	+6.1 %
Pr-145	1.51E14	1.47E14	1.50E14	+2.7 %	+0.7 %	+2.0 %
Sm-149	7.19E15	6.40E15	6.25E15	+12.4 %	+15.1 %	−2.3 %

Note: The last column is the benchmark's own ADDER-to-TRITON deviation for reader's reference.

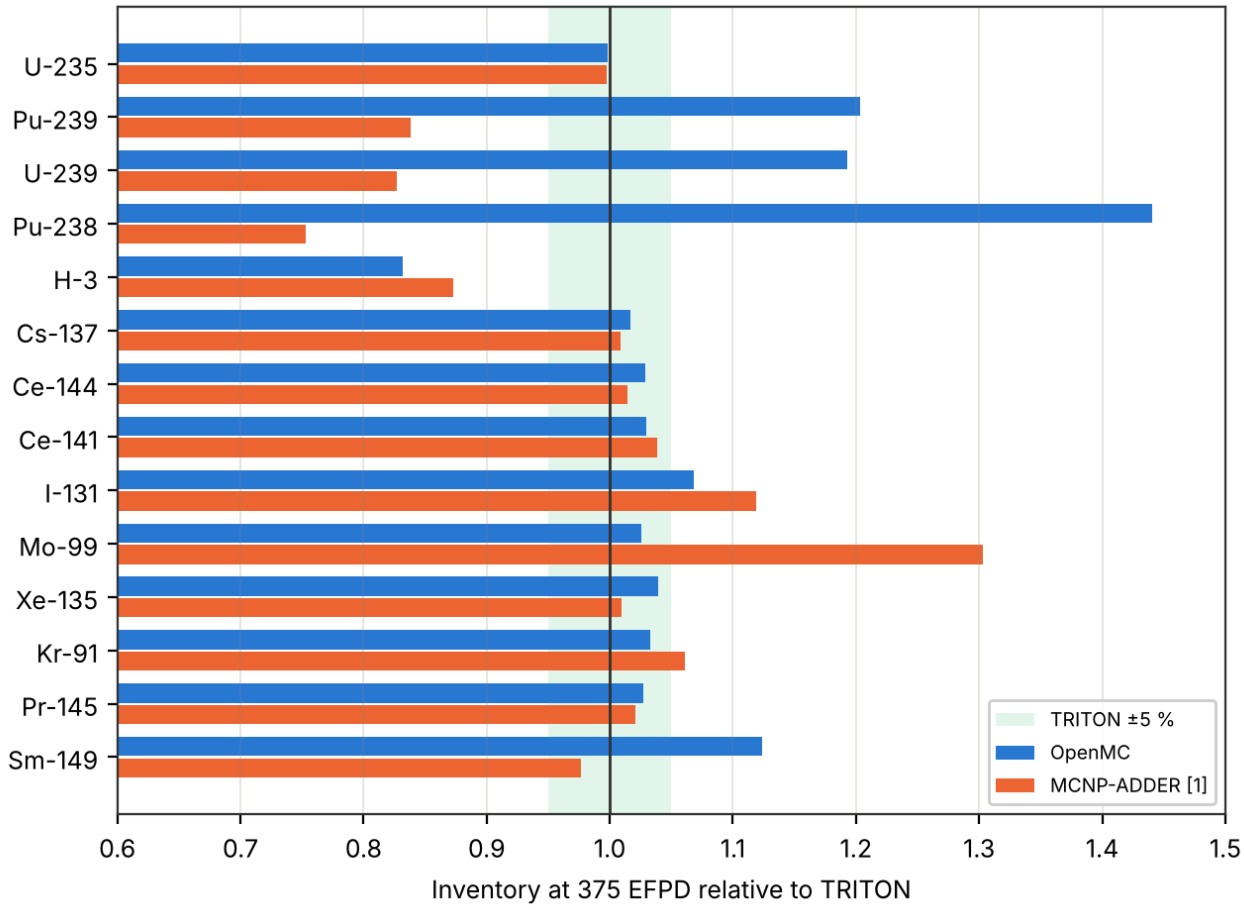

Figure 3. Inventories at 375 EFPD relative to TRITON for Case A (The shaded band is ±5 % of TRITON).

Table 7. Agreement statistics over the 14 nuclides of Table 6 for Case A.

COMPARISON	WITHIN ±5 %	WITHIN ±30 %	MEDIAN |DEVIATION|
OpenMC vs TRITON	8 / 14	13 / 14	3.6 %
OpenMC vs MCNP-ADDER	9 / 14	11 / 14	3.7 %
MCNP-ADDER vs TRITON (benchmark)	7 / 14	13 / 14	5.0 %

It can be seen from Table 6, Figure 3 and Table 7 that U-235 and seven of the nine fission products agree with TRITON to within 5 %; of the other two, I-131 is +6.8 % and Sm-149 +12.4 %. The inventories of the actinides U-239, Pu-239 and Pu-238 computed by OpenMC are 19.3–44.1 % above those computed by TRITON, whereas the MCNP-ADDER actinide inventories are 16.2–24.7 % below TRITON. The Sm-149 inventory calculated by OpenMC is 12.4 % above TRITON. These observations are discussed in Section 5.1.

