Developing Modeling Capability to Predict Life of Batteries

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Background and Approach

- The world-wide demand for high-power, high-energy batteries is increasing rapidly.
  - Lithium-ion batteries, for example, are being considered for automotive applications.
- The desired 15-year life capability remains a challenge.
- A goal of the Advanced Technology Development Program (now Applied Battery Research) is to develop methods of accurately predicting the life capability of lithium-ion batteries.
- Life prediction must be successfully achieved with a high level of confidence within only one or two years of accelerated aging.
  - The technique must also be applicable for electric, hybrid-electric, and plug-in hybrid electric vehicle applications.
- **Approach**:
  - Develop a statistically robust modeling methodology and tool which allows life prediction within confidence levels.

Goal and Prerequisites

- The goal of Technology Life Verification Testing (TLVT) is to verify battery life capability with high confidence and minimal testing.
  - Focus: USABC battery life of 15-year, 150,000 miles with a target confidence level of 90% within one or two years of testing.

- Prerequisites to TLVT are as follows:
  - Life-limiting wear-out mechanisms must be identified and characterized (e.g., standard USABC testing).
  - A life model (empirical or physical) that reflects typical degradation over time as a function of the identified life-limiting wear-out mechanisms.
  - Error model that accounts for both measurement error and manufacturing variability.
  - Sufficient supply of batteries, test channels, and temperature chambers for aging experiments.

Core Matrix

- Testing is based on a full factorial matrix that adequately covers identified stress factors at various acceleration rates.
  - Stress factors can include temperature, state-of-charge, energy throughout, pulse power rating, etc.
- The limiting value of the degradation mechanisms must also be identified so that the stress level is not increased to a point where a battery's failure rate is different than anticipated normal-use conditions.
- Monte Carlo simulations generate a large number of independent simulation trials using random perturbations to model parameters, measurement error, and manufacturing variability.
- Simulations are verified with actual battery testing and analysis for lack-of-fit using statistical methods that create multiple realizations of test data to assess the uncertainty of the life-on-test estimates.

Supplemental Matrix

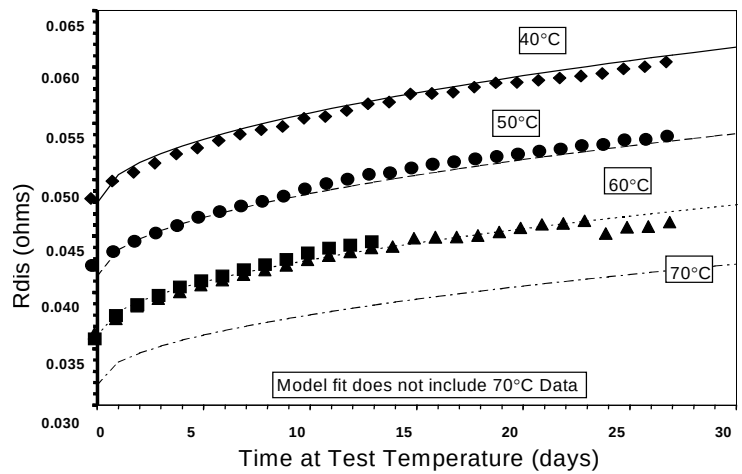
- The supplemental matrix is intended to verify various assumptions about performance degradation in the life prediction model.
  - Path dependence effects
  - Low temperature operation
  - Cold cranking

- If these assumptions are proven invalid, the model needs to be re-developed, and the core matrix simulation and testing need to be repeated.

