Fuel Cells & Electrolysers

3D Transient Simulation of a Planar SOFC: Linking Microstructure to Multiphysics Performance

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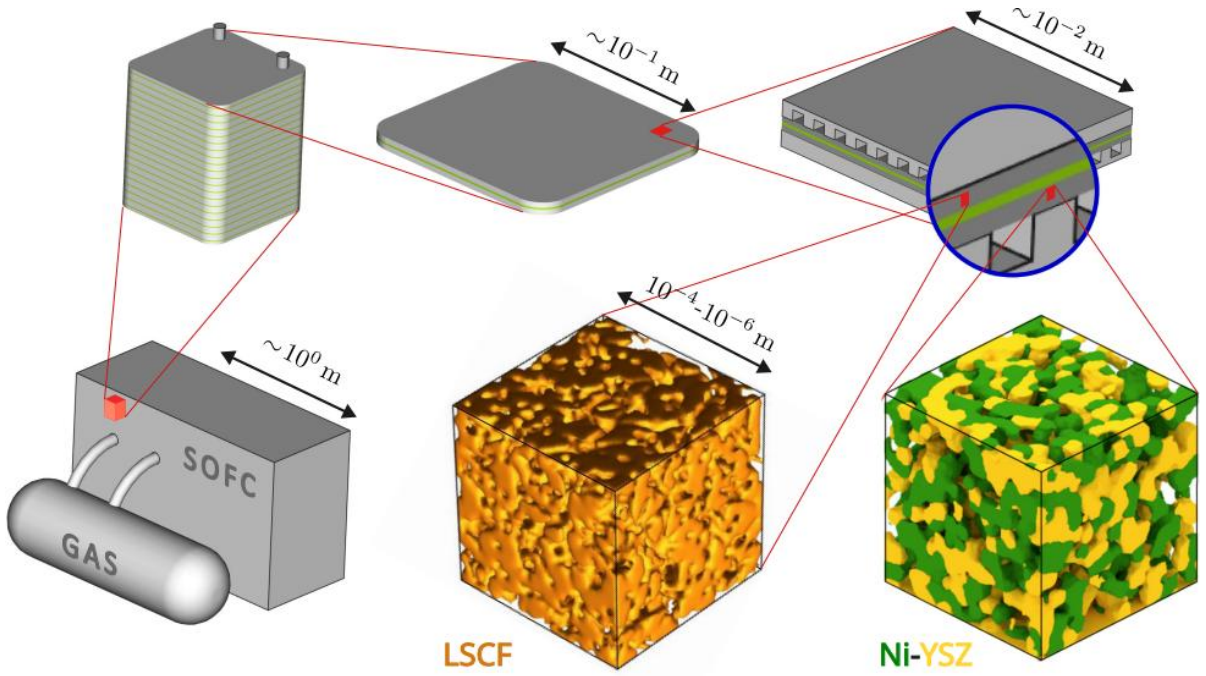
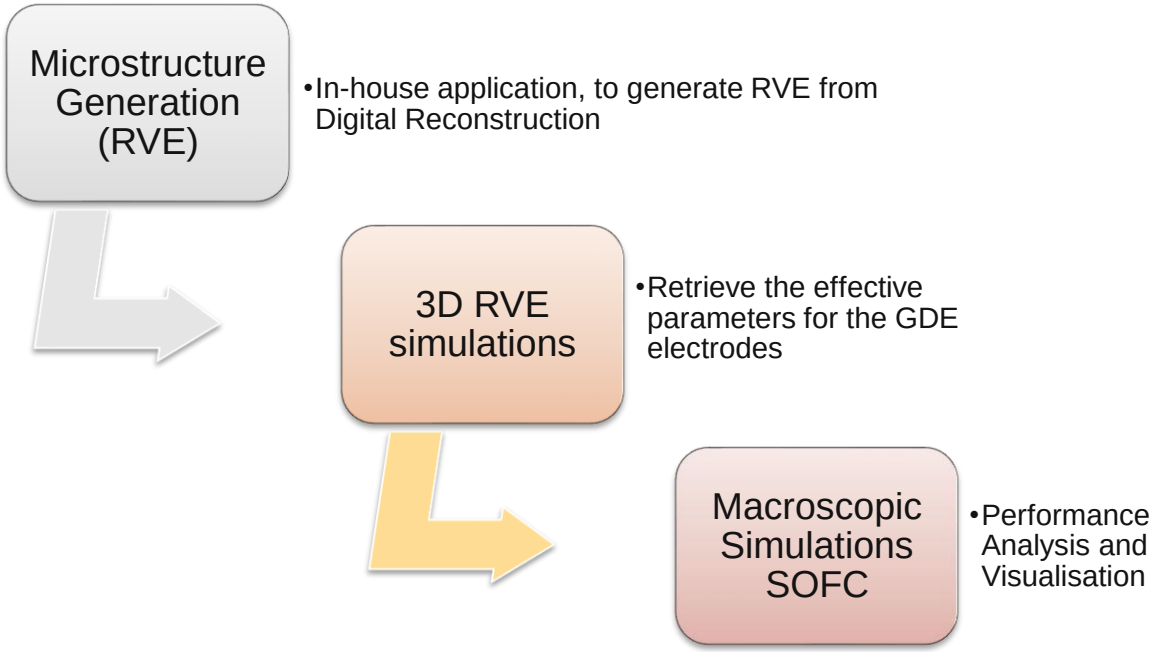
SOFC Simulation in COMSOL®

