11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

PRELIMINARY NUMERICAL ANALYSIS RELEVANT TO AN ELECTRONEUTRAL COMPUTATIONAL HOMOGENIZATION FORMULATION FOR LI-ION BATTERY CELLS.

Grazioli D.[1], Salvadori A.[2] and Bower A.[3]

[1] DICATAM, University of Brescia, via Branze 43, 25123, Italy, davide.grazioli@ing.unibs.it
[2] Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands, a.salvadori@tue.nl
DICATAM, University of Brescia, via Branze 43, 25123, Italy, alberto.salvadori@ing.unibs.it
[3] School of Engineering, Brown University, Providence, RI 02912, USA, allan_bower@brown.edu

Key words: *Computational Homogenization, Multi-scale processes, Multi-physics processes, Li-ion batteries, numerical simulations.*

In recent contributions the Computational Homogenization technique [1] was tailored to model the multi-physics processes that take place in Li-ion batteries. The formulation originally proposed in [2] was recently extended to take into account electroneutrality, quasi-static Maxwells equations, time dependent scale transitions and scale separation in time. Inspired by [3], in the present note some preliminary numerical analysis, accompanied by constitutive assumptions at the microscale, are shown.

The microscale complex formulation (with seven separate fields involved) has been broken down in simpler subproblems towards a full two-scale implementation. Among the considered subproblems, the *ionic conductivity of the organic electrolyte in Li-ion batteries* and the *one-dimensional intercalation in a single active particle* are dealt with.

The former has been modeled by several authors, mainly stemming from the porous electrode theory [4]. Under electro-neutrality conditions this complex system of equations can be reduced to simple diffusion equations with modified diffusion coefficient, using electroneutrality in place of Gauss's law. The problem is here dealt with following the extended microscale modeling of [2].

In the one-dimensional intercalation of Lithium in a single active particle balance [5] equations are limited to mass and force. Coupling between stress evolution and diffusion of neutral Lithium into the particles is therefore considered, whilst the influence of migration in the intercalation influx into the particle is here neglected. This assumption is actually

crude although widely used in the literature in order to focus on the mechanical effects of intercalation in a single particle without modeling a whole cell.

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