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A 3D Electrochemical-Thermal Coupled Model for Pouch-Type Lithium-ion Batteries with Counter-Tab Configuration

Supplementary information

Mesh independence analysis

A mesh independence analysis was conducted for both the sub-cell and the cell domains to ensure sufficient element resolution for accurate results. For the sub-cell domain, terminal voltage at the end of a constant current (CC) discharge at 2C-rate – from 80% to 20% State of Charge (SOC) window – was used as a control variable. For the cell effective domain, the maximum cell temperature (T_{\max}) served as the control metric. For the sub-cell, 1,444 quadrilateral elements were employed, with a distribution ratio of 3 between the positive and negative electrodes to enhance resolution for Li-ion diffusion. In the effective cell domain, 5,584 tetrahedral and triangular elements were utilized to solve the energy conservation equation. The mesh independence analyses are summarized in Table A1, the final mesh configurations are illustrated in Fig. A1.

Table A1. Mesh independence analyses: sub-cell and cell domains.

Sub-cell	V_{term} (V)	3.1648	3.1428	3.1945	3.1854	3.1862
	N of elements	684	924	1,204	1,444	1,684
Cell	T_{\max} (°C)	42.5598	42.3857	42.3602	42.3593	42.3588
	N of elements	378	553	2,127	5,584	37,895

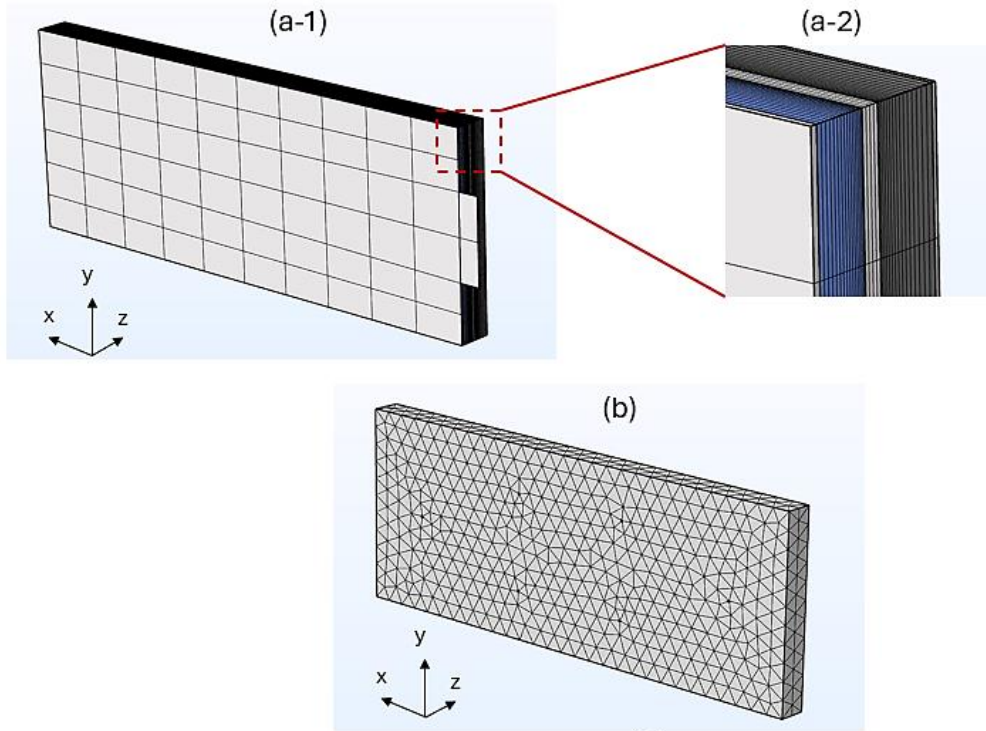


Fig. A1. Meshes for the numerical domains in the 3D electrochemical-thermal coupled model. (a-1) Mesh for the sub-cell domain in the electrochemical model. (a-2) Detail of the distribution ratio of electrode layers within sub-cell thickness for the electrochemical model. (b) Mesh for the cell effective domain in the thermal model.