Multiscale approach



Multiscale representation of SOFC
showing system's scale spans 6 order of magnitude



Workflow illustrating the computational approach
from microstructure to SOFC unite cell

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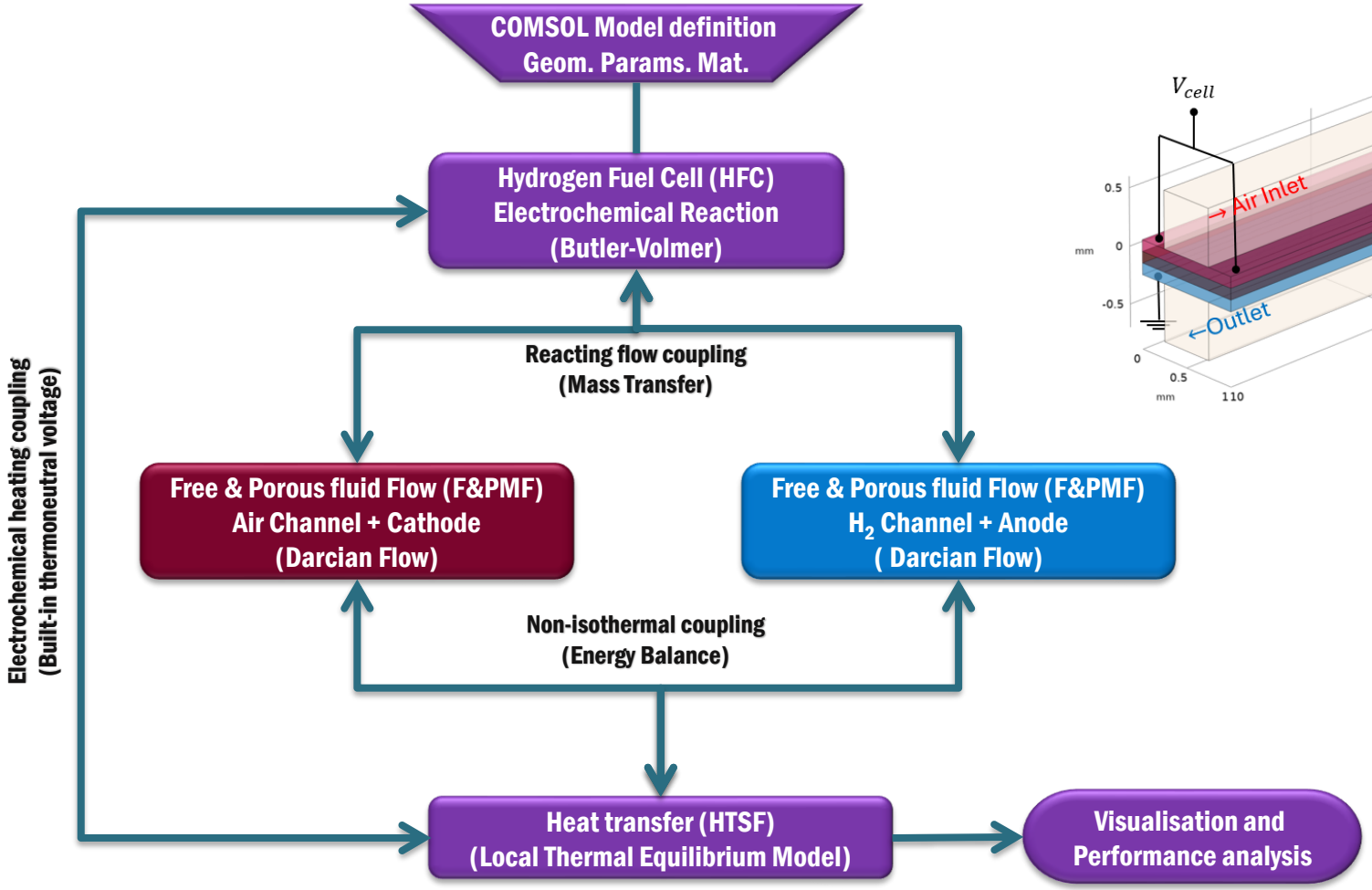
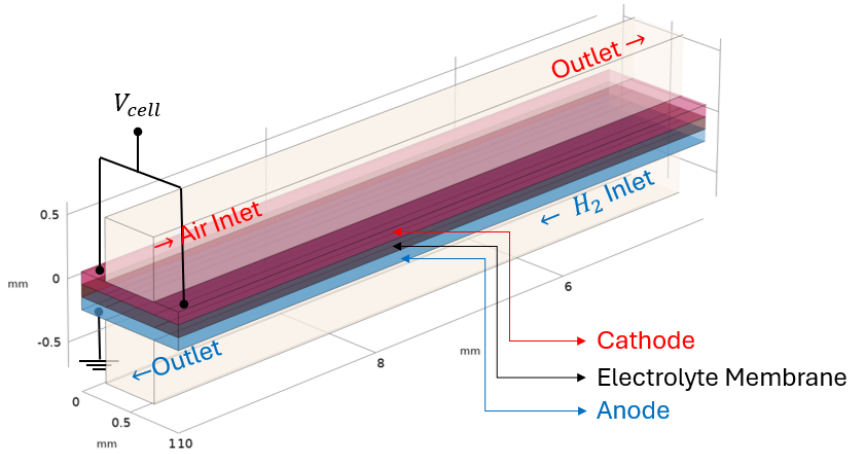
Multiphysics modelling of SOFC

