

Multiphysics Modeling of PVT Growth of SiC Crystals Coupled with Data-Driven Process Optimization

Physics-based simulation combined with proprietary data-driven process optimization

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Abstract

Physical Vapor Transport is the dominant route for high-quality SiC single crystals, but heat transfer, gas-phase transport and phase transition are strongly coupled. A COMSOL Multiphysics® model is used to investigate an industrial-scale, literature-based PVT reactor. The model combines induction heating, conduction and radiation, transport of Si, SiC₂ and Si₂C, and sublimation–recrystallization kinetics. Reactor design and graphite material properties are linked to temperature gradients, species fluxes, growth rate and crystal morphology. Proprietary SGL optimization tools, developed independently of COMSOL, complement the physics-based model through rapid parameter exploration, sensitivity analysis and data-driven optimization.

Methodology

The axisymmetric reactor model couples four physical blocks:



MF + HT Induction heating, conduction, radiation, regulation	SiC(s) ⇌ Si(g) + C(s) 2SiC(s) ⇌ SiC₂(g) + Si(g) 2SiC(s) ⇌ Si₂C(g) + C(s)	Stoichiometric growth at crystal surface Transient source ageing PDE-based source evolution Δt = 2 h
FP Porous flow in source, porous graphite and growth chamber		
TCS Transport of Si(g), SiC ₂ (g) and Si ₂ C(g)		

The transient workflow alternates between electromagnetic heating, heat transfer, porous-gas flow, species transport and source-evolution calculations using a two-hour update interval.

