

# Development of a Step-by-Step Estimation Approach for Battery Simulation Based on Experimental Data

Compare step-by-step parameter estimation modeling approach with general estimation approach results on the point of time efficiency and accuracy view for Li-ion battery.

D. Shin, J. Lee

CAE Solution Team, ALTSOFT Inc., Seoul, Republic of Korea

## Introduction

For modeling battery simulation, material properties and simulation parameters such as electrical conductivity, diffusion coefficient, exchange current density and electrode particle radius are required. Since obtaining these information by measurement is limited, it is necessary to estimate appropriate simulation parameters based on experimental data. However, it is difficult to estimate all parameters at once due to many numbers of variables to estimate.

In this work, we studied a step-by-step parameter estimation modeling approach by using the Battery Design Module and Optimization Module of COMSOL Multiphysics®. Common parameters between “Newman Model” and “Single Particle Model” were estimated first and remaining parameters were estimated through the “Newman Model”. The results of in this step-by-step approach were compared with general estimation approach results on the point of time efficiency and accuracy view.

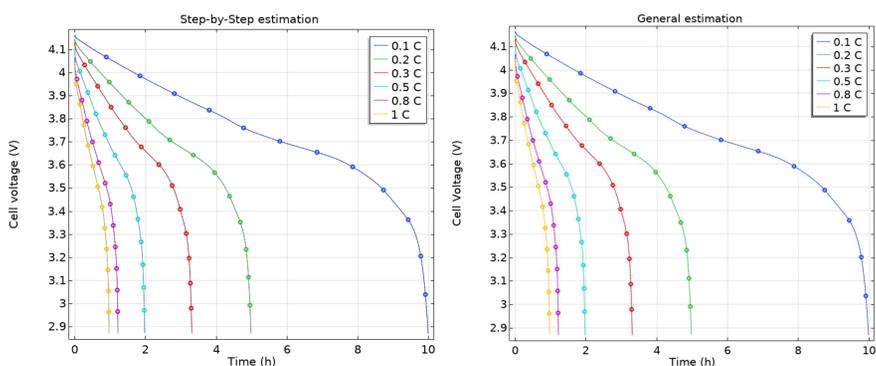


Figure 1. Parameter estimation results. Step-by-step approach (Left) and General estimation approach (Right)

## Methodology

For battery simulation, “Lithium-Ion Battery” and “Single Particle Model” interface in Battery Design Module are used. Experimental data uses low C-rate data; 0.1C, 0.2C, 0.3C, 0.5C, 0.8C, and 1.0C. The material of each electrode is graphite (Negative) and NMC (Positive). The parameters to be estimated are electrical conductivity, diffusion coefficient, exchange current density, and electrode particle radius. In general estimation approach, all parameters are estimated in one step. However, in step-by-step approach, the parameters are estimated separately; Exchange current density and particle radius are estimated by using “Single Particle Model”, and the others are estimated by using “Lithium-Ion Battery”. BOBYQA solver is used as the optimization solver. Relative tolerance of optimization solver is 0.005.

## Results & Conclusion

At Figure 1, both approaches are matched well with the experimental data. Also, Table 1 shows the standard deviation of the two approaches compared to experimental data are small. Therefore, it is confirmed that both approaches are close to the experimental data. On the other hand, for computation time, Step-by-Step estimation takes about 40% of the time compared to the general estimation.

In this simulation, test are conducted with 10 parameters, but in actual problem, it is necessary to simulate more parameters such as temperature dependence and volume fraction. In this case, Step-by-Step approach can be considered as an alternative to obtain faster while maintaining the accuracy of parameter estimation.

	Step-by-Step Estimation	General Estimation
Computation time	About 2h (5min / 1h 50min)	About 5h
Standard deviation compared to experimental data	9.65e-4	6.32e-4

Table 1. Simulation time & Standard deviation comparison between Step-by-Step and general approach.

## REFERENCES

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