Process Flow of Segregated Approach in COMSOL®





COMSOL Physics Modules:
- Hydrogen Fuel Cell (HFC)
  - Applied within:
- Free & Porous Media Flow (F&PMF)
  - Applied within anode side :
  - Applied within Cathode side :
- Heat Transfer in Solids and Fluids (HTSF)
  - Applied within:

COMSOL Multiphysics Coupling:
- Reacting Flow (F&PMF + HTSF)
  - Applied within anode side :
  - Applied within Cathode side :
- Non-isothermal Flow (F&PMF + HTSF)
  - Applied within anode side :
  - Applied within Cathode side :
- Electrochemical Heating (HFC + HTSF)
  - Applied within:

Computational Domain Specification

(Anode and Cathode assigned separate computational domain)

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Microstructure modelling of SOFC

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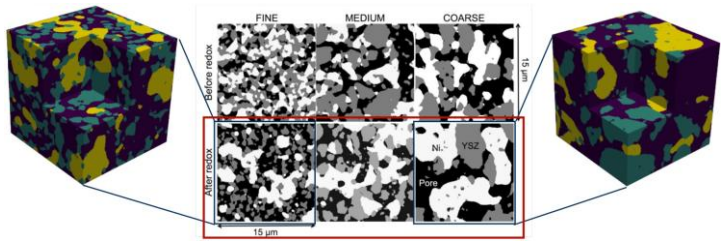
3D Microstructure Generation and homogenisation

