Simulation of the Temperature Dependence of Li-Ion Cell Performance

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The charge and discharge performance of lithium-ion cells can be simulated using first-principles' models with good fidelity to experimental results [1-3]. However, these simulations have not accounted for behavior over a wide range of temperatures. Typical lithium-ion cells are expected to perform from –30°C to +60°C. In order to simulate cell performance over a wide temperature range, the temperature dependence of a number of parameters (diffusion coefficients, rate constants, electrolyte conductivity) must be accounted for.

The temperature dependence of many physical and kinetic parameters can usually be well represented by an Arrhenius equation. For example, the temperature dependence of a rate constant, *k*, can be expressed

$$k = k_o \exp\left[\frac{-E_a}{RT}\right] \qquad (1)$$

In order to account for temperature-dependent behavior, the parameters listed in Table 1 were expressed in Arrhenius form. The Arrhenius constants were obtained by fitting to experimental discharge and charge curves.

Table 1 Arrhenius Constants for Temperature-Dependent Parameters

	k_o		E_a, kJ/mol
Parameter	Units	Value	
Pos. rate constant	A/m^2	7.73e+34	180.0
Neg. rate constant	A/m^2	1.65e+18	105.0
Pos. SEI	$1/ohm\text{-}m^2$	243.9024	1.0
Neg. SEI	$1/ohm\text{-}m^2$	3.311	1.0
Pos. Diff. Coeff.	m^2/s	2.282e-07	41.295
Neg. Diff. Coeff.	m^2/s	3.676e-06	45.740
Elyte Cond.	S/m	1878.313	23.000
Salt Diff Coeff.	m^2/s	1.0889e-08	2.76632

Experimental discharge and charge curves for 2.1 Ah 18650 cells (see Table 2) were used to adjust the Arrhenius constants listed in Table 1. The data fitting was done using the regression feature of Battery Design Studio® [4]. The simulation model is similar to that presented by Newman et al. [1-2] except that solid-phase diffusion of lithium was modeled using the lumped-parameter approach of Wang et al. [5].

The simulation model was able to produce very reasonable behavior over the entire range of experimental results. Figures 1-2 compare simulation results to a series of experimental results.

Table 2 Range of Experimental Data Used to Fit Simulation Model Parameters

Temp., °C	Disch. Rate, A	Charge Rate
-30	0.42	No charging
-20	0.42-1.05	No charging
-10	0.42-1.05	No charging
0	0.42-4.2	1.68 A / 4.2 V
20	0.42-4.2	1.68 A / 4.2 V
40	0.42-4.2	1.68 A / 4.2 V
60	0.42-4.2	1.68 A / 4.2 V

Figure 1 Comparison of Simulated and Experimental Discharge/Charge Curves at 20°C.

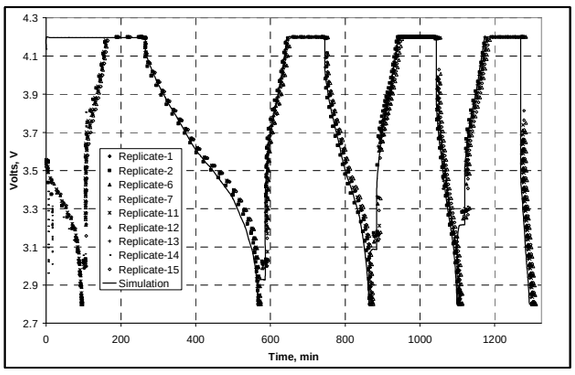
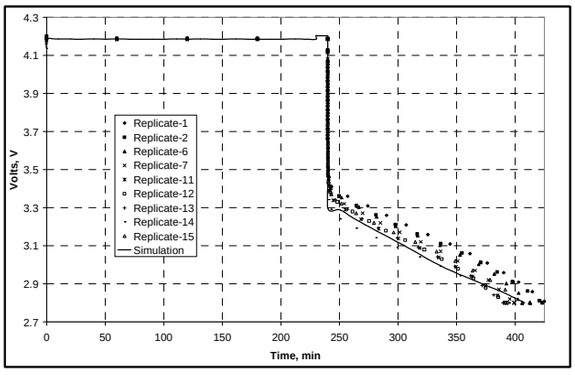


Figure 2. Comparison of Simualated and Experimental Discharge Curves at –30°C.



References:

[1] T. F. Fuller, M. Doyle, J. Newman, *J. Echem. Soc.*, Vol. 141 (1) 1 (1994).
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[4] Battery Design Studio® from Battery Design Co., www.batdesign.com
[5] C. Y. Wang, W. B. Gu, B. Y. Liaw, *J. Echem. Soc.*, Vol. 145 (10) 3407 (1998).