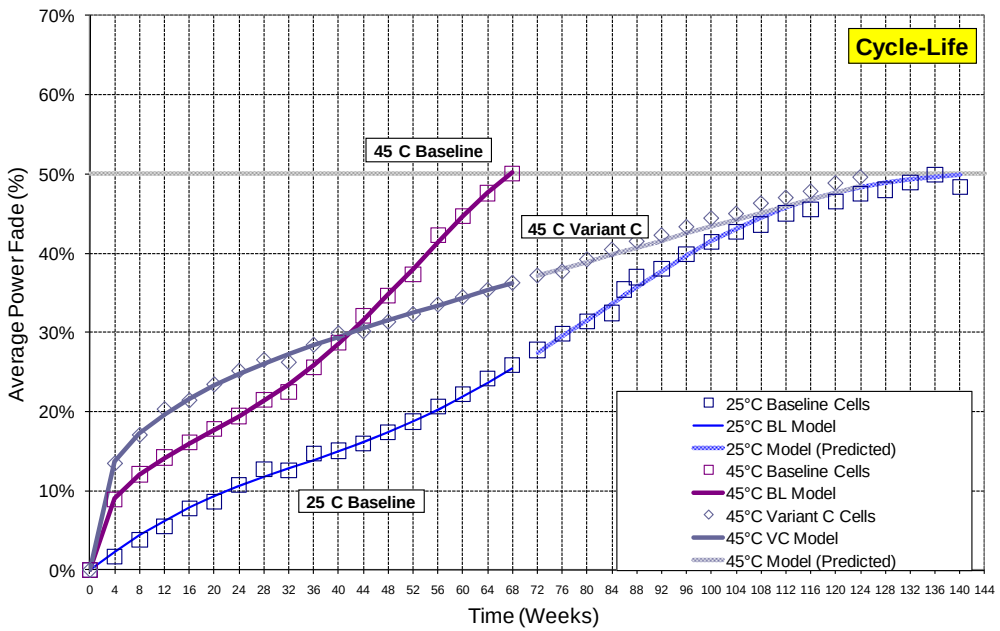
Data Analysis – Life Modeling

- Various electrochemical performance models have been developed, and can support the TLVT effort

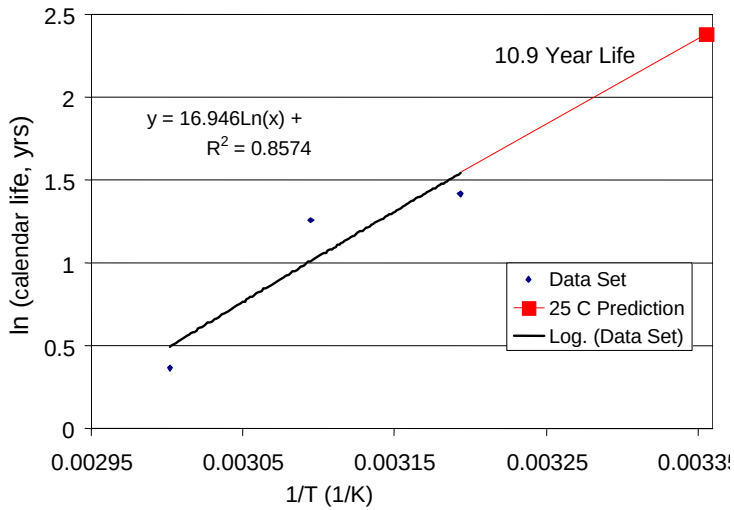
Calendar Life Discharge Resistance Data and Model Predictions for ATD Gen 1 Cells at 80% SOC



Available Power Fade at 300 Wh for the ATD Gen2 Cells



Calendar Life Model for Saft HP-12 Li-Ion Cells.



Data Analysis – Life Modeling (cont.)