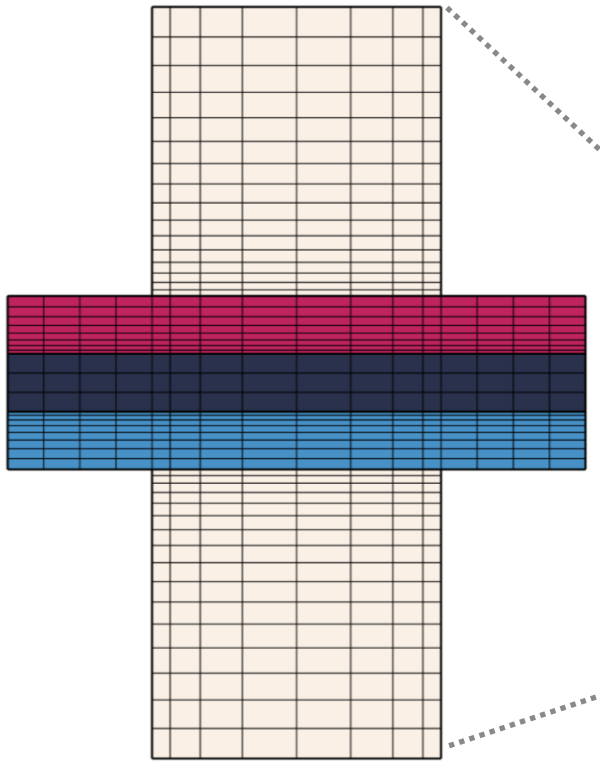


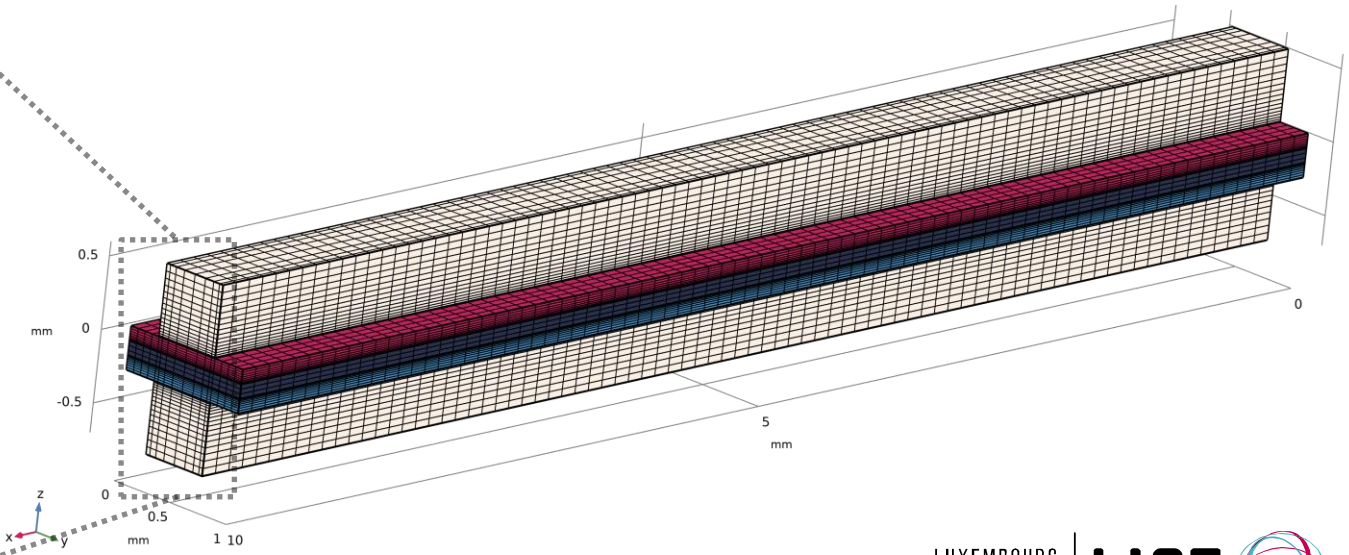
3D RVE

Homogenisation

	$k(T)$ (W/m.K)	$\sigma^e(T)$ (S/m)	$\sigma^l(T)$ (S/m)	κ^{eff} (μm^2)	τ (1)	ϵ (%)
Membrane 8YSZ	$2.04.10^{-3}T + 8.28$	0	$3.34.10^{+4}e^{-10300/T}$	1.2	1.4	25.0
41.6%8YSZ + 32.5%Ni (a)	$\underline{\underline{k}}^{(a)}(T)$	$\underline{\underline{\sigma}}^{e(a)}(T)$	$\underline{\underline{\sigma}}^{l(a)}(T)$	$\underline{\underline{\kappa}}^{\text{eff},(a)}(T)$	1.4	25.9
