

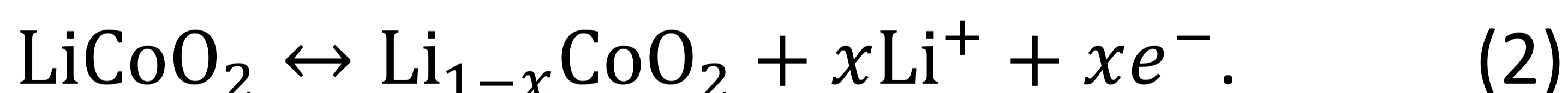
Two-dimensional Simulation of All-solid-state Lithium-ion Batteries

L. Tong

Keisoku Engineering System Co., Ltd., Chiyoda-ku, Tokyo, Japan

Introduction: There is great interest in developing all-solid-state lithium-ion batteries. They are ideal micro-power sources for many applications in portable electronic devices, electric vehicles and biomedical engineering. In this work, we present a simulation research based on a two-dimensional model of all-solid-state lithium-ion batteries using COMSOL Multiphysics®. The calculation of current density and the transport of lithium species are coupled. The charge/discharge curves (cell voltage vs. time) for various charge/discharge rates are obtained and analyzed.

Computational Methods: The simulations for the charge/discharge processes of an all-solid-state lithium-ion battery are carried out, in which the negative electrode comprises metallic lithium and the positive electrode is constructed by the polycrystalline film of LiCoO_2 . The electrolyte is a solid-state Li_3PO_4 film. The electrochemical reactions at the negative and positive electrodes can be represented by



The chemical reaction in the electrolyte is $\text{Li}^0 \leftrightarrow \text{Li}^+ + e^-$. The transport of Li^+ and e^- is solved by the Nernst-Planck equation. The transport of lithium species in the positive electrode is described by the Fick's law. In calculations, the negative electrode domain is not involved. The calculation of current density taken in the electrolyte is coupled with the solution of the transport of lithium species in the positive electrode.

Results: Calculations are performed for the charge/discharge processes of the all-solid-state lithium-ion battery, in which the battery is charged up to 4.2 V and then the discharge is terminated by 3.3 V. The charge/discharge rates are 0.8, 1.2, 1.6, 2.4, and 3.2 C.

