NASA SBIR/STTR Technologies

Z1.01-9821 - Thermodynamically Consistent Electrochemical Models for Accelerating Development and Qualification of Power Generation and Storage Systems

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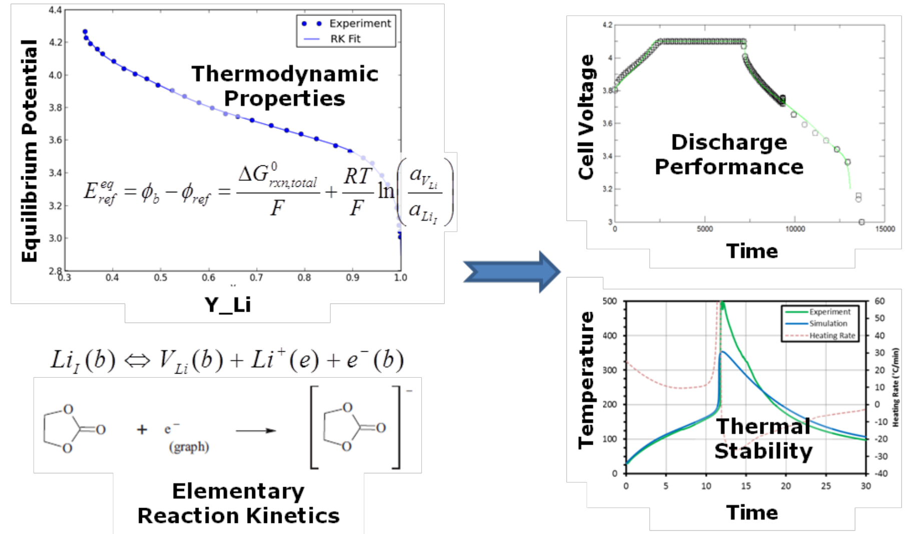
Identification and Significance of Innovation

NASA's unique missions, with extreme conditions and difficulty in replacing power system components require significant specific power improvements in conjunction with long life and performance at extremely high or low temperatures. For electrochemical systems, particularly batteries, many of these advancements are based on improvements to the active materials. Rapid evaluation and qualification of new materials remains an unresolved challenge. Qualification and acceptance of emerging materials, as well as development of new technologies, can be accelerated by the utilization of electrochemical models with a strong physical and chemical basis. Predictive models, incorporating the thermodynamics and electrochemistry that dictates device performance and degradation, are needed to accelerate development and insertion of these systems.

Estimated TRL at beginning and end of contract: (Begin: 2 End: 3)



Technical Objectives and Work Plan

The overall objective of this Phase I effort is to demonstrate the feasibility of improving thermodynamic and kinetic models of electrode and electrolyte materials in electrochemical systems to reduce the level of empiricism in performance simulations. Specific objectives are:

?Demonstrate an improved representation of battery anode and cathode material thermodynamics that better reflects the chemical changes occurring during intercalation;

?Demonstrate, consistent usage of thermodynamic and kinetic data in detailed mechanistic models of electrochemical processes and verify the model predictions against published data;

?Demonstrate application of the developed models, and the path forward to addressing additional performance and safety-limiting effects, to address important side processes including SEI growth during lithium-ion battery cycling and decomposition leading to thermal runaway.

To meet these objectives, the team will:

1.Develop improved thermodynamic representations of key battery materials;

2.Link a thermodynamic and electrochemical kinetics software library with battery cell models;

3.Verify the developed models by simulation of experimental characterization studies; and

4.Demonstrate the extension to predict rates and products of additional

NASA Applications

The developed models and software will directly benefit NASA electrochemical power generation and energy storage development teams. Sample applications include accelerating development by predicting the rates of both desirable and undesirable reactions for a given material system without extensive calibration; and accelerating transition of new materials from the laboratory to program-specific hardware by enabling confident estimation of performance under baseline and extreme conditions.

Non-NASA Applications

The developers of batteries for satellite applications will benefit from these models, due to demands for high specific energy and long cycle life. The commercial and government entities developing automotive batteries and fuel cells, and electrochemical grid-scale storage devices, will be able to leverage this technology for faster development and increased confidence in life projections.

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NON-PROPRIETARY DATA