LSCF 46% (c_1)	$\underline{\underline{k}}^{(c_1)}(T)$	$\underline{\underline{\sigma}}^{e(c_1)}(T)$	$\underline{\underline{\sigma}}^{l(c_1)}(T)$	$\underline{\underline{\kappa}}^{\text{eff},(c_1)}(T)$	1.6	46.6
LSCF 37% (c_2)	$\underline{\underline{k}}^{(c_2)}(T)$	$\underline{\underline{\sigma}}^{e(c_2)}(T)$	$\underline{\underline{\sigma}}^{l(c_2)}(T)$	$\underline{\underline{\kappa}}^{\text{eff},(c_2)}(T)$	1.6	37.5

Microstructure properties





Mesh Details of unit SOFC:
Boundary layers at interface
44000 Hexahedra elements

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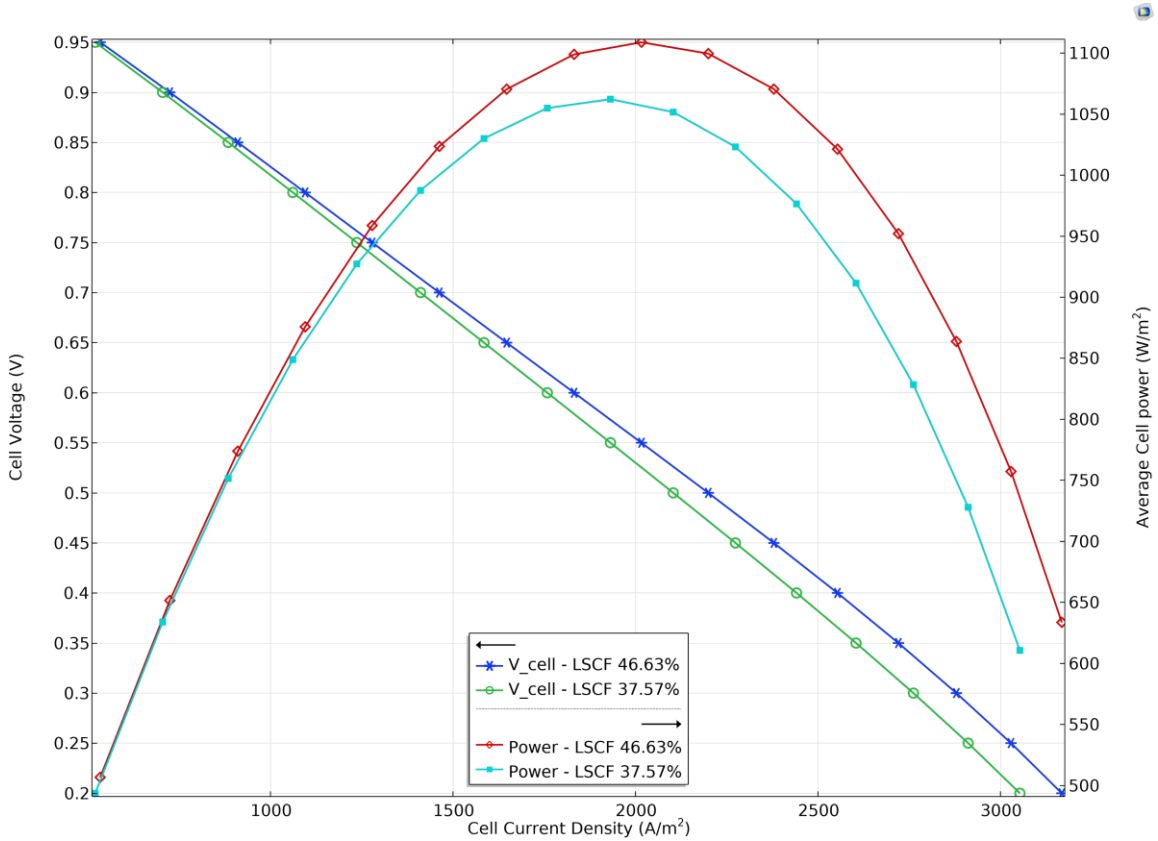
Unit SOFC PERFORMANCE

