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CFD Analysis of Multi-Phase Reacting Transport Phenomena in Discharge Process of Non-Aqueous Lithium-Air Battery

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Abstract : A computational fluid dynamics (CFD) model is developed for rechargeable non-aqueous electrolyte lithium-air batteries with a partial opening for oxygen supply to the cathode. Multi-phase transport phenomena occurred in the battery are considered, including dissolved lithium ions and oxygen gas in the liquid electrolyte, solid-phase electron transfer in the porous functional materials and liquid-phase charge transport in the electrolyte. These transport processes are coupled with the electrochemical reactions at the active surfaces, and effects of discharge reaction-generated solid Li2O2 on the transport properties and the electrochemical reaction rate are evaluated and implemented in the model. The predicted results are discussed and analyzed in terms of the spatial and transient distribution of various parameters, such as local oxygen concentration, reaction rate, variable solid Li2O2 volume fraction and porosity, as well as the effective diffusion coefficients. It is found that the effect of the solid Li2O2 product deposited at the solid active surfaces is significant on the transport phenomena and the overall battery performance.

Keywords : Computational Fluid Dynamics (CFD), modeling, multi-phase, transport phenomena, lithium-air battery
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