Results

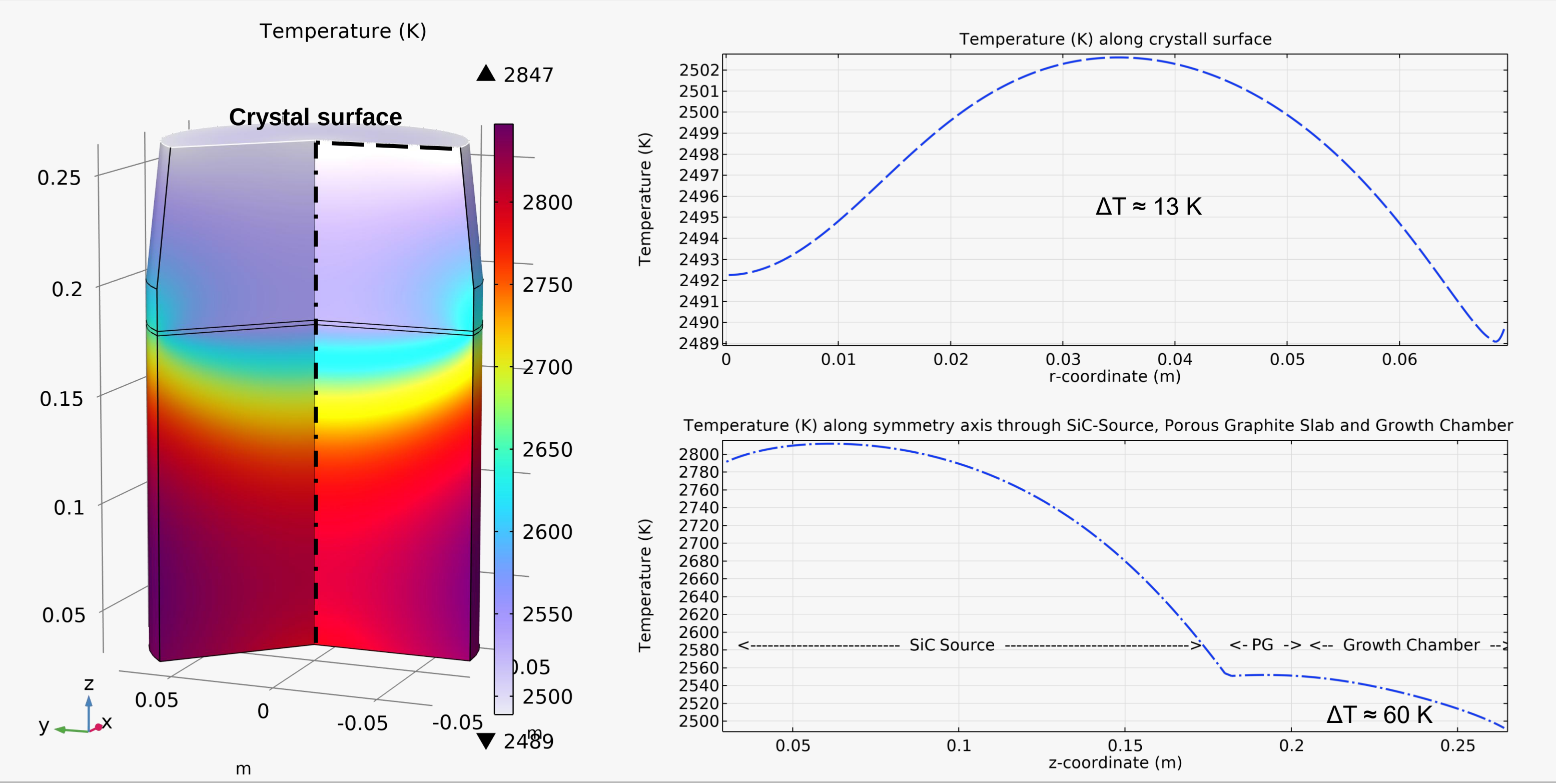


FIGURE 2. Thermal conditions governing SiC crystal growth. Temperature distribution in the PVT reactor, axial thermal gradient through source, porous-graphite slab and growth chamber, and radial temperature variation at the crystal surface.

A key design objective in PVT growth is the combination of a large axial temperature gradient and a small radial temperature variation at the crystal surface. The reference configuration provides approximately 60 K between source and crystal while maintaining a radial crystal-surface temperature difference of only approximately 13 K.

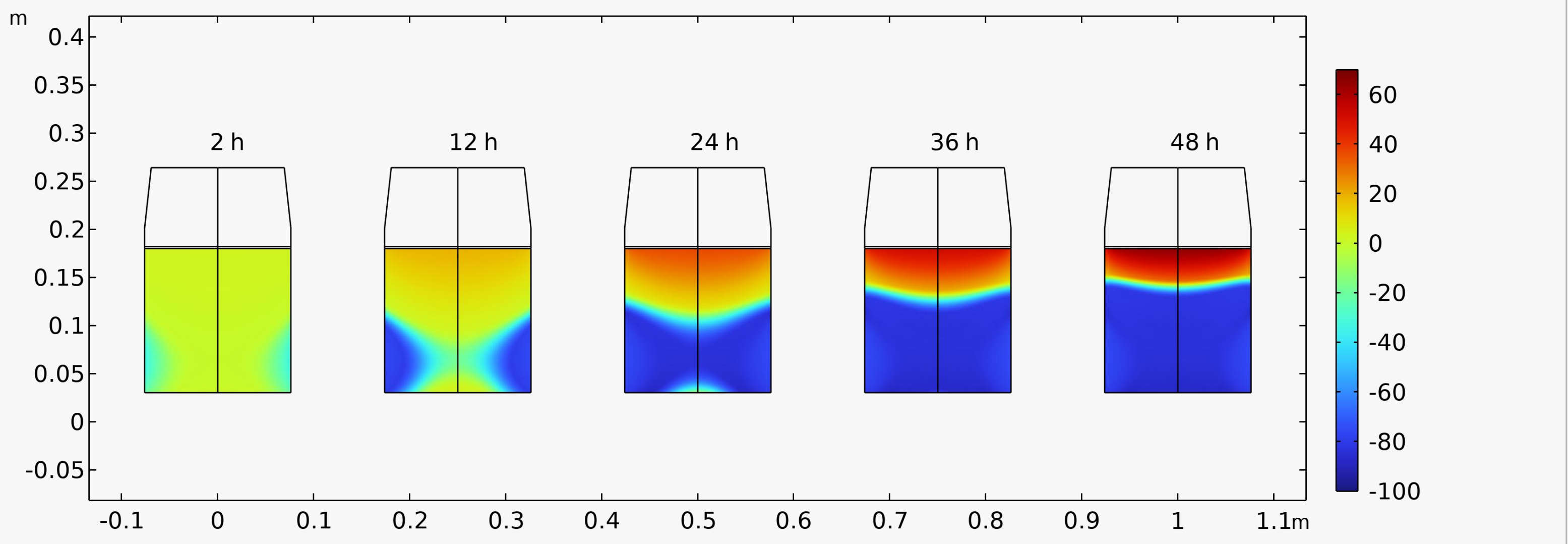


FIGURE 4. Relative enrichment and depletion of the SiC phase within the source.

Transient source evolution leads to local SiC depletion and formation of carbon-rich regions. The resulting changes in effective transport and thermal properties influence the sublimation process and contribute to the gradual reduction of crystal-growth rates observed in the reference simulation.