- A simple life prediction model based on a single stress factor (temperature, *T*):
  - $Y(t, T) = 1 + \exp(b_0 + b_1/T)\, t^{\rho} + e$
  - where Y(t, T) is the degradation parameter (e.g., resistance) at time (*t*) and temperature (*T*)
  - ρ is the power of time ($\rho = 0.5$ for typical ATD cells)
  - b_0 and b_1 are model parameters
  - *e* is the error term

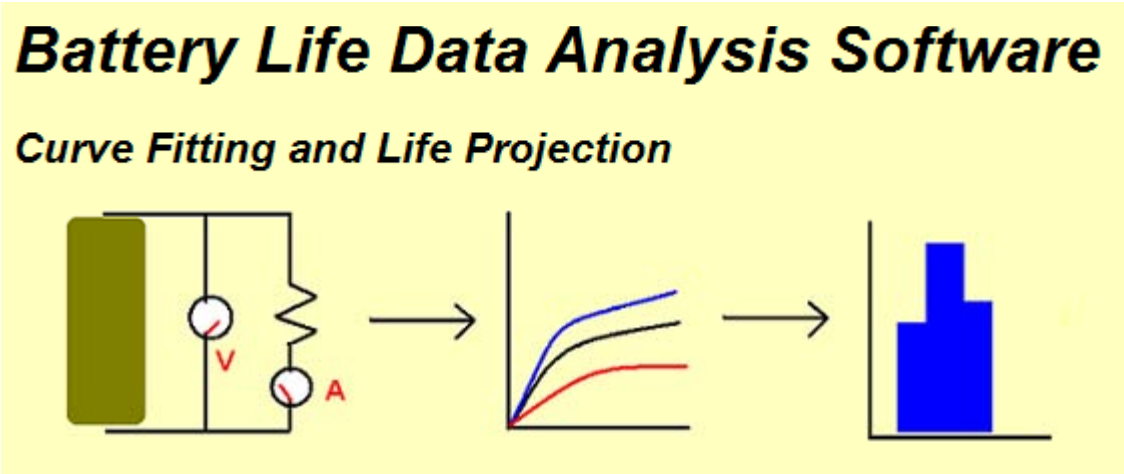
- This model can be generalized to include multiple stress factors ($X_i \ldots X_n$):
  - $Y(t, X_1, X_2, \ldots, X_n) = 1 + \exp(b_0 + b_1X_1 + b_2X_2 + \ldots + b_nX_n)t^{\rho} + e$

Data Analysis – Error Modeling

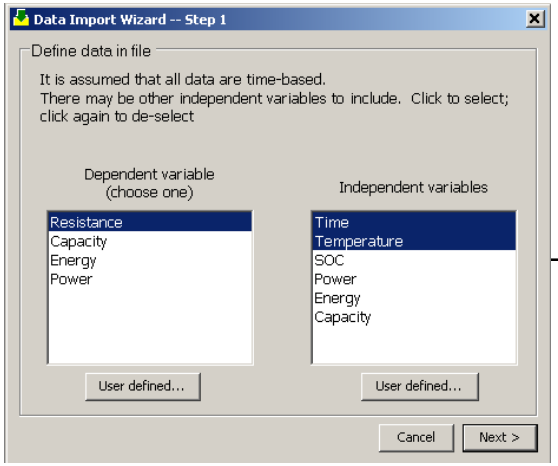
- The error model should include a combination of cell-to-cell effects (δ) and measurement error (ε):
  - $e = Var\,(Y(i, t)) = \sigma_\delta^2\,(Y_{pop}(i,t)-1)^2 + 2\,\sigma_\varepsilon^2$
  - where *Var(Y(i,t))* is the variance of *Y* at time *t* for the ith experimental condition defined by the combined levels of the stress factors
  - σ_δ^2 is the variance of the cell-to-cell effects
  - σ_ε^2 is the measurement error variance
  - Y_{pop} (i, t) is the value of *Y* at (i,t) predicted by the life model

