

Development of a Size-Resolved Noble Metal Transport Code for a Passive Molten Salt Fast Reactor and Its Coupling with Serpent Depletion Calculations

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1. Introduction

Passive Molten Salt Fast Reactors (PMFRs) are integral-type molten salt reactor systems operating under natural circulation without external pumping [1-4]. Because the compact, integrated configuration leaves little room for external fission product cleanup loops, in-vessel strategies are required to manage the insoluble noble metal fission products (Mo, Ru, Rh) that would otherwise deposit on structural surfaces and heat exchangers.

In a previous study [5], a one-dimensional flotation code with fixed particle sizes and a constant external source was developed for the PMFR riser and compared against a water-based helium bubbling experiment. That work identified two key limitations: the absence of particle growth, which controls the size-dependent removal physics, and the absence of a link to neutronic calculations that determine the noble metal source. The present paper reports a complete redevelopment of the code (NMT ver1.2) addressing both. The new code solves the full natural-circulation loop, derives zone-wise noble metal generation directly from Serpent [6] burnup matrices, tracks the particle size distribution with a 77-bin coagulation model, and removes particles through diffusive bubble flotation and wall deposition integrated into a loop transport solver. A two-way, cycle-based coupling with Serpent — depletion on a fuel-salt zoning that exactly matches the transport mesh, with the removed inventories fed back into the compositions — is demonstrated over one year of operation, including dissolved noble-gas (Xe/Kr/He) stripping. Every module was verified against analytic or independent numerical references with machine-precision conservation criteria before integration.

2. Modeling for Noble Fission Product Transport and Removal

2.1. Loop thermal-hydraulics

The loop (core, riser, heat exchanger, downcomer) is discretized into 35 axial nodes. For the prescribed thermal power $Q = 300$ MWth and core temperature rise $\Delta T = 175$ K ($783.15 \rightarrow 958.15$ K), the circulating mass flow follows from the energy balance

$$\dot{m} = \frac{Q}{C_p(T)\Delta T} \quad (1)$$

Thermophysical properties of the NaCl-KCl- UCl_3 fuel salt (mole fractions 0.363/0.255/0.382) are evaluated from component correlations with standard mixing rules. Helium bubbling in the riser (mass fraction 5×10^{-5}) is modeled with a drift-flux formulation ($C_0 = 1.2$), and the pressure field is integrated from the cover-gas pressure with Shiba-Yamazaki friction. The converged field ($\dot{m} = 3038$ kg/s, riser void fraction $\alpha = 0.562$, bubble velocity 5.0 m/s) satisfies mass and energy balances to 0.000% and 0.007%, and is frozen for all subsequent modules.

2.2. Noble metal generation from Serpent

The noble metal source is extracted from Serpent depletion matrices (depmtx output): for element Z the generation rate is the sum of production in-flows of the burnup matrix A ,

$$gen_A(Z) = \sum_{i \in Z} \sum_{j \neq i} A_{ij} N_j \quad (2)$$

where $\bar{N}$ is the trapezoidal average of the step-boundary nuclide densities. Because the diagonal of A holds the loss terms, gen_A is nonnegative by construction, unlike the net inventory difference $(N_1 - N_0)/\Delta t$ used previously, which becomes negative wherever inventory decay exceeds local production (e.g., Ru in the riser).

2.3. Size-resolved growth

The particle population of each element is discretized into 77 volume bins (atomic-diameter base, volume-doubling tail) and evolves by Brownian coagulation with the Smoluchowski kernel

$$\beta_{ij} = \frac{2kT}{3\mu} \left(2 + \frac{d_i}{d_j} + \frac{d_j}{d_i} \right) \quad (3)$$

using the Fixed Pivot assignment of Kumar and Ramkrishna [7]. Explicit time integration of the coagulation equation is stiff (stability requires $\beta n \Delta t < 1$, i.e., sub-ms steps at the PMFR generation rates), so a volume-sequential semi-implicit scheme after Jacobson [8] was adopted:

$$n_k^{t+\Delta t} = (n_k^t + \Delta t P_k) / (I + \Delta t L_k) \quad (4)$$

where P_k and L_k are the production and loss operators evaluated with already-updated smaller bins. The scheme is unconditionally positive and conserves particle volume algebraically at any Δt ; the largest bin is treated as a volume-conserving absorbing bin. At the production time step (0.1 s) the semi-implicit solution reproduces the sub-stepped explicit reference within 0.0001% in total number while using three orders of magnitude fewer steps (10 min $\rightarrow$ 0.8 s for the full mesh).

