Digital Twin for Transient Heat Diffusion in Composite Heater–Insulation Assemblies

Draft Methodology (for Energies submission)

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1 System Overview

We simulate transient heat conduction in heterogeneous solids with (i) prescribed heater temperature ramps (Dirichlet), (ii) convection and linearized radiation at exposed faces (Robin), and (iii) optional thin, low-conductivity gaps to represent imperfect contacts. The solver uses FiPy finite volumes on gmsh-generated unstructured tetrahedral meshes, with temperature-dependent properties from a material catalog.

Geometries considered: (a) baseline single-layer: $10 \times 10 \times 25$ cm geopolymer core, heater rod ($r = 0.8\,\text{cm}$), brick-dust bedding ($r = 1.0\,\text{cm}$), silica blanket shell ($t = 1.3\,\text{cm}$); (b) double-layer: same core, shell $t = 2.6\,\text{cm}$; (c) four-block 120 cm "naked" stack: core $10 \times 10 \times 120$ cm, heater $r = 1.25\,\text{cm}$, bedding $r = 1.3\,\text{cm}$, three 2 mm low-k gaps.

2 Governing Equations

2.1 Heat Equation

For each material region:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q, \tag{1}$$

with density ρ [kg/m^3], heat capacity c_p [J/kg·K], conductivity k [W/m·K], and volumetric source q (set to zero; the heater is imposed via Dirichlet).

2.2 Dirichlet Heater Ramp

Heater temperature:

$$T_h(t) = \begin{cases} T_0 + (T_{\max} - T_0)\, t/t_{\text{ramp}}, & t < t_{\text{ramp}}, \\ T_{\max}, & t \geq t_{\text{ramp}}. \end{cases} \tag{2}$$

An efficiency factor $\eta_h \in (0, 1]$ may be applied: $T_{\max,\text{eff}} = \eta_h T_{\max}$.

2.3 Robin Boundary: Convection + Linearized Radiation

On a surface Γ with outward normal $\mathbf{n}$:

$$-k_{\text{face}}\, \mathbf{n} \cdot \nabla T = h(T - T_\infty) + h_{\text{rad}}(T - T_\infty), \tag{3}$$

where h is the convective coefficient, T_∞ ambient temperature, and linearized radiation term

$$h_{\text{rad}} = 4\sigma\varepsilon T_\infty^3, \tag{4}$$

with emissivity ε and Stefan–Boltzmann constant σ. Effective coefficient: $h_{\text{eff}} = h + h_{\text{rad}}$. Face conductivity k_{face} is taken from the adjacent cell material.

2.4 Low-Conductivity Gaps

Imperfect contacts are represented as explicit thin layers (material `air_gap`) with low k, adding conduction resistance without explicit contact-resistance models.

3 Material Properties (Catalog Snapshot)

- Geopolymer: $\rho \approx 1960\,\text{kg/m}^3$; $c_p \approx 950\,\text{J/kg K}$ to $1050\,\text{J/kg K}$; $\alpha \approx 4.4 \times 10^{-7}\,4\,7\text{e} - 7m^2/s$.
- Nichrome: $k \approx 14\,\text{W/m K}$ to $16.5\,\text{W/m K}$; $c_p \approx 440\,\text{J/kg K}$ to $500\,\text{J/kg K}$; $\rho = 8400\,\text{kg/m}^3$.
- Silica blanket: $k = 0.04\,\text{W/m K}$ to $0.40\,\text{W/m K}$ (260 °C–1200 °C); $\rho = 128\,\text{kg/m}^3$; $c_p = 900\,\text{J/kg K}$ to $1150\,\text{J/kg K}$.
- Brick powder (bedding): $k = [0.28, 0.27, 0.26, 0.25, 0.24]$ W/m·K (20 °C–700 °C); $\rho \approx 1560\,\text{kg/m}^3$ to $1620\,\text{kg/m}^3$; $c_p \approx 880\,\text{J/kg K}$ to $990\,\text{J/kg K}$.
- Air gap: $k = [0.026, 0.030, 0.034, 0.038, 0.042]$ W/m·K; $\rho = 1.2\,\text{kg/m}^3$; $c_p = 1000\,\text{J/kg K}$.
- Emissivity default $\varepsilon = 0.9$.

4 Boundary Conditions Used

- Baseline / 2L: convection on `outer_shell` with $h = 17\,\text{W/m}^2\,\text{K}$; +z insertion face $h = 23\,\text{W/m}^2\,\text{K}$; $T_\infty \approx 26\,°\text{C}$; $\varepsilon = 0.9$.
- Naked 4-block: convection on `geopolymer_core` directly; $h = 18\,\text{W/m}^2\,\text{K}$; $\varepsilon = 0.9$.

5 Meshing and Quality

- gmsh 3D tetra meshes; global size typically 10 mm; rod refinement 2 mm; gaps 2 mm thick.
- Quality metric: radius ratio; accepted min ≥ 0.2 (observed 0.20–0.39), mean $\sim$ 0.80–0.86.
- Cell distances floored to 10^{-6} to avoid divide-by-zero in FiPy face terms.
- Exports: `.msh` (v2.2) and `.vtu` (preview).

6 Solver Workflow

1. Parse scenario YAML (geometry, mesh controls, heater schedule, BCs, probes, time controls).
2. Build gmsh model, fragment, tag physical groups, generate mesh.
3. Convert to FiPy mesh (Gmsh3D); regularize distances.
4. Interpolate material fields (k, c_p, ρ) per cell (temperature-dependent).
5. Impose heater Dirichlet ramp; advance transient (implicit scheme).
6. Apply Robin BCs with $h_{\text{eff}} = h + 4\sigma\varepsilon T_\infty^3$.
7. Stream telemetry (NDJSON), optional live plot; write summary JSON.

7 Assumptions and Limitations

- Heater as uniform Dirichlet (no electrical/coil geometry); efficiency factor η_h can approximate unmodeled losses.
- Contact resistance via explicit low-k gaps (no TCR model).
- Radiation linearized around ambient; nonlinear form not yet used at very high T.
- No phase change or dehydration; no fluid flow; convection coefficients uniform.
- Probes are point samples; no sensor mass/lag.

8 Planned Extensions

Nonlinear radiation BC; heater efficiency parameter in scenarios; true contact conductance model; data-driven heater power; calibration/optimization vs experimental NDJSON; adaptive refinement near heater/gaps.

9 Validation Plan

Compare ramps/plateaus vs experimental datasets (1L/2L, long stack) with RMSE per probe and timing to milestones (100 °C, 200 °C, etc.). Sensitivity: vary h, bedding k, gap k/thickness, η_h. Stability checks with smaller dt on stiff cases.

10 Key Formulae

- Heat: $\rho c_p \partial T/\partial t = \nabla \cdot (k \nabla T)$.
- Heater: Dirichlet ramp to $\eta_h T_{\max}$.
- Robin: $-k\nabla T \cdot n = (h + 4\sigma\varepsilon T_\infty^3)(T - T_\infty)$.
- Linearized radiation: $h_{\text{rad}} = 4\sigma\varepsilon T_\infty^3$.

11 Citations

[CITATION] FiPy FVM solver; [CITATION] gmsh; [CITATION] Mesh quality (radius ratio); [CITATION] Linearized radiation BC; [CITATION] Thermal properties; [CITATION] Contact resistance.