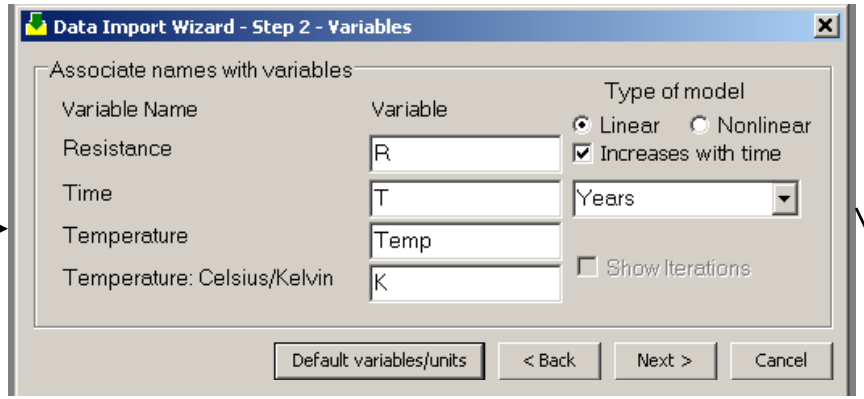
Data Analysis – Software

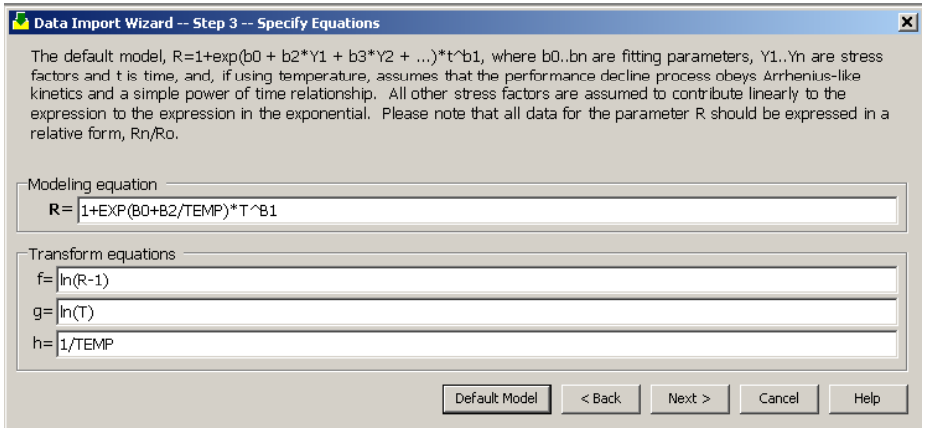
- The Battery Life Estimator (BLE) software has been developed as a user-friendly tool for analysis and simulation of battery test data.
- The software operates with the assumption that all data are time-dependent (i.e., time is a variable in the model equation).
- The simple model assuming a single stress factor has been included in the software as a default model, though other models can be input by the user as well.



Data Analysis – Software (cont.)

