Effect of Intercalation Diffusivity When Simulating Mixed Electrode Materials in Li-Ion Batteries

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Introduction: Physics based models is a strong tool when studying lithium ion batteries. A drawback is the difficulty in estimating and measuring the needed parameters. This contribution investigates the effect of large differences in the solid diffusion coefficients when simulating mixed electrode materials.

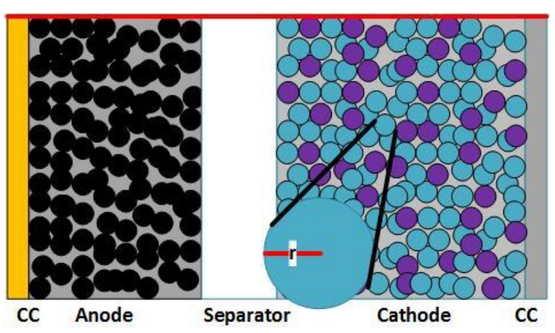

Figure 1. Battery cell schematics. Red lines indicate simulated structure.

Case	$D_{LMO}(m^2/s)$	$D_{NMC}(m^2/s)$	$D_G(m^2/s)$
1	1e-13	1e-13	1e-13
2	1e-13	1e-15	1e-13
3	1e-15	1e-13	1e-13
4	According to [1] from 1.5e-14 to 9e-16	According to [2] from 4e-14 to 3e-16	1e-13

Table 1. Description of the different cases.

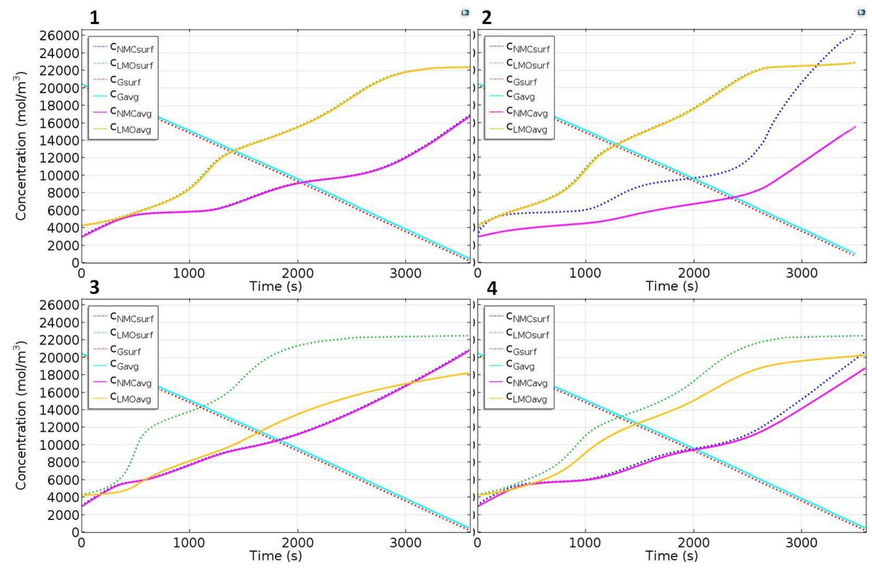

Figure 4. Lithium concentration in the materials during constant discharge with 1C current.

Model: The battery cell is modeled in 1D in the COMSOL lithium ion battery node. The lithium concentration in the active particles are solved in an additional 1D pseudo dimension. The simulated structures are indicated by the red lines in fig. 1.

- Anode - Graphite on copper
- Cathode - 50/50 NMC/LMO on alumina

Results: The influence of two different time constants is more prominent when the material with a steep potential curve has faster time constant. Fig. 2. shows the charge pulse response for four simulated cases, see table 1.

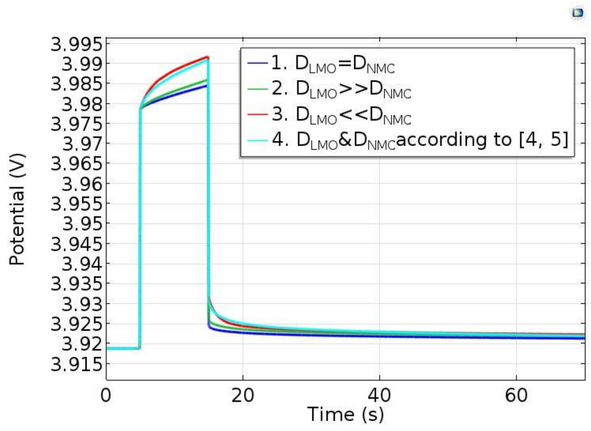

Figure 2. 1C 10 s charge pulse response at 50 % SOC.

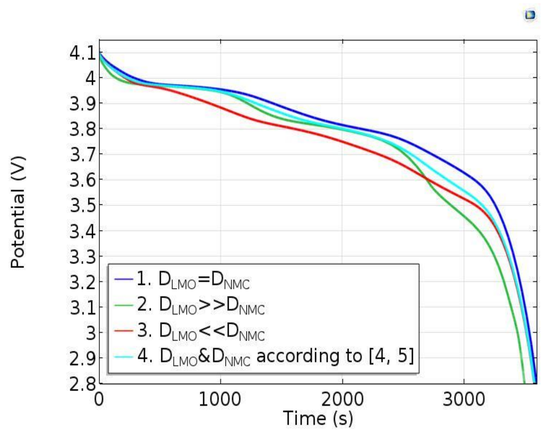

Figure 3. 1C constant discharge potential cures.

The slow diffusion coefficient results in a concentration buildup on the surface of the active particles, see fig. 4. This causes a higher voltage drop and results in a lower capacity for case 2 and 3.

Conclusions: When simulating mixed electrode materials extra care need to be addressed to the different materials diffusion coefficients.
The diffusion coefficients concentration dependence should not be neglected for LMO and NMC mixtures.

References:

1.P. C. Goonetilleke et al., Effects of Surface-Film Formation on the Electrochemical Characteristics of LiMn2O4 Cathodes of Lithium Ion Batteries, Journal of the Electrochemical Society, 156, A709-A719, (2009)
2.Shao-Ling Wu et al., High Rate Capability of Li(Ni1/3Mn1/3Co1/3)O2 Electrode for Li-Ion Batteries, Journal of the Electrochemical Society, 159 , A438-A444, (2012)