Impedance Simulation of A Lithium-ion Battery-Validity of Solid Phase Diffusion Coefficient Estimation

Qingzhi Guo, Venkat R. Subramanian, J. W. Weidner and R. E. White
Center for Electrochemical Engineering
University of South Carolina, Columbia, SC 29208

Introduction

The transport process in lithium-ion batteries has been attracting more and more attention. Two different perspectives are commonly used: the equivalent-circuit model and the macroscopic model. Due to the difficulty of the former model in correlating the equivalent-circuit parameters to the fundamental properties of a real battery, the macroscopic modeling has played an inspiring role in previous impedance simulations. Doyle *et al* [1] used a macroscopic model for the first time to simulate the impedance of a full lithium rechargeable battery, which consists of one porous electrode, with the application of the concentrated electrolyte theory to the solution phase. The possibilities of estimating many important parameters from full battery impedance response were also discussed. Meyers *et al* [2] are the first ones to derive an analytical expression for the impedance response of a full lithium rechargeable battery with the application of the macroscopic porous electrode theory. But, for the real characteristics of a lithium battery, concentrated electrolyte theory cannot be ignored.

Doyle *et al* simulated the impedance response of a $Li|PEO_{18}LiCFSO_3|LiTiSO_2$ cell. They concluded that only when the actual value is less than the order of 10^{-13} cm^2/s, one could get a reliable estimate of solid phase diffusion coefficient. However, they did not study the effect of other parameters on the reliability of estimation of D_s.

In this communication we have two objectives: first, we have extended Newman's macroscopic modeling for impedance simulations to a lithium-ion battery consisting of two porous electrodes, carbon and $Li_yMn_2O_4$ and we have classified the parameters as globally specific and locally specific. Second, we have studied the effect of parameters, such as the porosity, thickness, solid phase conductivity and specific surface area of the porous electrode, on the reliability of the estimation of solid phase diffusion coefficient. In our simulation we have used Maple for our numerical calculations [3]. We solve twenty equations with ten interior node points specified for each of the three regions in a lithium-ion battery.

Results and Discussion

1.Classification of parameters on the impedance response of the full-cell
2. Estimation of Solid Phase Diffusion Coefficient Using The Modified Warburg Method

Conclusion

The impedance responses of a lithium-ion electrode with two porous electrodes are simulated in this paper for the first time. Based on the simulation, the parameters are classified as globally specific and locally specific. And, the effects of these parameters are studied.

The estimation of solid phase diffusion coefficient from the impedance response of a T-cell consisting of only one porous electrode by the modified Warburg method is discussed. And, the validity of the modified Warburg method is analyzed. Effect of different parameters on the reliability of diffusion coefficient measurement is analyzed. Preparation of porous electrodes by using thinner porous electrode and small specific surface area is recommended. Ranges for the specific surface area "a" and electrode thickness δ for reliable estimation of D_s are provided.

References

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Fig. 8. The Error of Estimation with Different Values of Specific Surface Area