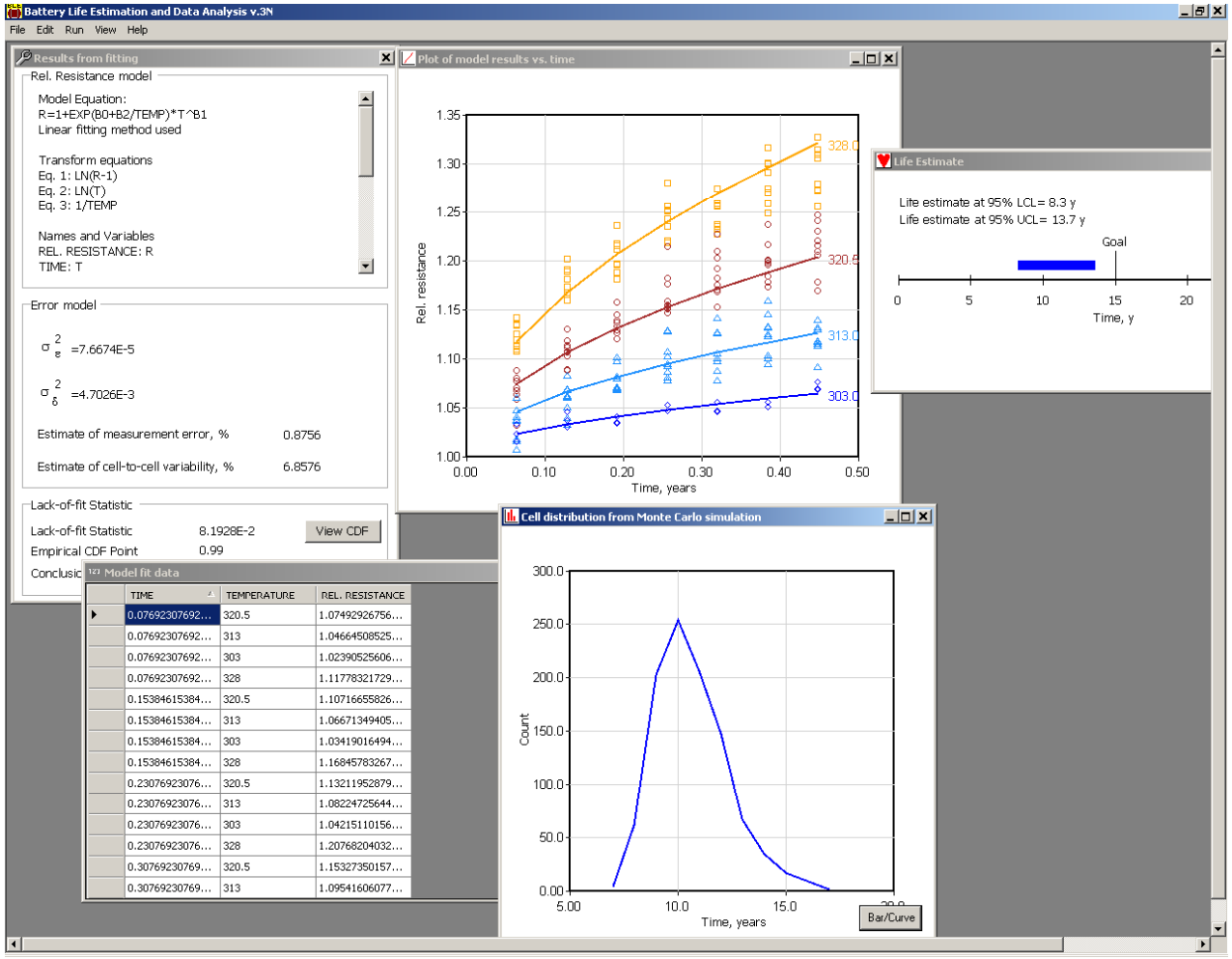






Data Analysis – Software (cont.)

- On-screen results (these can be copies to other documents for reports):



Example*

- The default model was applied to a set of cells that were calendar-life aged at various temperatures.
- The 30°C data were not used to construct the model.

