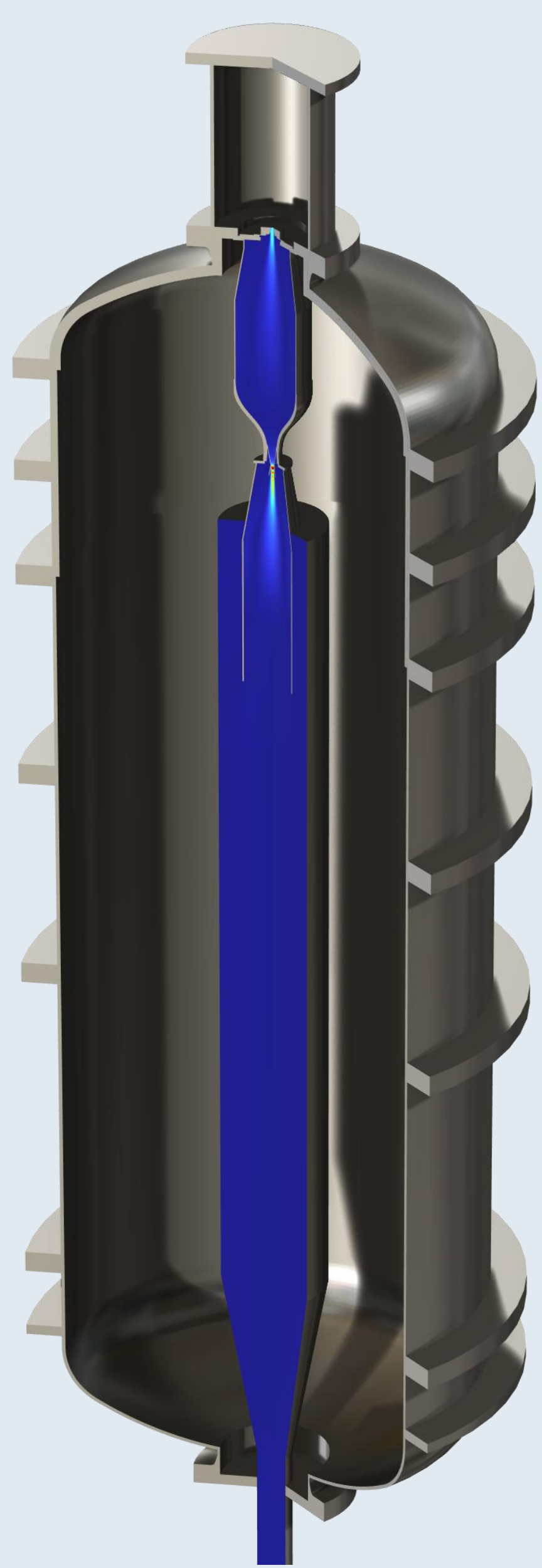




Digital Twin of an Argon–Hydrogen Plasma Reactor

A COMSOL Multiphysics® twin of GREEN14’s DC hydrogen-plasma reactor — reaction chamber, supersonic nozzle and a custom phase-change particle-tracing layer — coupled to AI surrogates.

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Abstract

GREEN14 builds digital twins for metallurgy. The proof of concept is an argon–hydrogen plasma reactor that melts, reduces, atomizes and quenches critical raw material in a single step, delivering premium spherical powder with controlled composition chemistry. The reactor is monitored by thermocouples and pressure sensors that provide a daily real-world data source, and is modeled in COMSOL Multiphysics® as the core multiphysics solver, complemented with AI models for seamless data assimilation and

optimization. We present the COMSOL twin of the reaction chamber and converging–diverging nozzle, together with a custom phase-change particle-tracing layer validated on Ti-6Al-4V (Ti-64), and show how the COMSOL–AI synergy can drive self-consistent optimization loops toward (i) autonomous live control and (ii) process optimization.



FIGURE 1. The GREEN14 pilot reactor at KTH.

Numerical Model

Compressible RANS (COMSOL High Mach Number Flow, SST) on a 2-D axisymmetric domain, with conjugate heat transfer in the water-cooled walls and optically-thin gas-phase radiation as a volumetric source. The single-fluid argon–hydrogen plasma is in local thermodynamic equilibrium, with properties from Cantera (cross-checked with Mutation++) over 300–30 000 K. A power-based supersonic inlet fixes the delivered plasma power; the outlet is held at 75 mbar; each coil is a 1-D coolant PDE for the coil-to-wall contact conductance. Particles follow a custom one-way phase-change model (drag, evaporation, breakup). COMSOL is complemented by AI: calibration, SINDy source-term discovery and neural surrogates.