Power Density and I/V figure-of-merit

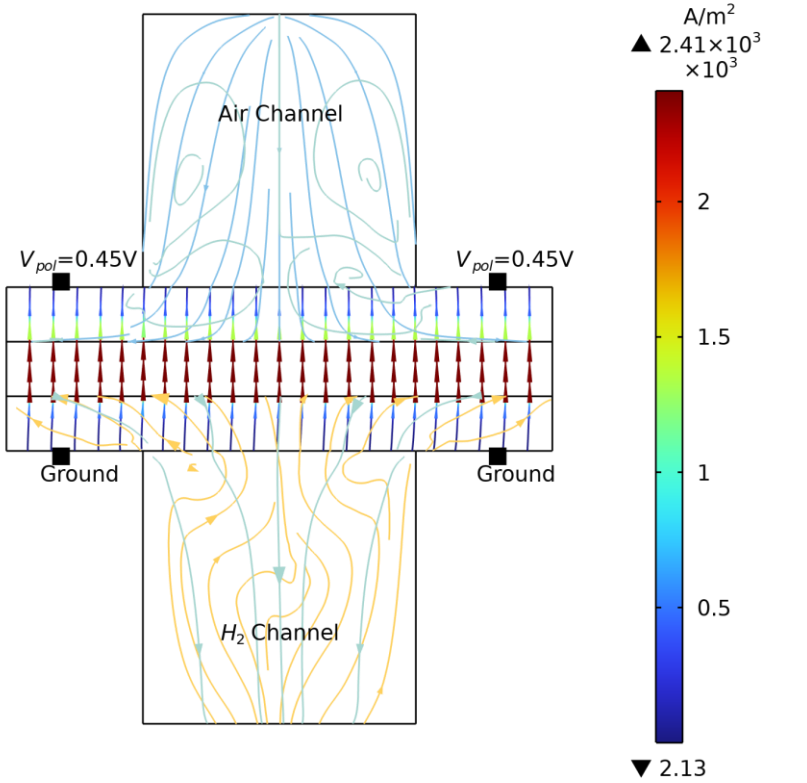


Polarization curve and Average power-density distribution generated from the COMSOL simulation, showing the relationship between current density and cell voltage for different LSCF microstructures .