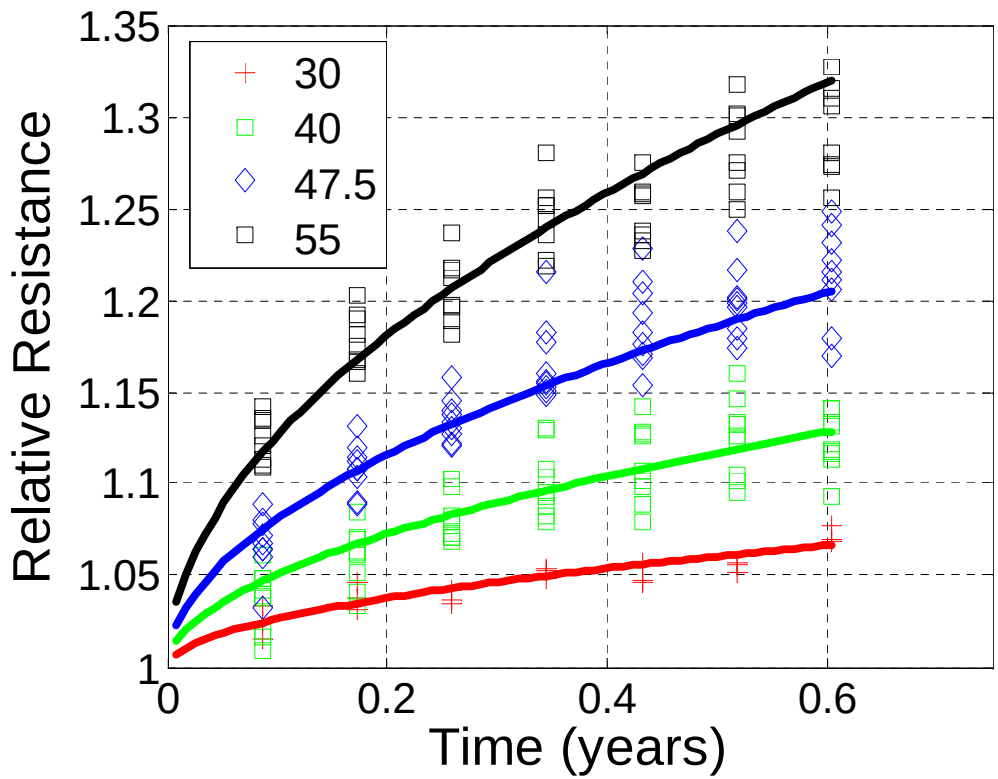
$$\hat{Y} = 1 + \exp\left\{\hat{\beta}_0 + \hat{\beta}_1 \cdot \frac{1}{T}\right\} \cdot t^{0.5}$$

$t = \text{time (years)}$

$T = \text{temperature (K)}$

$$\hat{\beta}_0 = 18.11$$

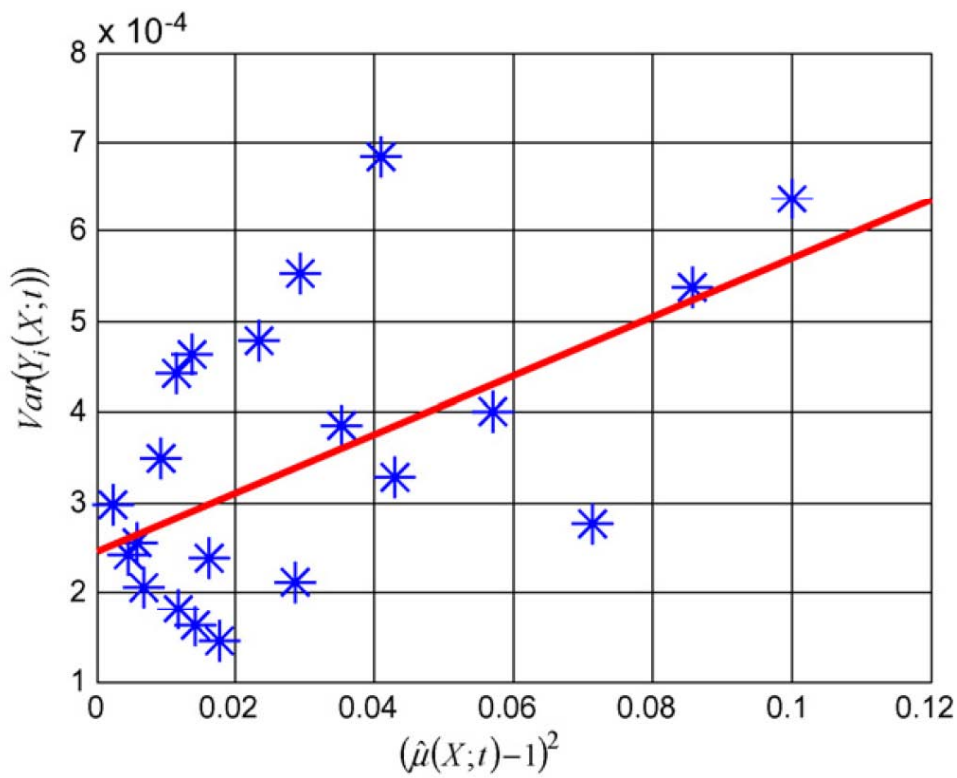
$$\hat{\beta}_1 = -6236$$



* E.V. Thomas, I. Bloom, J.P. Christophersen, V.S. Battaglia, *J. Power Sources*, 184 (2008) 312–317

Example (cont.)