4.2 Case B: MSRE U-235 power history and salt-sample measurements

4.2.1 Experiment and benchmark description

During operation, small samples of fuel salt were drawn from the pool in the fuel-pump bowl by lowering metal capsules through the sampler-enricher, and were analysed radiochemically by gamma spectrometry at ORNL. ORNL-4865 [2] lists 23 samples from the U-235 operating period: mostly ladle samples, plus four freeze-valve (FV) samples. For each nuclide in each sample it gives the activity in disintegrations per minute (dpm) per gram of salt, corrected to a reference time. The ratio of the measured value to the ORNL-calculated value from 1975 is also given. Measurement uncertainties are not reported.

The benchmark describes the setup of this case in detail [1]; a short summary is given here. It digitised the U-235 power history from ORNL progress reports, with an estimated resolution of ±2 h in time and ±0.5 MW in power. The 791-day operating history is summarised in 91 steps: 53 at power and 38 at zero power, during which the fission products only decay [1]. Full power was taken as 7.34 MWth, the level ORNL estimated from isotopic changes (heat balances gave about 8 MW). MCNP-ADDER modelled flowing fuel (nine loop regions at 167.1 kg/s) with no chemical removal, and assumed samples were taken at noon on their reported dates. Of the 23 samples, the benchmark compared 18: 8-5 and 12-6 were excluded because their values did not show the decay expected after long shutdowns; 6-17, 7-10 and 14-63FV were omitted. Three suspected typographical errors were corrected (order of magnitude corrections for Ru-103 and Mo-99), and Ce-143 at 11-58 and 14-66FV was excluded. Results are given only as per-nuclide average deviations [1]. TRITON was not run on Case B.

4.2.2 Inputs

We use the 91 depletion steps of the benchmark, reproduced in Table 8 from [1]: 53 steps at power and 38 at zero power, with stationary salt normalised to the 4,590 kg loop inventory and no chemical removal. On zero-power steps OpenMC only decays the inventory, without a transport solve, so the 791-day history required 54 transport solves. Each salt sample is compared at the end of the step it is listed against. The benchmark's schedule and its text differ on two samples. Sample 12-6 appears in the schedule but is excluded from the comparison in the text [1]. Sample 14-66FV is not labelled in the schedule, but the text implies it was compared for Ba-140, Sr-89 and Zr-95, since only its Ce-143 value is excluded. We follow the text: 12-6 is excluded and 14-66FV is included. With this selection, our number of samples for each nuclide matches the benchmark's for all 13 nuclides (Table 9). ORNL-4865 dates Sample 14-66FV to the end of run 14 [2], which corresponds to the end of the benchmark history, so it is compared at the end of the last step. Sample names, a pair of numbers separated by a dash, are taken as-is from ORNL-4865 Table 6.7.

Table 8. Depletion steps, with the power and duration of each step and the salt samples compared at its end, for Case B [1].

STEP	POWER [MWTH]	DURATION [H]	SAMPLE	STEP	POWER [MWTH]	DURATION [H]	SAMPLE
1	0.2500	10		47	7.3400	108	
2	0.0000	14		48	0.0000	360	
3	0.5000	12		49	5.5843	28	
4	0.0000	12		50	0.0000	20	
5	1.0000	28		51	6.8106	324	**11-8**
6	0.0000	1772		52	7.3400	192	**11-12**
7	0.0694	72		53	7.0576	183	
8	0.0000	24		54	0.0000	9	
9	2.5000	30		55	6.8674	140	
10	0.0000	42		56	0.0000	48	**11-22**
11	2.5000	48		57	0.0000	28	
12	0.0000	24		58	7.2390	912	**11-45**
13	5.0000	12		59	7.3400	264	**11-51**
14	0.0000	12		60	6.7936	72	**11-52**
15	5.0000	12		61	7.3400	96	**11-54**
16	0.0000	60		62	7.3400	72	**11-58**
17	5.0000	96		63	0.0000	1032	
18	0.0000	252		64	0.0000	34	
19	5.2500	72		65	4.8462	26	
20	0.0000	12		66	0.0000	12	
21	6.5000	84		67	7.0000	36	
22	0.0000	48		68	0.0000	48	
23	5.0000	38		69	7.0000	360	
24	0.0000	42		70	0.0000	12	
25	6.3976	132	**6-19**	71	7.0000	120	**12-27**
26	0.0000	414		72	6.9008	524	
27	7.3400	30		73	0.0000	922	
28	0.0000	12		74	7.3400	60	
29	6.9938	278	**7-7**	75	0.0000	78	
30	0.0000	104		76	7.1945	772	
31	7.2015	318	**7-12**	77	0.0000	68	
32	0.0000	12		78	7.1892	216	**14-20FV**
33	7.3400	48		79	7.3400	72	**14-22**
34	0.0000	2120		80	7.1298	204	
35	5.3281	64		81	0.0000	210	
36	0.0000	6		82	7.3400	258	**14-30FV**