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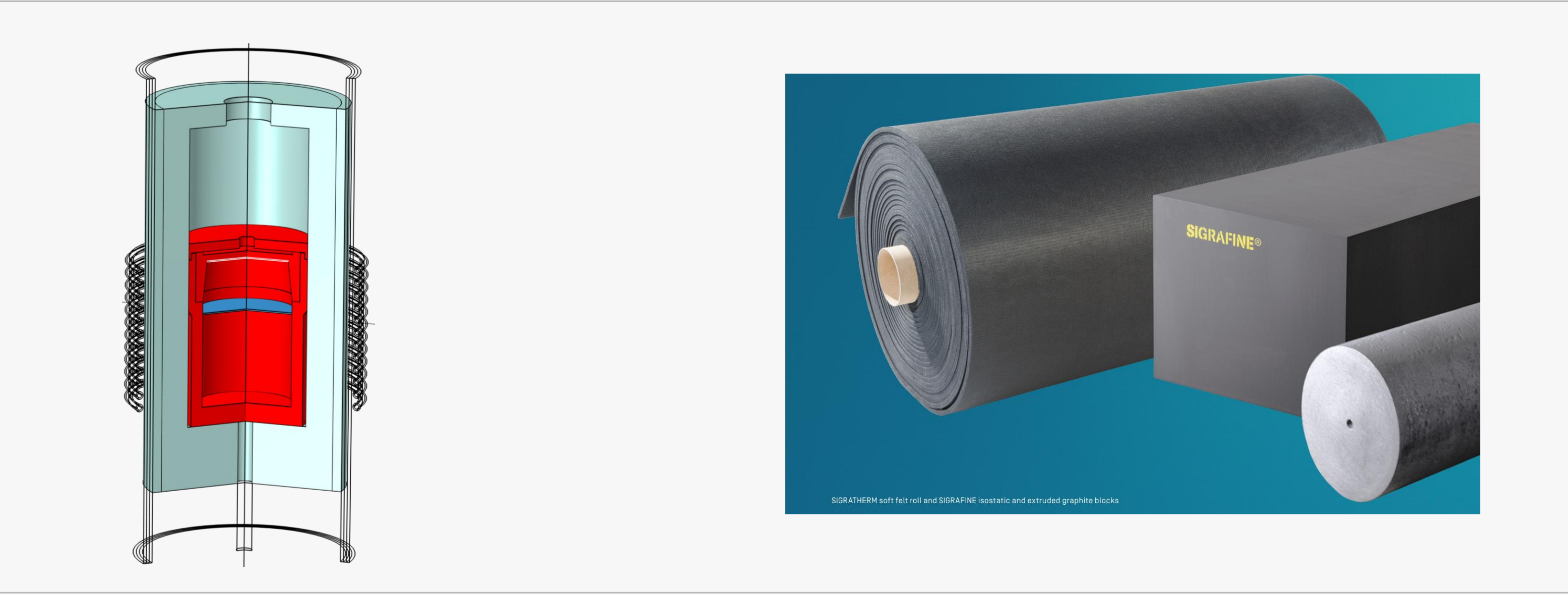


FIGURE 1. PVT reactor model and representative graphite materials for semiconductor crystal-growth applications.