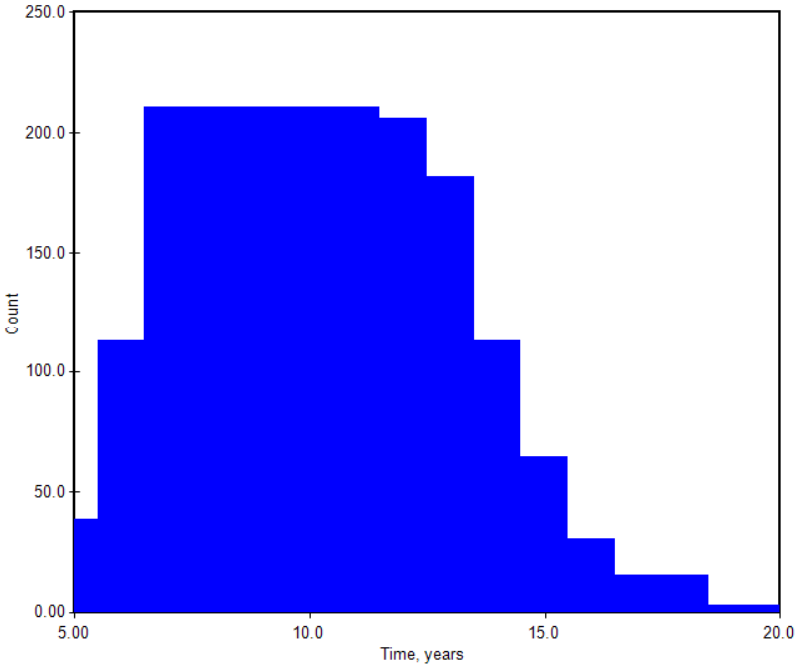
- The fitted error model shows the sample variance of observed relative resistance versus the square of the difference between the expected relative resistance and unity.
- The estimated error model parameters are given by the slope and half of the intercept of the fitted line.
  - $\hat{\sigma}_{\delta}^{2}$ = 3.2 x 10^{-3}
  - $\hat{\alpha}^{2}$ = 1.2 x 10^{-4}



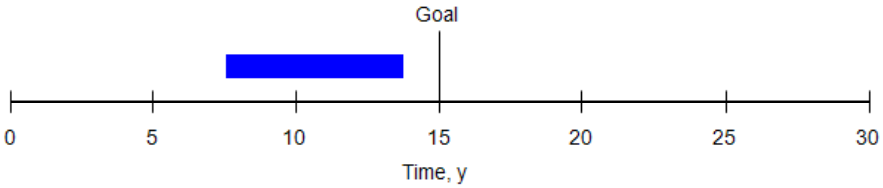
Example (cont.)

- Life estimation was completed with 1000 Monte Carlo simulations using the default models.
- These cells were projected to have a life capability between 7.6 and 13.8 years.

Monte Carlo simulations
(1000 simulations)



Life estimate at 95% LCL= 7.6 y
Life estimate at 95% UCL= 13.8 y



Summary and Future Work

- The Technology Life Verification Testing methodology was designed to predict battery life capability within a short period of accelerated aging.
- A software tool that is based on statistically robust methods of curve fitting and life simulations has been developed.
- The software tool is commercially available on the Argonne Software Shop website.

- **Future Work**:
  - Expand the library of models to the software tool
  - Incorporate comments and suggestions from software users.