Unit SOFC PERFORMANCE

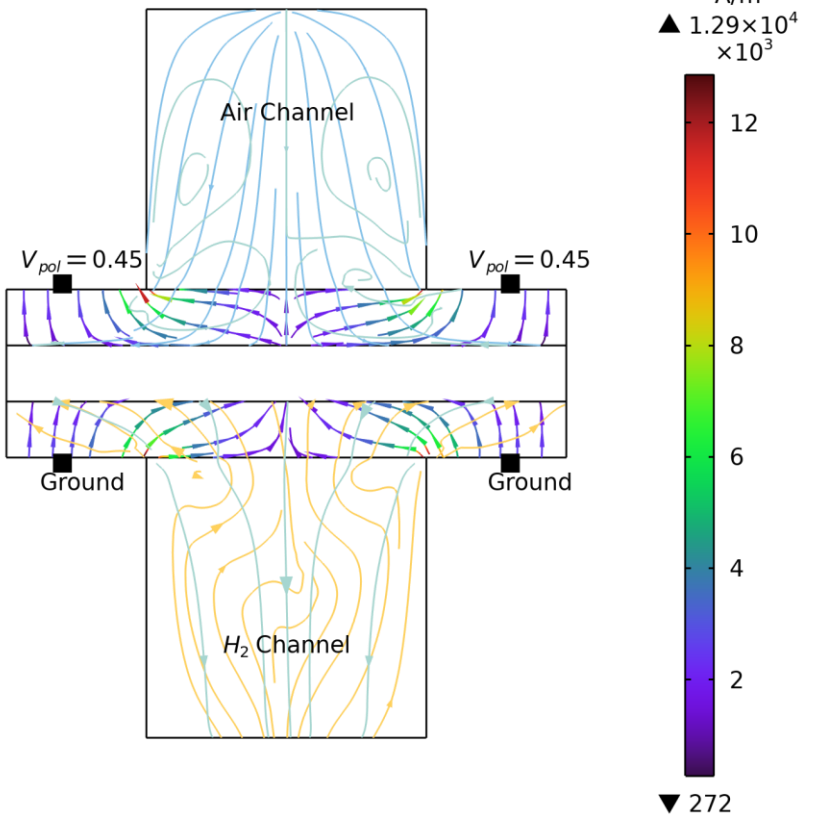
Component fluxes and current density streamlines on transversal cross-cut of the SOFC

$J_{O^{2+}}$ streamlines



H_2O streamlines:
H_2 streamlines:
O_2 streamlines:

J_{e^-} streamlines:



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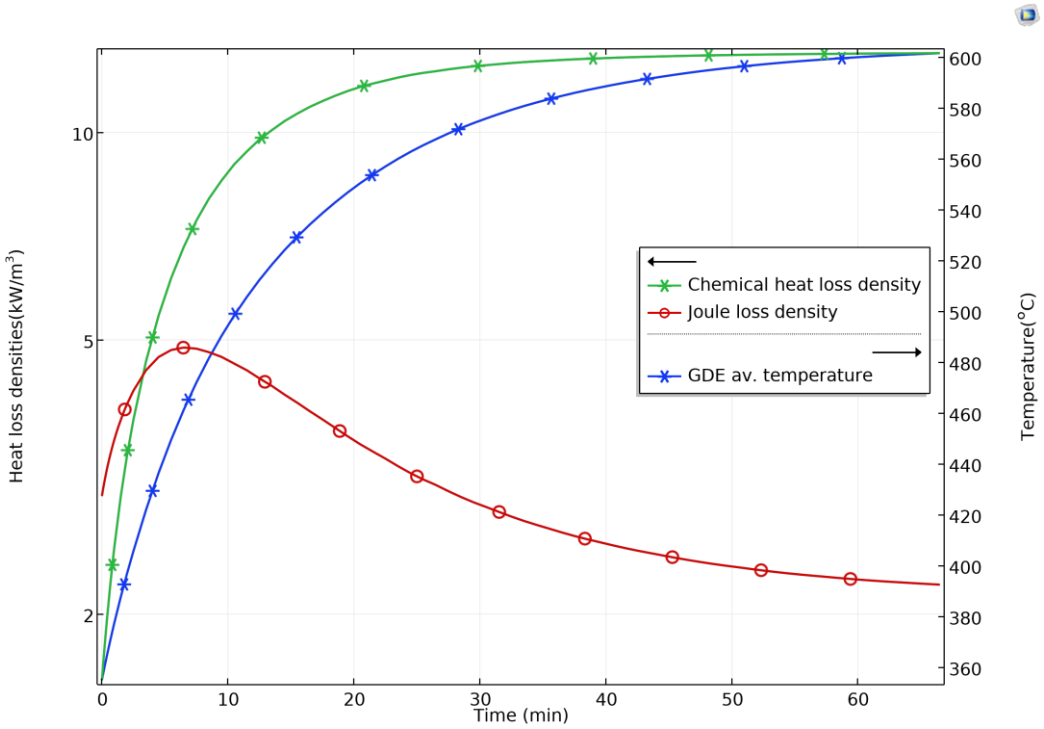
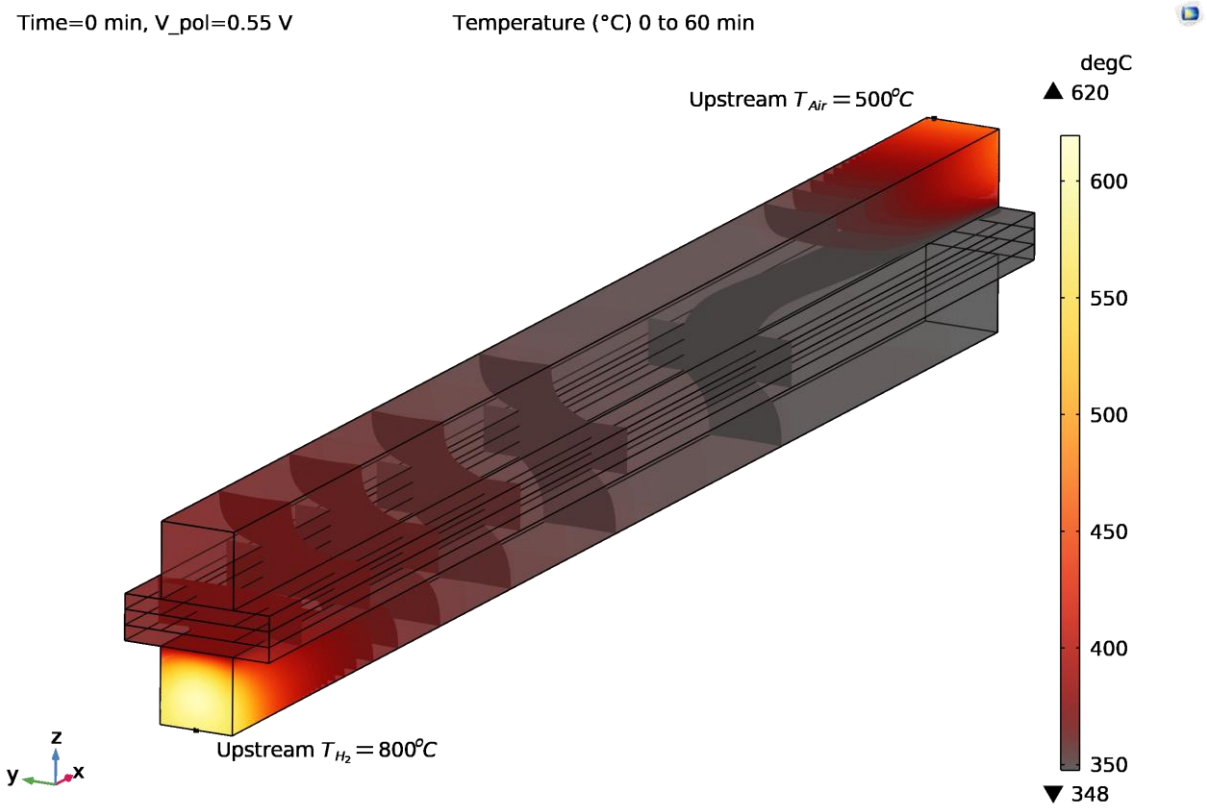
UNIT SOFC Heat&loss Management