2.4. Removal mechanisms

Coagulation-limited particle sizes remain in the nanometer range (Section 5), where the inertial collision-attachment flotation chain of the previous model [5] predicts negligible rates ($\sim 10^{-18} \text{ s}^{-1}$). Flotation is therefore remodeled as diffusive interface mass transfer to the rising bubble swarm. Per size bin,

$$\lambda_f = Sh_b \frac{6\alpha D_p}{D_b^2} \quad (5)$$

with the Higbie penetration form $Sh_b = 2 + (2/\sqrt{\pi})Pe_b^{1/2}$ [9] for the mobile bubble surface, where D_p is the Stokes-Einstein diffusivity. The inertial chain is retained as a parallel channel with its dimensional inconsistency corrected through a swept-volume kernel. Wall deposition uses a turbulent Sherwood correlation on each wetted node, and Stokes settling biases the advective flux of every bin. All removal sinks are integrated by exact integrating-factor half-steps within Strang splitting, so the removed volume and its flotation/wall attribution are accounted exactly.

2.5. Loop transport

The 77-bin populations of the three elements are advected around the 35-node loop with a donor-cell scheme whose face flow rate is

$$Q_{face} = \dot{m}/\rho_{donor} \quad (6)$$

which telescopes to exact number conservation for arbitrary axial density variation. Axial diffusion is neglected ($Pe \sim 10^9$). Each time step performs the local semi-implicit coagulation-generation-removal update (OpenMP over nodes) followed by the per-bin advection sweep; the CFL limit of the sweep is monitored.

3. Coupled Calculation with Serpent

The coupling replaces precomputed depletion data with Serpent 2.2 [6] calculations executed directly by the framework. The PMFR full-core depletion model (ENDF/B-VII.1) was rezoned so that the burnable fuel salt division coincides with the transport mesh: 10 axial core zones of 19.5 cm and 10 riser zones of 85.5 cm. The

zone-to-node mapping thereby degenerates to the identity. Because the salt makes $\sim 4,500$ loop transits per burnup step, all zone compositions are volume-averaged (complete mixing) at every step boundary; this mixed-boundary scheme reproduces a continuous-circulation reference solution of the coupled multi-zone burnup system to 0.13% at a small fraction of its cost.

Each coupling cycle runs Serpent first for one step of adaptive length (1 d during the precursor build-up, widening to 5 d as the source drift falls below 2%/d), then evaluates the transport code at that cycle's generation. Since the particle field relaxes within 300-400 s (runtime-verified, $|dI/dt|/G < 10^{-4}$), removal is booked quasi-statically as the steady rate times the cycle length, with wall deposits ledgered per node. The circulating Mo/Ru/Rh inventories and the dissolved Xe/Kr/He inventories then REPLACE the corresponding isotope densities in the composition (isotope ratios preserved) before the next Serpent run. Dissolved noble-gas stripping uses the same Higbie interfacial channel with the atomic diffusivity; its steady loop state is solved exactly (node-balance residual $\sim 10^{-16}$).

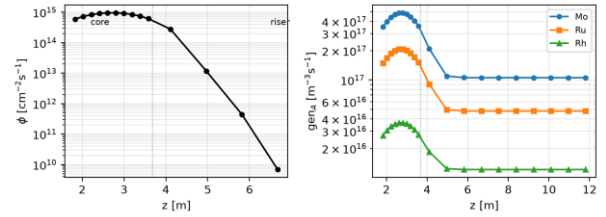


Fig. 1. Axial flux and noble metal generation gen_n from the coupled mixed-boundary Serpent depletion (day 10).

4. Verification

Development followed a fixed per-module workflow: implementation, a standalone example isolating the module, verification by an independent reviewer process, review of that verification, and only then an integration example coupling the module to the previously verified chain. Ten example sets are maintained with the code. Mass conservation was the leading acceptance criterion throughout: the semi-implicit coagulation conserves volume to $|massCons-1| \leq 2 \times 10^{-14}$ at any time step including the absorbing-bin regression; the transient solution was cross-validated against four independent references (sub-stepped explicit, two independent stiff ODE integrations) to within 0.001%; the loop advection conserves a passive population to 2×10^{-15} over 20 loop transits and reproduces the continuous decay operator to 4×10^{-13} ; and the fully coupled system closes the (salt + removed)/injected balance to $\leq 2.5 \times 10^{-12}$ over the 1200 s production run. In the year-long coupled run, every cycle additionally closed the generation-removal ledger to $\leq 7.7 \times 10^{-10}$ and held a bin-spectrum stationarity diagnostic below 1.5×10^{-6} .