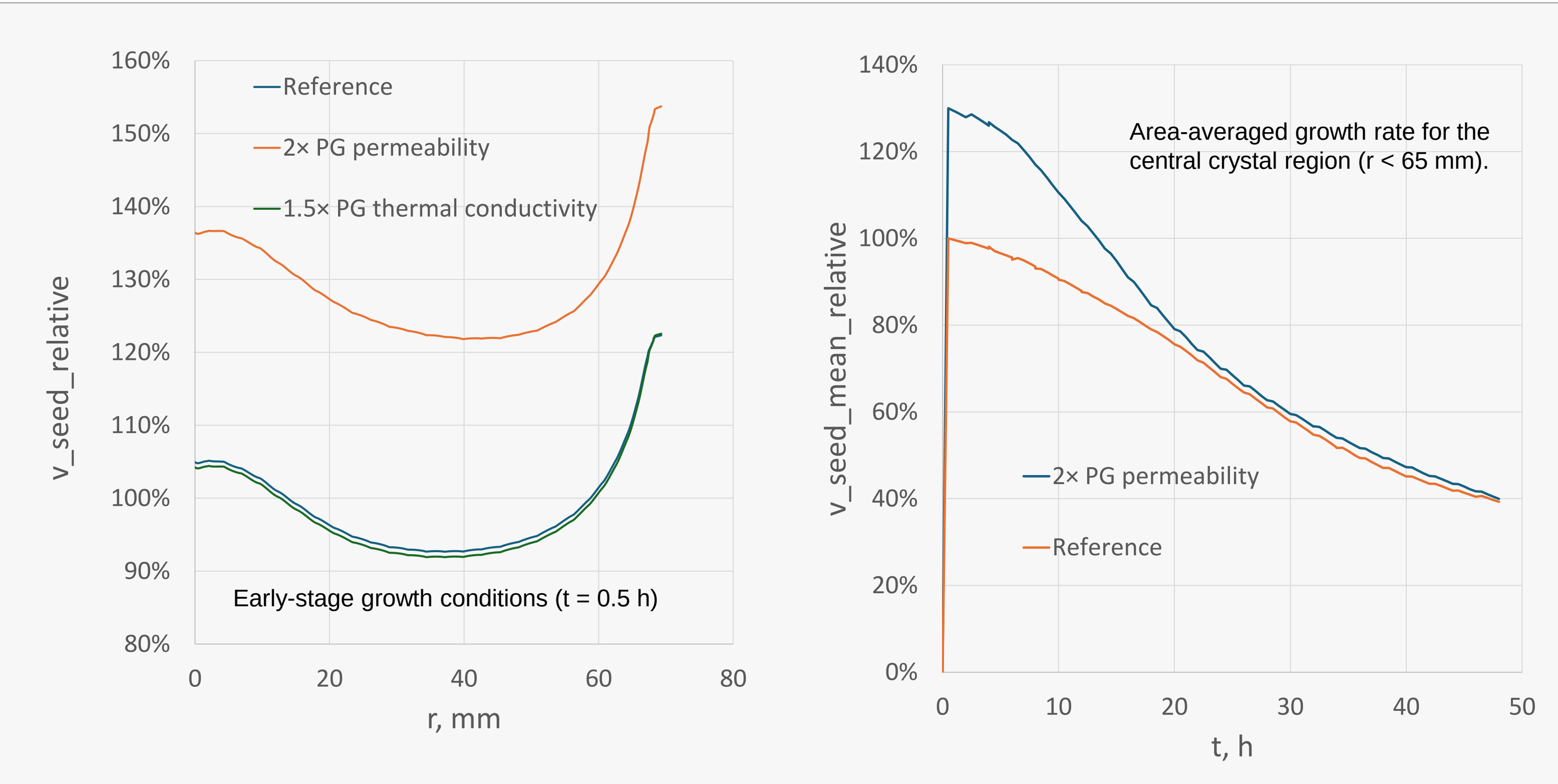
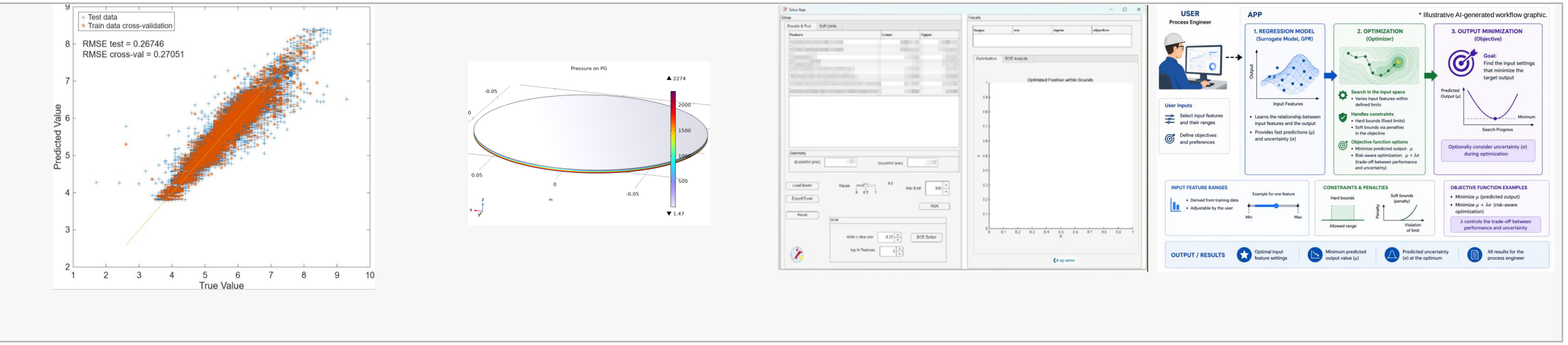


FIGURE 3. Influence of porous-graphite properties and transient source evolution on crystal growth (without accounting for the C supply from porous graphite).

Changing porous-graphite permeability modifies heat and mass transport conditions inside the reactor and thereby affects crystal-growth rates. While doubling the PG permeability significantly increases the initial growth rate, both configurations exhibit a continuous decline and gradually converge during transient operation. This behaviour indicates that SiC source evolution increasingly governs the process response during long-duration growth runs and should be considered when defining thermal process conditions.

Data-Driven Optimization



Proprietary SGL data-driven tools, developed independently of COMSOL, are used to optimize permeability, mechanical performance and impurity levels of graphite-based materials. The workflow combines production data, simulation results and machine-learning methods to accelerate material and process development.

Conclusions

- Coupled MF, HT, FP and TCS simulations provide detailed insight into heat and mass transport during SiC PVT growth.
- Porous-graphite properties influence heat and mass transport and thereby affect crystal-growth rates.
- Transient source evolution significantly affects the predicted long-term growth behaviour and should be considered in long-duration growth simulations.
- Physics-based simulation and data-driven optimization jointly support the development of advanced graphite materials and crystal-growth components.