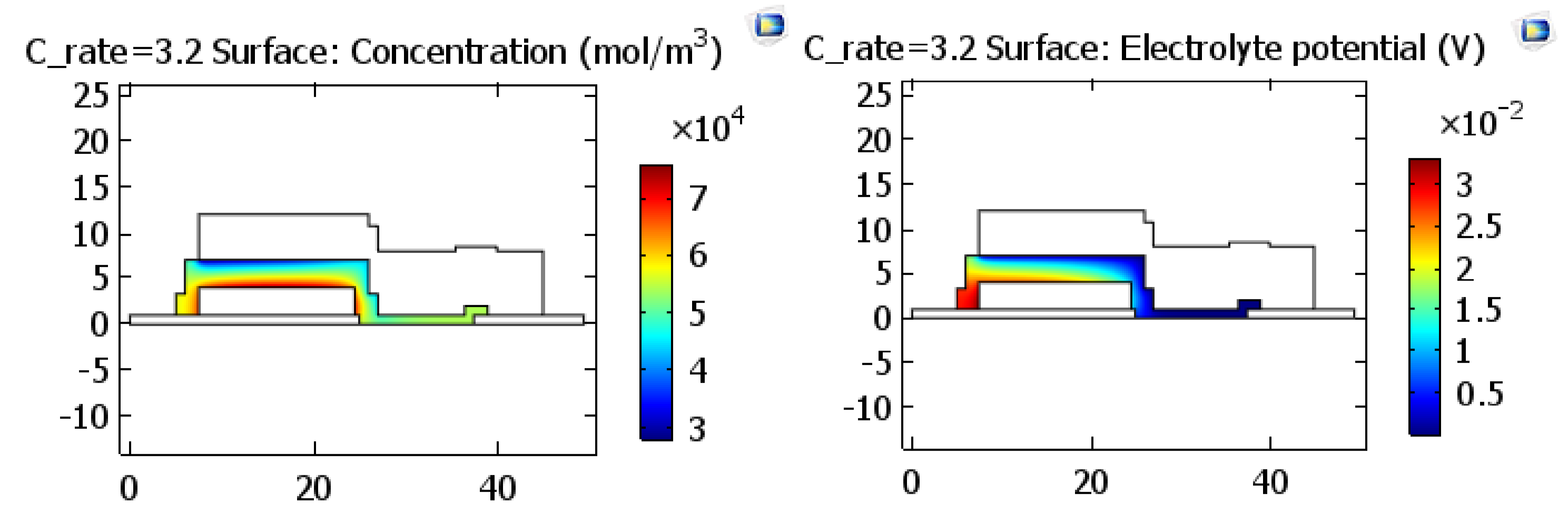


Figure 1. Concentration of lithium ion and potential in the electrolyte at the end of charge

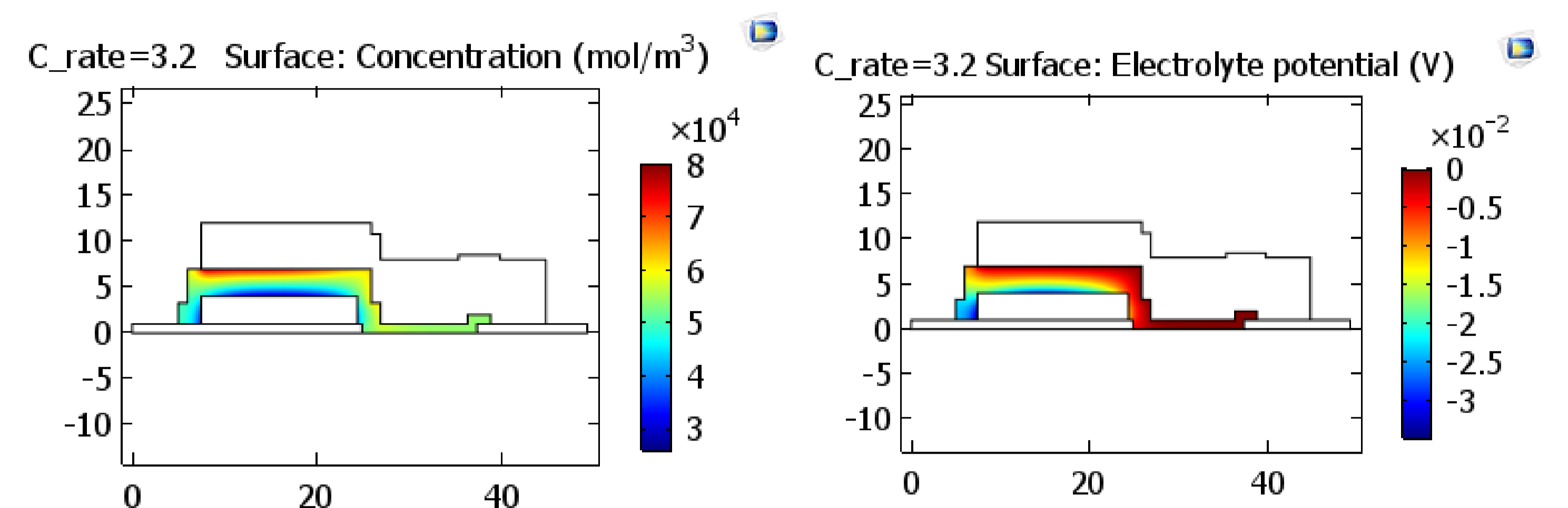


Figure 2. Concentration of lithium ion and potential in the electrolyte at the end of discharge