STEP	POWER [MWTH]	DURATION [H]	SAMPLE	STEP	POWER [MWTH]	DURATION [H]	SAMPLE
37	5.8814	354		83	7.3400	192	
38	0.0000	188		84	4.9896	960	
39	6.7710	120		85	0.0000	196	
40	0.0000	24		86	5.0000	434	
41	7.3400	28		87	7.3400	284	
42	0.0000	30		88	5.0000	154	
43	7.3400	24		89	0.0000	72	
44	0.0000	664		90	1.8750	48	
45	7.3400	326	**10-12**	91	7.2469	312	**14-66FV**
46	7.3400	288	**10-20**				

Note: Following Section 4.2.2, Sample 12-6 (end of step 63 in [1]) is not compared and Sample 14-66FV is compared at the end of step 91.

4.2.3 Results

Figures 4(a) and 4(b) show OpenMC's calculated activity of each of the 13 nuclides over the whole history, at the end of every depletion step, with the measured activities and the ORNL-calculated values from 1975 at the sample times. In each panel, lines join OpenMC's activities at the end of each depletion step, and circles mark OpenMC at every sample in Table 8 and at Sample 12-6 (end of step 63), which is not compared. Triangles are the measured activities and crosses the ORNL-calculated values from 1975, both from ORNL-4865 Table 6.7 [2], for the samples used in [1]. Shaded bands mark the zero-power steps, each axis is clipped six decades below the operating level, and the half-life of each nuclide is given in the panel title. Nuclides with half-lives of hours to a few days (Sr-91, Sr-92, I-133, I-135, Ce-143) follow the power closely: they reach a steady activity within days at power and fall by many orders of magnitude during long shutdowns, so their activity in a sample depends mainly on the power in the preceding hours. Longer-lived nuclides (Sr-89, Zr-95, Ce-141, Ce-144, Cs-137) accumulate over the history and dip only modestly during shutdowns. The deviations from the measurements and from the reference calculations are quantified in Section 4.2.4.

