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THERMO-ELECTROCHEMISTRY-SWELLING-FLOW ANALYSIS OF BATTERY CELLS: AN INTERDISCIPLINARY MULTI-SCALE CHALLENGE

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As multiple industries are urged to address environmental and climate issues, the interest in electrification and energy storage is nowadays exponentially increasing, fostering the development of an interdisciplinary ecosystem spanning from material science to assemblies and systems engineering. Battery cell engineering constitutes a cardinal ingredient in the ongoing transformation. In such context, the trade-off between safety, costs and performance constantly challenges engineers. The full 3D digitalization of battery cells becomes therefore an enabler for reduced design times and continuous improvements.

For instance, in the analysis of the electrochemical performance of battery cells, the full 3D digitalization helps engineers to understand and control the effects of charging-discharging cycles, while limiting time-consuming experimental tests. In addition to the coupling across multiple physics, a thermo-electrochemistry modelling strategy also embodies a multi-scale coupling. Based on the porous electrode theory introduced in [1-2], 3D detailed variables such as temperature, electric potentials in solid phase and electrolyte, ionic concentration in electrolyte, swelling mechanism and electrolyte flow are strongly coupled within a full 3D homogenised multi-material macro-scale level, along with being function of molecule concentration (e.g. lithium's) in the solid phase within a 1D-FE2 particle micro-scale level.

As described in Allu et al. [3], multiple coupling strategies are possible. In the order of increasing accuracy, we identify the 1-way electrochemistry-to-thermomechanics coupling, 2-way concurrent explicit coupling, 2-way concurrent iterative coupling and monolithic coupling. With the present works, the Authors propose a thermo-electrochemistry-swelling-flow "pseudo-4D" multi-scale procedure, implemented in the finite element analysis software Abaqus. Simulation results are compared to experimental tests for validation.

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