5. Results

Fig. 2 shows the axial particle field after 360 s of generation-driven growth: total number densities of 10^{17} m^{-3} order and coagulation-limited mean diameters saturating near 0.5 nm in the core and 0.3 nm in the riser, confirming that the removal physics must operate in the diffusive regime.

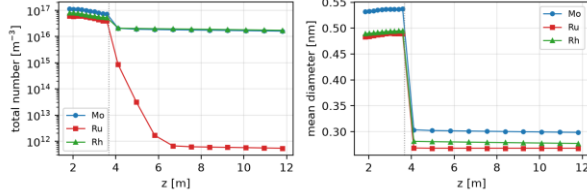


Fig. 2. Axial total number density and coagulation-limited mean diameter after 360 s of growth.

In the coupled calculation the particle field tracks a quasi-steady state whose inventory follows the slowly saturating generation. Table I summarizes the one-year coupled results at the reference bubble diameter $d_b = 5$ mm: circulating inventories of 10^{-10} m^3 order, flotation carrying 99.94% of the marginal removal, and 7.88 kg of Mo, 3.08 kg of Ru and 0.37 kg of Rh removed to the off-gas over the year, against gram-level wall deposits that peak at the riser inlet (0.39 g/m^2 of Mo). Gas stripping removes 17.0 kg of Xe, 4.9 kg of Kr and 5.6 g of He per year. Fig. 3 shows the loop steady profile, and Fig. 4 the one-year reactivity trajectory and cumulative removal: reactivity falls from +580 to -150 pcm, crossing critical near day 250 as burnup overtakes the (fast-spectrum, hence small, $+46 \pm 35$ pcm) Xe-stripping gain.

Table I: One-year coupled results ($d_b = 5$ mm)

	Mo	Ru	Rh
Salt inventory [m^3]	2.63e-10	6.87e-11	5.87e-12
Removed 1 yr, flotation [kg]	7.88	3.08	0.37
Removed 1 yr, wall [g]	4.5	1.9	0.3
Marginal flotation share [%]	99.94	99.94	99.94
Ledger closure (worst)	5.0e-10	5.0e-10	5.0e-10

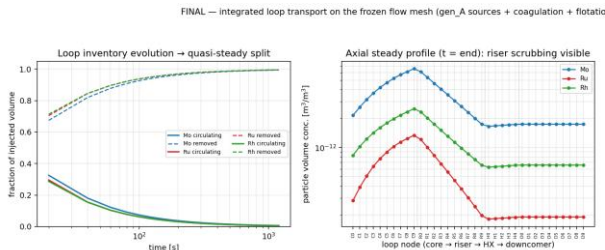


Fig. 3. Integrated loop transport: inventory evolution toward quasi-steady state and axial steady profile.

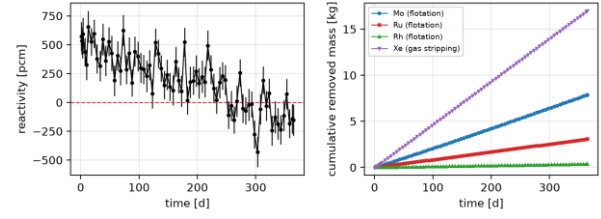


Fig. 4. One-year coupled run: reactivity trajectory and cumulative removed masses (noble metals by flotation; Xe by gas stripping).

Fig. 5 resolves the year-end state around the loop, with particles and gases on a common atomic scale: every species is loaded through the core, peaks at the riser inlet, is scrubbed down the riser, and reloads through the bubble-free HX and downcomer legs by decay of the circulating precursor inventory — He alone stays flat there, since its production needs flux. The steady size spectra (Fig. 6) peak at the atomic size and fall by twenty decades within about 100 nm: removal outpaces coagulation growth (particle residence of order 10^2 s versus months to reach micron sizes), which pins the population in the diffusive regime.

