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Mechanical and Aerospace Engineering Department  
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Theoretical and Numerical Analysis of Thermal Runaway Propagation in Li-Ion Battery Packs.

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Abstract

Thermal runaway in Li-ion cells is a well-known and widely researched phenomenon that directly impacts the safety, reliability and performance of electrochemical energy storage and conversion devices. Onset of thermal runaway occurs when overheating of the cell results in initiation of exothermic reactions, leading to even greater heat generation. This Ph.D. dissertation contributes towards studying thermal runaway propagation in Li-ion battery packs at multiple scales and highlights important preventive measures through experimentally validated numerical simulations. In the first part of this work, thermal runaway fire propagation in large scale Li-ion storage facility is studied. Effective mitigation techniques and standards to prevent and mitigate battery fire in different scenarios are developed. In the second part, a comprehensive theoretical approach based on Tank-in-series model to analyze thermal response of a Li-ion cell to overcharge is studied. In the third part, multi-mode heat transfer simulations of the onset and propagation of thermal runaway in a pack of cylindrical li-ion cells are carried out to study effects of cell arrangement, impact of flow of vent gases, effects of radiative shielding and impact of combustion of vent gases on thermal runaway propagation in a Li-ion battery pack.

Thermal safety of large battery storage and transportation systems requires a careful investigation of the multiple highly coupled processes that occur during thermal runaway. Given the cost and hazard associated with measurements, simulation models such as the one presented here may play a key role in guiding preliminary design and optimization. In the first part, a numerical simulations-based investigation of large-scale thermal runaway propagation during large-scale storage or transportation of Li-ion batteries are presented. The model captures thermal runaway onset and fire due to combustion of vent gases and predicts the transient temperature field in proximity of pallets containing a large number of cells. The model is used to understand the parameters that affect thermal runaway propagation and potential techniques for fire suppression.

In the second part, Electrochemical and thermal coupled overcharge to thermal runaway model to predict thermal and electrochemical response of a li-ion battery to an overcharge abuse scenario is presented. A lumped thermal model in conjunction with well-established tank in series electrochemical model is used to comprehensively quantify heat release during thermal runaway onset due to overcharge by exothermic electrochemical reactions in a cell. Finally, a systematic simulation framework to account for different electrochemical and heat transfer processes and their interactions with each other is developed in order to accurately predict onset and propagation of thermal runaway in 18650 Li-ion battery packs.