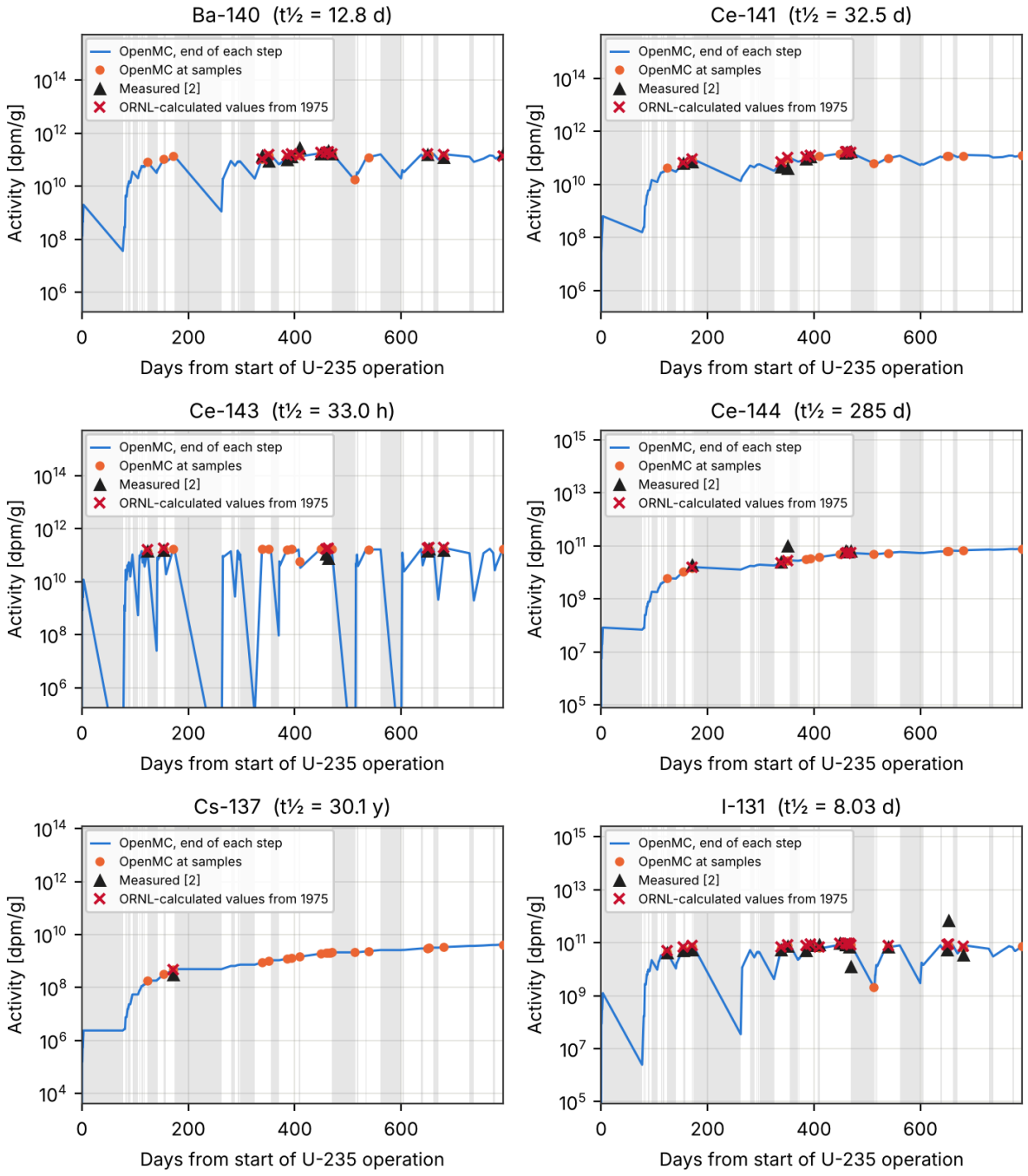

Figure 4(a). Activities in dpm per gram of salt over the full history, Ba-140 to I-131, for Case B.