Simulation of unit SOFC cold start



History of cold start of SOFC



Contours of temperature across the SOFC

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UNIT SOFC Heat&loss Management

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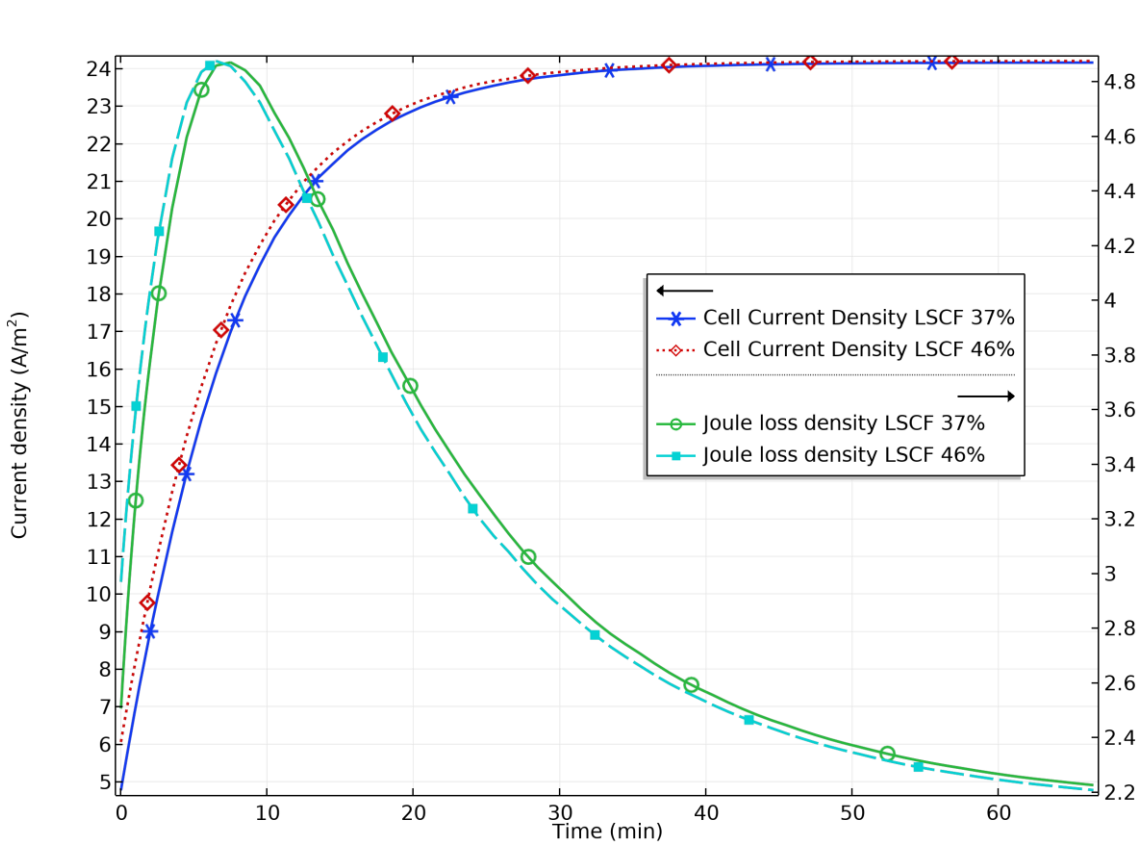
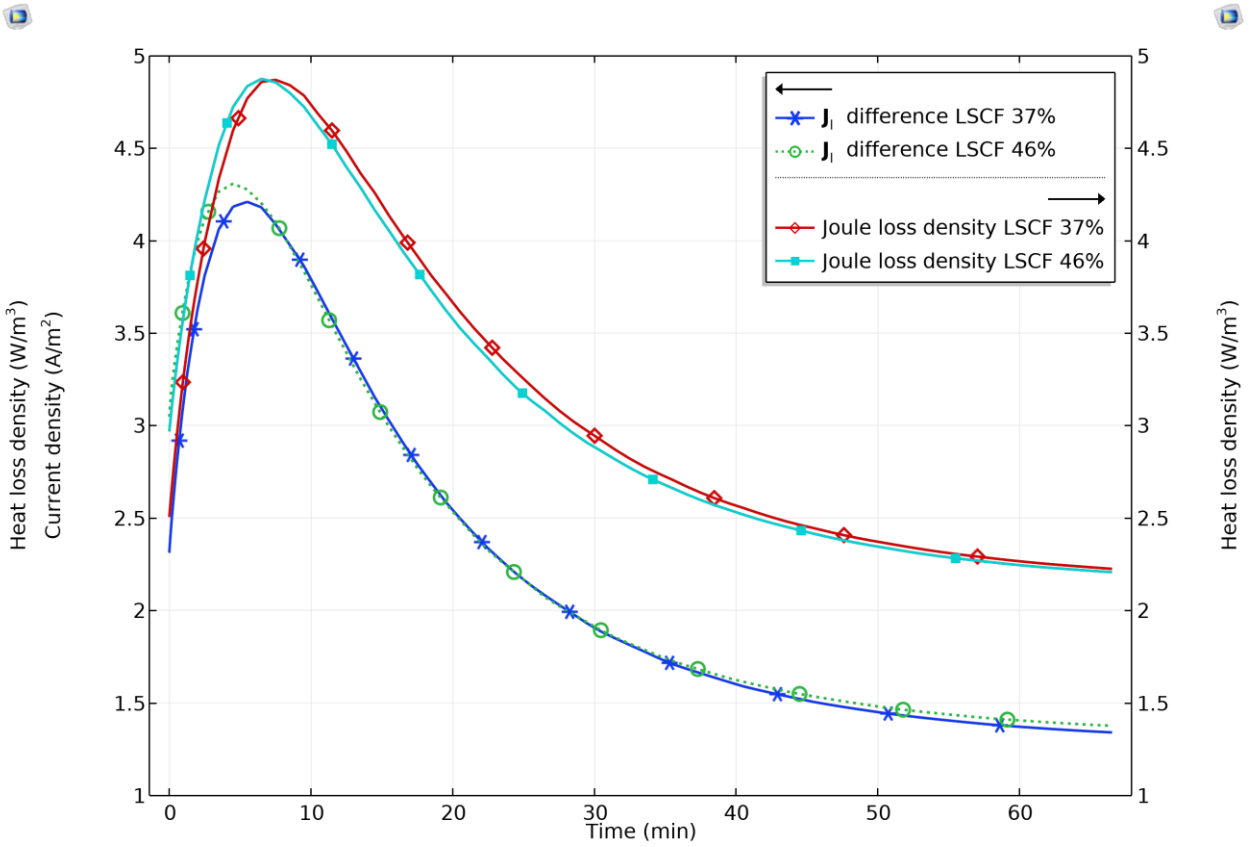
Cold start: Recombination dominance losses.





Comparison of Joule losses and current density distributions for two LSCF microstructures

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CONCLUSION

- The early dominance of Joule heating and recombination effects emphasizes the need for optimized electrical/ionic transport to reduce startup inefficiencies.

- Chemical heat loss stabilization demonstrates the system's thermochemical efficiency during steady-state operation.

- Temperature dynamics reveal effective heat transfer mechanisms crucial for rapid operational temperature achievement.

- Bridging microstructural analysis with macroscopic simulations, the model shows how microstructure impact overall efficiency. And the coupled analysis of fluid dynamics, heat transfer, and electrochemical reactions provided actionable insights for optimizing flow distribution and minimizing parasitic losses.

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