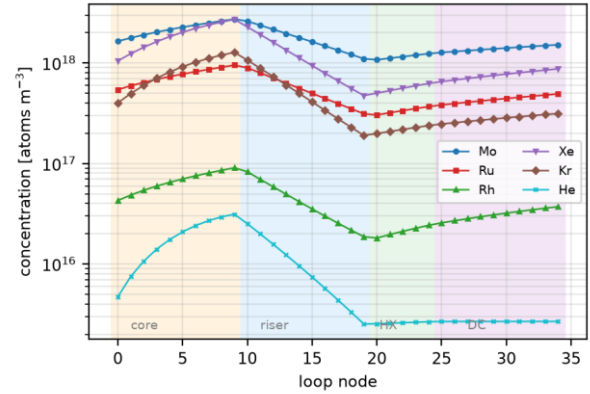


Fig. 5. Species concentrations around the loop at $t = 1$ year (particles and dissolved gases, atoms/m^3).

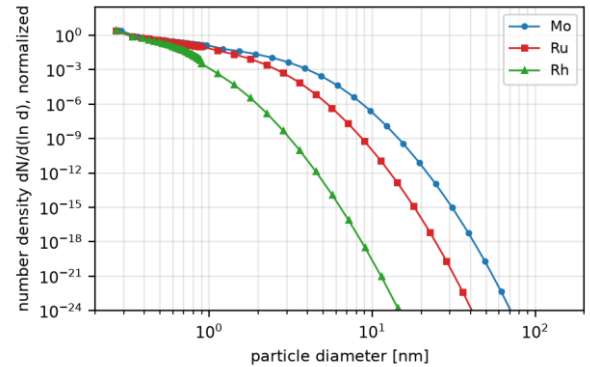


Fig. 6. Loop-integrated steady size distributions at $t = 1$ year.

The fouling pattern (Fig. 7) follows the mass-transfer flux $j = k_d C$: within each leg the deposit tracks the local concentration, while the steps at region boundaries reflect the discontinuous hydraulic environment through $k_d \propto \text{Re}^{0.83}/D$. The maximum areal density occurs at the

riser inlet (0.39 g/m^2 of Mo per year, where both C and k_d are high), and the narrow downcomer collects a three-fold higher areal density than the wide core — a direct guide for inspection and decontamination planning.

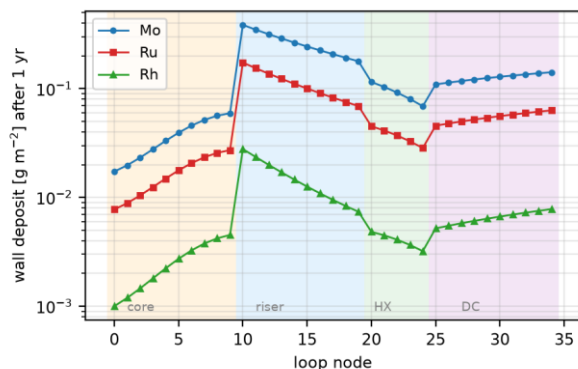


Fig. 7. Wall-deposit areal density per node after one year.

A bubble-diameter sensitivity (2.5/5/10 mm at fixed void fraction) shows the cumulative flotation removal moving from 96-98% to 50-61%, scaling approximately as $d_b^{-3/2}$, which identifies the delivered bubble size as the dominant design lever of the helium bubbling system. The bubble diameter, particle-bubble induction time, and heat exchanger geometry remain the principal model inputs awaiting experimental confirmation.

6. Conclusions

A size-resolved noble metal transport code for PMFR systems was developed, integrating a frozen natural-circulation flow field, Serpent-burnup-matrix-derived generation, an unconditionally volume-conserving semi-implicit coagulation solver, diffusive flotation and wall deposition, and exactly conservative loop advection. All modules passed independent verification with conservation closures at machine precision, and the coupled system reaches a quasi-steady state in which helium bubbling removes over 99% of the generated noble metal volume at the reference bubble size. A one-year coupled calculation with Serpent was performed on a shared 20-zone mesh with complete mixing at step boundaries and adaptive cycle lengths: removal feeds back into the depletion compositions each cycle, dissolved Xe/Kr/He stripping is included, and every cycle closes its mass ledger below 10^{-9} . Future work will move the exchange from files to messages in a single MPMD MPI execution, replace the fixed bubble diameter with an experimentally informed model, and extend validation to molten salt conditions.

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