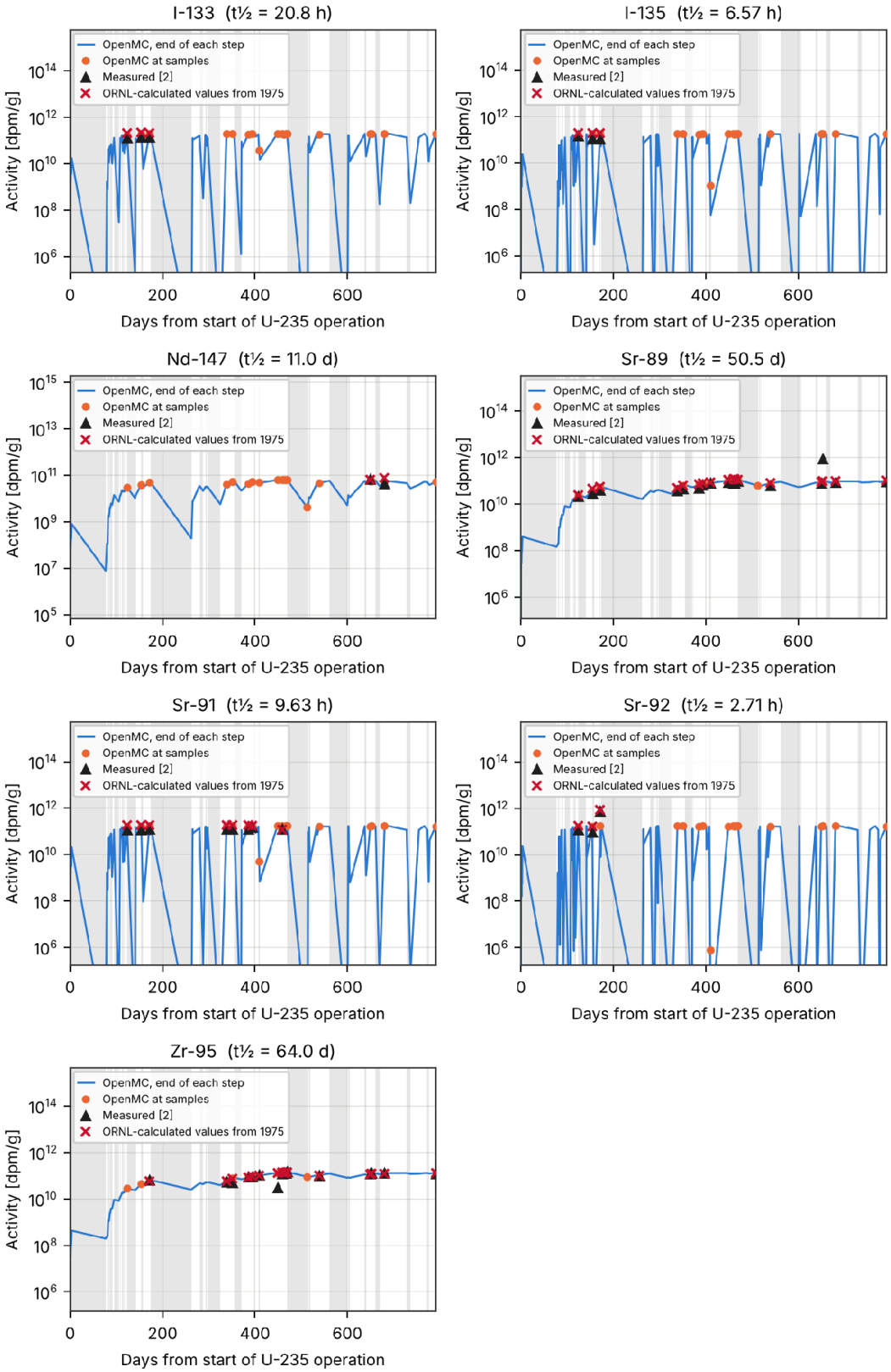

Figure 4(b). Activities, continued: I-133 to Zr-95, for Case B.

4.2.4 Comparison with MCNP-ADDER and the measured activities

Table 9 compares OpenMC, nuclide by nuclide, with the measured activities, with the ORNL-calculated values from 1975 and with MCNP-ADDER. To make the numbers directly comparable with the benchmark, we use the method of the benchmark [1]: at each sample, the deviation of the calculation from the reference is computed as (calculated − reference) / reference, and this deviation is then averaged over the samples the benchmark used for that nuclide. Positive values mean the calculation is higher than the reference.

Comparing OpenMC with MCNP-ADDER needs one extra step, because the benchmark does not publish ADDER's activity at each sample: it gives only ADDER's two average deviations per nuclide, from the measurements and from the ORNL-calculated values from 1975. The ORNL-calculated values can therefore serve as a common yardstick. If OpenMC lies a fraction d_{OpenMC} from it and ADDER a fraction d_{ADDER}, the ratio of OpenMC to ADDER is $(1 + d_{OpenMC}) / (1 + d_{ADDER})$, so the deviation of OpenMC from ADDER is

$$d_{OpenMC\ vs\ ADDER} = \frac{1+d_{OpenMC}}{1+d_{ADDER}} - 1$$

The formula is exact for a single sample; applied to averages over samples, as here, it is an approximation. Figure 5 shows the deviations of both codes from the measurements.

Table 9. Mean deviations by nuclide, using the benchmark sample selection for Case B [1].

NUCLIDE	SAMPLES	OPENMC VS MEASURED	ADDER VS MEASURED [1]	OPENMC VS ORNL-CALCULATED VALUES FROM 1975	ADDER VS ORNL-CALCULATED VALUES FROM 1975 [1]	OPENMC VS ADDER
Ba-140	12	+0.2 %	−10.0 %	−5.9 %	−8.5 %	+2.9 %
Ce-141	9	+19.5 %	+18.0 %	−8.8 %	−10.0 %	+1.3 %
Ce-143	7	+33.2 %	+27.8 %	−8.8 %	−12.4 %	+4.1 %
Ce-144	6	−24.1 %	−25.6 %	−3.8 %	−5.7 %	+2.0 %
Cs-137	1	+52.0 %	+54.0 %	+3.4 %	+4.7 %	−1.3 %
I-131	17	+42.7 %	+38.5 %	−11.6 %	−14.0 %	+2.9 %
I-133	3	+35.6 %	+32.5 %	−14.0 %	−16.1 %	+2.4 %
I-135	3	+40.8 %	+37.6 %	−11.2 %	−13.3 %	+2.4 %
Nd-147	2	−0.6 %	−1.9 %	−25.3 %	−26.3 %	+1.3 %
Sr-89	17	+13.9 %	+12.8 %	−5.9 %	−6.8 %	+1.0 %
Sr-91	8	+29.0 %	+23.0 %	−1.8 %	−6.4 %	+4.9 %
Sr-92	3	+8.1 %	+9.5 %	−30.2 %	−29.3 %	−1.3 %
Zr-95	16	+26.9 %	+21.4 %	+3.1 %	−1.4 %	+4.5 %

Using the ORNL-calculated values from 1975 as a common reference, OpenMC and MCNP-ADDER differ from each other by −1.3 % to +4.9 % on all 13 nuclides, with OpenMC on average 2.1 % higher

(Table 9, last column). Against the ORNL-calculated values themselves, the largest deviations are −30.2 % for OpenMC and −29.3 % for ADDER, both for Sr-92. Against the measurements, both codes show the same pattern of deviations (Figure 5): OpenMC from −24.1 % (Ce-144) to +52.0 % (Cs-137), and ADDER from −25.6 % to +54.0 % for the same two nuclides.