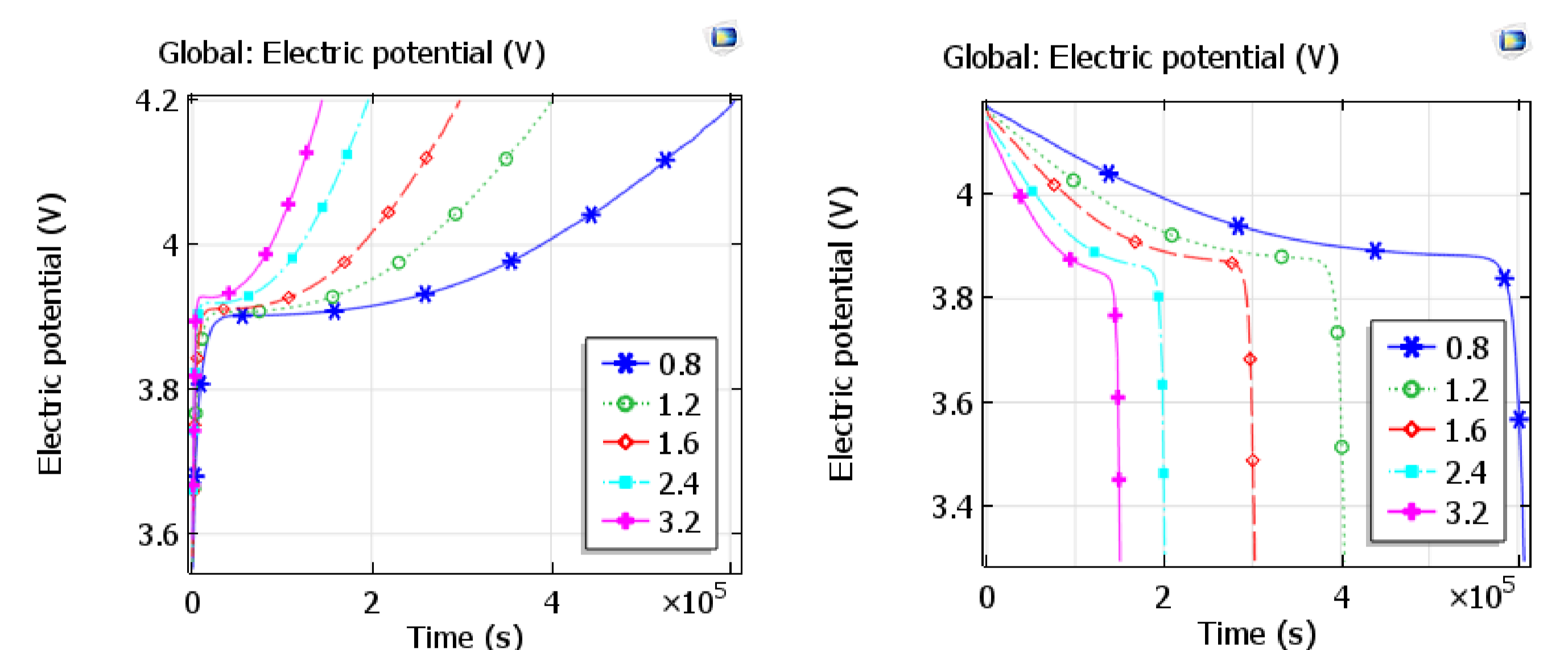


Figure 3. Charge/discharge curves (cell voltage vs. time) for various charge/discharge rates

Conclusions: Results show the charge/discharge characteristics of an all-solid-state lithium-ion battery. The cell voltage by charge has a steep rise until about 3.9 V and then spreads around corresponding to the different charge rates. For discharge, the cell voltage before depletion is shifted downwards for higher discharge rates.

References:

1. N. J. Dudney, *Mater. Sci. Eng. B* **116**, 245-249 (2005)
2. A. Patil, et al., *Mater. Res. Bull.* **43**, 1913-1942 (2008)
3. D. Danilov, et al., *J. Electrochem. Soc.* **158** (3), A215-A222 (2011)
4. J. B. Bates, et al., *Solid State Ion.* **135**, 33-45 (2000)