Variations in cell thermal performance with the electrode particle radius

The particle radius of the electrode material, which defines the specific surface area (Equation (11) in Table 1), impacts both mass conservation in the solid phase and charge conservation in solid and liquid phases. Larger particle radii reduce specific area, leading to higher polarization voltage and thus greater polarization heat generation – the dominant form of irreversible heat generation compared to ohmic losses²⁴. Fig. A2 illustrates that changes in particle radius primarily affect the magnitude of the volumetric heat generation rate (Q_{gen}) rather than its temporal evolution, with comparable effects for the cathode (r_p^+) and anode (r_p^-) electrodes. In turn, these increments in Q_{gen} imply higher cell maximum temperature (T_{max}) and maximum spatial temperature gradients (ΔT_{max}) with higher particle radii.

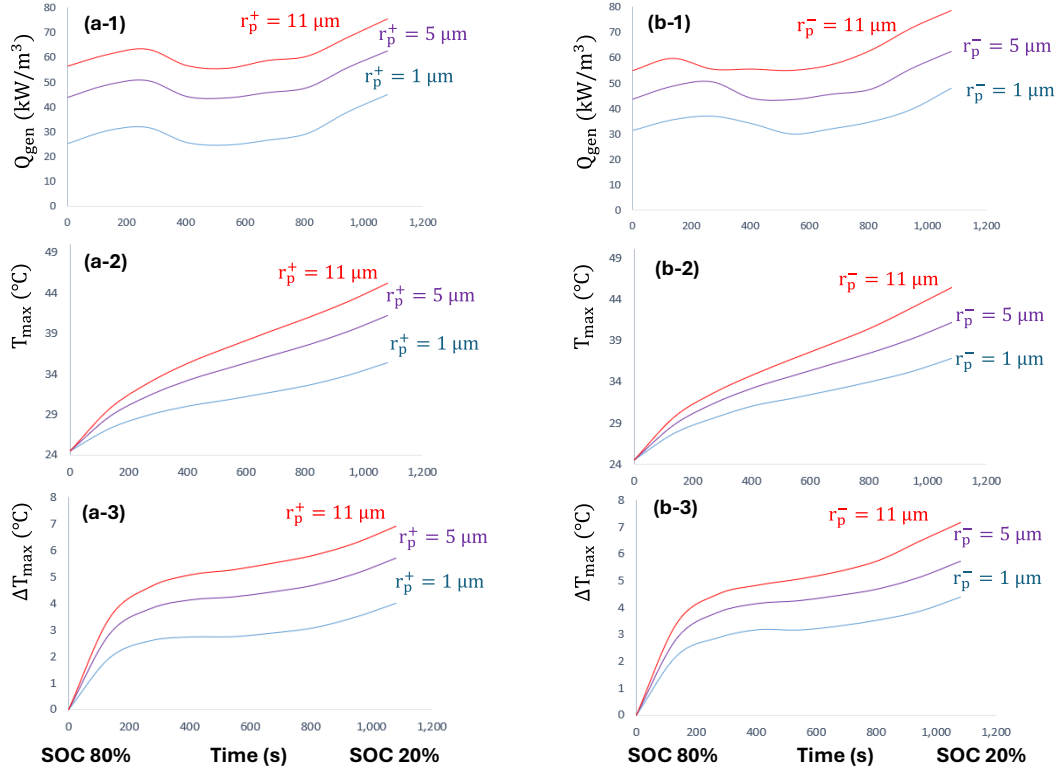


Fig. A2. Sensitivity analysis of cell thermal performance with respect to changes in the electrode particle radii, examining their impact on the cell volumetric heat generation rate (Q_{gen}), maximum temperature (T_{max}), and maximum spatial temperature gradient (ΔT_{max}). Effects of variations in the positive electrode particle radius (r_p^+) are presented in (a-1) Q_{gen} ; (a-2) T_{max} ; and (a-3) ΔT_{max} , and in the negative electrode particle radius (r_p^-) are presented in (b-1) Q_{gen} ; (b-2) T_{max} ; and (b-3) ΔT_{max} .

P2D electrochemical model applied to a 3D sub-cell based on COMSOL's interface "Lithium-ion Battery"

Current initialization: Steady State Step.

Convergence criteria: Backward difference formula BDF.

$$\text{error} < \text{RelTol} \cdot |u| + \text{AbsTol}$$

BDF: Temporal method for Discharge. Each time step, an algebraic system is generated and solved through a Direct Method Pardiso (Newton-based).