

Newsletter Issue No. 2

Space Technology & Propulsion Insights

Unlocking Peak Core Efficiency: Predictive Multiscale Modeling for High-Temperature Space Nuclear Propulsion

Sustaining high-performance Nuclear Thermal Propulsion (NTP) with a specific impulse of 900 seconds or greater is widely recognized as a critical enabler for human Mars exploration. Reaching this milestone, however, requires reactor cores to operate continuously with propellant temperatures approaching 3,000 K under intense fluid shear. At these operational extremes, the primary bottleneck to flight qualification is not raw neutronic output—it is the dynamic, high-temperature chemical wear occurring at the interface where supercritical hydrogen meets refractory fuel elements.

To prevent structural failure across multi-burn flight profiles, design architectures frequently apply conservative temperature deratings. While protective, derating core temperatures by even a few hundred degrees directly erodes specific impulse, reduces allowable payload mass, and lengthens interplanetary transit durations. The solution lies in replacing empirical margin assumptions with high-fidelity, predictive modeling that captures non-equilibrium interfacial degradation before physical hardware ever enters a hot-fire test cell.

Bridging the Multiscale Physics Gap

A persistent challenge in space nuclear engineering has been the disconnect between macroscopic computational fluid dynamics (CFD) and microstructural materials science. Standard core design workflows often depend on static thermodynamic equilibrium tables or empirical Arrhenius corrosion rates derived from non-prototypic test chambers. These approximations fail to capture dynamic, non-equilibrium boundary phenomena—most notably the rapid generation of reactive atomic hydrogen radicals and the resulting localized carbon depletion within advanced carbide and cermet fuel matrices.

Addressing this gap requires a computational architecture that seamlessly scales from the reactor channel down to atomic surface kinetics:

Channel-to-Boundary Fluid Ingestion: The operational workflow begins by directly extracting localized thermal-hydraulic boundary conditions—

including surface temperature gradients, local pressures, and wall shear profiles—from established reactor-scale platforms like OpenFOAM and MCNP. It then computes real-time boundary-layer gas dissociation kinetics to accurately quantify the incident flux of reactive radicals actively impinging on fuel surfaces.

Accelerated Machine-Learned Interfacial Kinetics: Rather than incurring the prohibitive computational latency of standard electronic-structure calculations across an entire fuel element, modern scientific software pipelines utilize transfer-learned, equivariant machine-learning interatomic potentials. By bootstrapping established refractory databases and applying targeted sampling to high-temperature non-equilibrium transition states, the system rapidly predicts localized chemical wear and carbon-extraction energy barriers with sub-chemical accuracy.

Stochastic Surface Recession and Defect Transport: At the microstructural scale, rejection-free lattice kinetic Monte Carlo solvers simulate non-equilibrium surface recession rates in real time. Coupled directly with transient diffusion solvers, this pipeline monitors subsurface hydrogen migration and grain-boundary saturation, identifying localized embrittlement thresholds well before structural integrity is compromised.

Engineering-Grade Software Tailored for Mission Primes

High-fidelity physics is only as valuable as its usability within existing engineering workflows. Developing this capability as a modular, open-architecture scientific software suite ensures that NASA centers and aerospace prime contractors can readily integrate predictive degradation curves into their core design loops:

1. **Interoperable by Design:** Built to ingest outputs natively from NASA-standard neutronic and thermal-hydraulic tools, eliminating custom translation layers and proprietary lock-in.
2. **GPU-Accelerated High-Throughput Execution:** Leveraging modern parallel computing architectures allows reactor design teams to run comprehensive material trade studies across thousands of candidate operational cycles in hours rather than weeks.
3. **Rigorous Historical Benchmark Validation:** Calibrating interfacial recession kinetics against documented archival ground-test datasets from historical nuclear rocket testing programs establishes empirical confidence and accelerates technology readiness level advancement.
4. **Mission-Ready Margin Optimization:** Delivering deterministic mass-loss and embrittlement profiles gives reactor engineers the data-driven justification

needed to maintain core operating temperatures at peak thresholds without compromising flight safety margins.

Accelerating the Path to Interplanetary Flight

As NASA and its industry partners continue advancing space nuclear propulsion architectures for crewed deep-space missions, software tools that deliver physics-grounded operational certainty will play a foundational role in reducing development risk and expensive ground-test cycle times.

By delivering verified, multiscale visibility into the most demanding boundary layer in aerospace propulsion, agile scientific software developers are providing the analytical backbone needed to preserve high specific impulse, optimize fuel cladding longevity, and keep Mars transit architectures on a definitive path to flight.

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