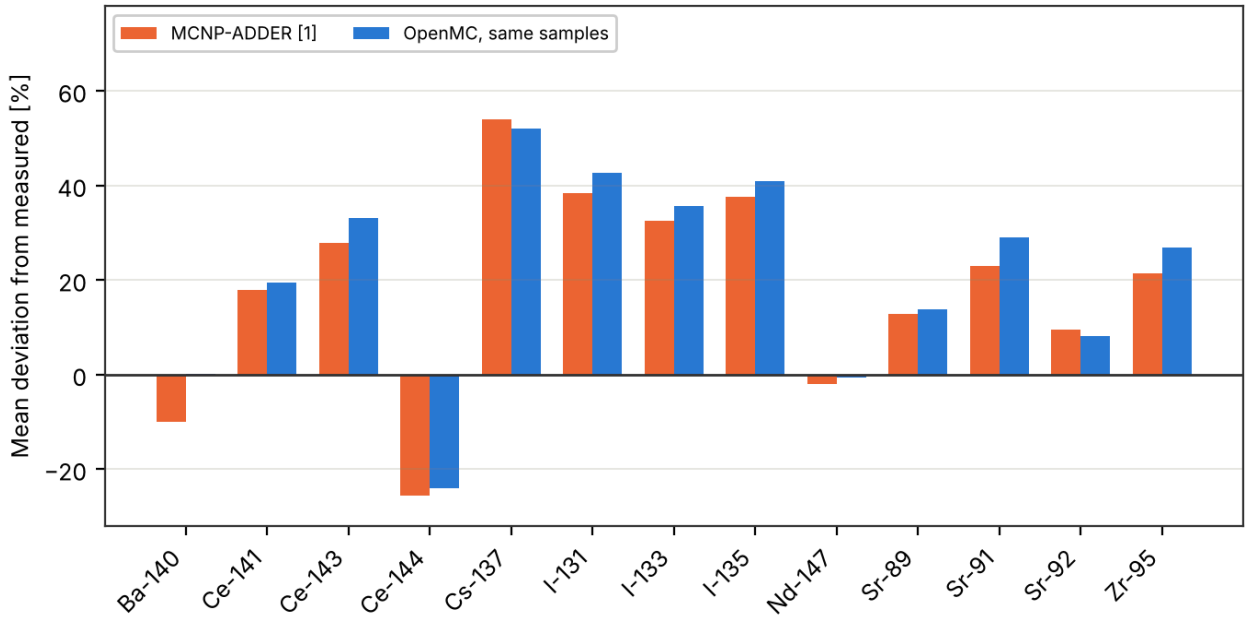

Figure 5. Mean deviation from the measured activities by nuclide, MCNP-ADDER [1] and OpenMC on the same samples, for Case B.

5. Discussion

The two cases test different parts of the model. Case A tests the neutronics and depletion solver in isolation, by comparing with other codes (TRITON and ADDER) under the same idealised operating conditions. Case B tests whether the model, driven by the real power history, reproduces what was measured in the salt; since its quantities depend mainly on fission yields, fission rate and decay, it is largely insensitive to transport detail but highly sensitive to normalisation and salt chemistry.

5.1 Case A: burnup and fission products agree; actinide mismatch points to a harder spectrum

The U-235 inventory calculated in OpenMC matches the TRITON calculation to within 0.2 %, and eight of the nine fission products sit 1.7–6.8 % above it, most of them within the plot-reading error (see Table 6). Sm-149 is predicted higher, at +12.4 %. The median deviation of OpenMC from TRITON is 3.6 %, against 5.0 % for MCNP-ADDER. OpenMC also agrees with TRITON on Mo-99 (+2.5 %), and lies 21.3 % below MCNP-ADDER for that nuclide.

The fission products sit consistently a few percent above TRITON. A likely contributor is normalisation: TRITON's quoted 36.7 MW per metric tonne of initial heavy metal (MTiHM) implies a

loop inventory of about 4,850 kg, against our 4,590 kg as taken from the benchmark [1]. At the same power TRITON spreads fissions over 5.7 % more salt, lowering its concentrations by 5.4 %. This is close to the reading error, so it is suggestive rather than proven.

The inventory of U-239 calculated by OpenMC is 19.3 % above TRITON. Its level is set directly by the U-238 capture rate, so U-238 is capturing about a fifth more neutrons per atom in our model; about 5.4 % of the difference can come from the normalisation difference (TRITON used more salt to normalise power, as noted above). Pu-239, formed from U-239, shows a similar deviation (+20.4 %). Pu-238, which needs several successive captures, amplifies the difference to +44.1 %.