Results

Calibration. The unmeasurable plasma power and the coil-to-wall contact conductance are inferred from the measured chamber pressure and coil heat, matched to ~0.1% and ~0.4% across 11 hot tests.

Reactor fields & particles. The twin returns the temperature and Mach fields — a >12 000 K core with a supersonic shock-diamond train — into which Ti-64 particles are released, crossing the liquidus, evaporating and breaking up.

Product powder. Evaporation tightens the predicted size distribution (median 58 → 47 μm); collected particles are perfect spheres.

Surrogate & app. A large dataset over varied inputs trains a neural-operator surrogate, deployed in our in-house app for real-time process monitoring and control.

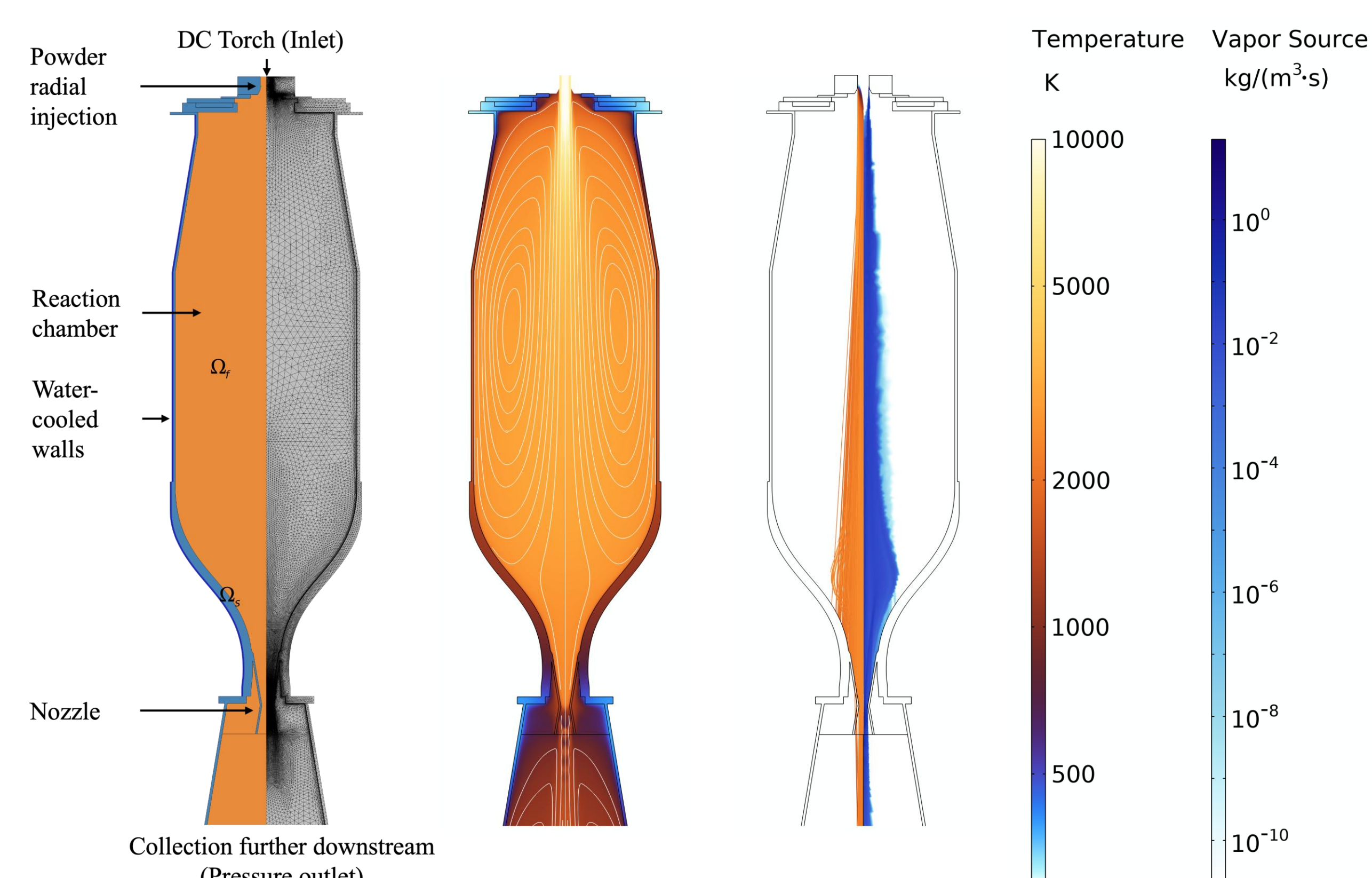


FIGURE 2. COMSOL twin (~22 kW): geometry & mesh, gas temperature + streamlines, Ti-64 particles + vapor source.

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