For the actinides, OpenMC lies consistently above TRITON and MCNP-ADDER below it, so the OpenMC-vs-ADDER deviations are large, up to +91.4 % for Pu-238; this value combines the two opposite deviations from TRITON. The ordering follows the geometry of the three models (Section 3). ADDER models a single fuel channel with reflecting boundaries, effectively an infinite lattice without leakage in which all the salt is next to graphite, and so has the softest spectrum. TRITON's two-dimensional slice includes radial leakage. Our three-dimensional model adds axial leakage and the salt in the plenums and downcomer, which sees little graphite; the partly inserted control rod contributes slightly. A harder spectrum raises epithermal (resonance) capture relative to U-235 fission, and so raises the actinide inventories. Sm-149 (+12.4 %) may be affected in the same way.

Tritium is 16.8 % below TRITON and 4.6 % below ADDER; the remaining shortfall probably reflects tritium routes absent from the chain used in our simulation, such as Li-7(n,n′α)t (the chain was patched only for Li-6(n,t)).

5.2 Case B: OpenMC reproduces the benchmark's comparison with experiment

OpenMC and MCNP-ADDER differ from each other by −1.3 % to +4.9 % on the 13 nuclides (Table 9, last column), despite very different geometry, nuclear data and fuel-motion treatment. This is expected: the activities are fixed almost entirely by fission yield, fission rate per gram of salt and decay. OpenMC is higher than ADDER for 11 of the 13 nuclides, by +1.0 % (Sr-89) to +4.9 % (Sr-91), and lower for Cs-137 and Sr-92 (both −1.3 %). A similar slight excess over ADDER appears in Case A for the long-lived fission products Ce-144 (+1.5 %) and Cs-137 (+0.8 %; Table 6), although in Case B Cs-137, from a single sample, is below ADDER. Plausible contributors are fission-yield differences (ENDF/B-VIII.0 against ORIGEN2.2 used in ADDER), a plutonium share of fissions that is likely larger in our model, as in Case A, and ADDER's flowing-fuel normalisation.

OpenMC sits 1.8–14.0 % below the ORNL-calculated values from 1975 for nine of the 13 nuclides, and 3.1–3.4 % above them for Zr-95 and Cs-137 (Table 9). One hypothesis, which we have not tested, is that the ORNL-calculated values from 1975 assumed the 8 MW design power rather than the 7.34 MW used here. If so, our activities would be 8.3 % lower (7.34/8) for every nuclide. This could account for a common offset, but not for the spread between nuclides. The loop inventory, uncertain by up to about 10 % [1], may also contribute. The two largest deviations, for Nd-147 (−25.3 %) and Sr-92 (−30.2 %), rest on only two and three samples respectively (Table 9).

5.3 Case B: deviations are consistent with salt chemistry for most nuclides, with some exceptions

In Case B, none of the codes simulates the removal of nuclides from the salt. In the operating reactor, wherever nuclides left the salt, the measured values would be lower than the calculated ones. For most nuclides, the deviations follow the chemistry:

- **Products that stay in the salt.** If the deviations come from material leaving the salt, which no code models, then nuclides whose whole formation chain stays in the salt should show no systematic deviation. Ba-140 (+0.2 %) and Nd-147 (–0.6 %; Table 9) fit this expectation: they are salt-soluble, and their only gaseous precursors decay within seconds, before reaching the pump bowl. The other four salt-soluble nuclides without major noble-gas precursors do not. Ce-141 (+19.5 %), Ce-143 (+33.2 %) and Zr-95 (+26.9 %) are calculated higher than measured, which would normally mean that some of the nuclide left the salt; but cerium and zirconium are salt-soluble, so the salt chemistry gives no route for them to leave. Ce-144 (–24.1 %) is calculated lower than measured, which removal from the salt cannot cause at all, because removal can only lower the measured value. These four nuclides are therefore exceptions to the salt-chemistry explanation, as is Sr-91 below.
- **Products of short-lived noble gases are depleted.** Cs-137 and Sr-89 form from Xe-137 and Kr-89 respectively, which have half-lives of a few minutes and are stripped into the off-gas at the pump bowl before they decay in the operating reactor. Since our simulation does not model this removal, the calculated activities are higher than measured (Cs-137 +52.0 %, from a single sample; Sr-89 +13.9 %). The converse, however, does not hold. Sr-91 forms from Kr-91, whose half-life is only a few seconds, so little of it should be stripped, and the calculated Sr-91 activity should be close to the measured value. Instead, it is 29.0 % higher (ADDER: +23.0 %). Because both codes, and the ORNL-calculated values from 1975, exceed the measurements by a similar amount, the excess is unlikely to come from either code. It points to a removal path for Sr-91 or its precursors in the operating reactor, or to a bias in the measurements.
- **Iodine.** Our calculations give 35.6–42.7 % more iodine than measured (I-131, I-133 and I-135), against 32.5–38.5 % for ADDER (Table 9). This indicates a removal mechanism for iodine or its precursors; the benchmark estimates that around 25 % of the iodine escaped the salt [1].

5.4 Modelling assumptions and their effect

- **Stationary fuel (inventories).** Method (a), described in Section 2.4, is exact for all nuclides compared with measurement (Case B), whose half-lives are at least 2.7 hours; the close agreement with ADDER's flowing-fuel results is consistent with this.
- **Decay heat in the power normalisation.** The 201.7 MeV per fission includes about 13 MeV of fission-product beta and gamma energy, implicitly in equilibrium with the fission rate. After start-ups the true fission rate is slightly higher for a given thermal power, an estimated effect of about 1 % on total fissions in Case B. The 7.34 MW level was itself derived from isotopic changes, effectively a fission rate, so no correction is applied.

- **Control rods.** In our simulation the control rods are modelled at their first-criticality positions, ADDER model contains no control rods. TRITON is described to account for the presence of control rods and structural alloys, but it is not clear to what extent it is done [1]. In the operating reactor the rods moved slightly throughout operation. These differences slightly change the spectrum.

6. Conclusions

An OpenMC 0.16 depletion model of the MSRE built on the OpenMSR three-dimensional CAD geometry has been benchmarked against the U-235 fuel-depletion benchmark [1].

1. **Code-to-code (Case A).** OpenMC reproduces TRITON's U-235 burnup to 0.2 % and eight of its nine fission products to within 1.7–6.8 % (Sm-149: +12.4 %), with a median deviation of 3.6 % against 5.0 % for MCNP-ADDER, and it agrees with TRITON on Mo-99 (+2.5 %), where MCNP-ADDER deviates by +30.3 %. It predicts 19.3–44.1 % more U-239, Pu-239 and Pu-238 than TRITON, pointing to a harder salt-averaged spectrum in the full three-dimensional model.
2. **Against experiment (Case B).** OpenMC and MCNP-ADDER differ by −1.3 % to +4.9 % on all 13 measured fission products, despite very different geometry, nuclear data and fuel-motion treatment. Against the measurements, OpenMC deviates by −24.1 % (Ce-144) to +52.0 % (Cs-137), following the same pattern as MCNP-ADDER.

Taken together, these results support the use of OpenMC with DAGMC CAD geometry for molten-salt fuel-depletion analysis. We suggest extending the simulation to the U-233 operation of the MSRE.

7. References

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Appendix A. Abbreviations and nomenclature

Table A1 lists the abbreviations used in this paper and Table A2 the symbols and units.

Table A1. Abbreviations.

ABBREVIATION	MEANING
ADDER	Advanced Dimensional Depletion for Engineering of Reactors (ANL depletion driver used with MCNP)
ANL	Argonne National Laboratory
CAD	Computer-aided design
DAGMC	Direct Accelerated Geometry Monte Carlo (CAD geometry interface for Monte Carlo codes)
EFPD	Effective full-power days
ENDF/B	Evaluated Nuclear Data File, version B (ENDF/B-VIII.0 in this paper)
FV	Freeze valve (salt-sample type in ORNL-4865)
HM	Heavy metal (uranium isotopes in this paper)
INOR-8	Nickel-molybdenum alloy of the MSRE vessel, later marketed as Hastelloy N
IRPhEP	International Reactor Physics Experiment Evaluation Project
MCNP	Monte Carlo N-Particle transport code
MSRE	Molten Salt Reactor Experiment
MTiHM	Metric tonne of initial heavy metal
NEAMS	Nuclear Energy Advanced Modeling and Simulation programme (US DOE)
ORIGEN2	Oak Ridge Isotope Generation and depletion code, version 2
ORNL	Oak Ridge National Laboratory
OSTI	Office of Scientific and Technical Information (US DOE)
PWR	Pressurised water reactor

ABBREVIATION	MEANING
SCALE	ORNL nuclear analysis code system
TRITON	Transport and depletion sequence of SCALE

Table A2. Nomenclature.

SYMBOL OR QUANTITY	MEANING [UNIT]
t½	Half-life [s, min, h, d, y]
Removal rate	First-order rate of chemical removal of an element from the salt [s^{-1}]
S(α,β)	Thermal neutron scattering law (graphite) [–]
Activity	Radioactive disintegrations per minute per gram of salt [dpm/g]
Concentration	Atom density averaged over the loop inventory [atoms/cm^3]
Power	Thermal power [MWth]
Energy	Cumulative thermal energy [MWh]
Specific power	Thermal power per tonne of initial heavy metal [MW/MTiHM]
Energy per fission	Recoverable energy per fission (201.7 MeV for U-235) [MeV]
d	Relative deviation, (calculated – reference) / reference [%]