Li-ion batteries are one of the most popular battery types on the market, due to their prime properties such as high capacity, low self-discharge rate, zero-maintenance, high energy density and long lifetime. However, safety still remains a major drawback, due to overheating and thermal runaway. The shortcomings of safety were reflected in the recent accidents, where fires and explosions were reported in cell phones, electric cars, laptops, e-hovers and even airplanes. The goal of this thesis is to generate knowledge, understanding and methods to ensure safety in Li-ion cells and packs.

For achieving the goal, two main mathematical models and a side model were developed as follows:
1. A lumped venting model for analyzing the thermal runaway behavior in a cylindrical Li-ion cell, which includes the venting of gases and solids. The venting model was developed by deriving the energy and the mass conservation equations, and the results were compared against experimental data from the open literature;
2. A simplified thermal runaway model for investigating the propagation of thermal runaway in a battery pack designed by NASA for astronaut spacesuits. A simplified model was initially built for single battery cells with an internal short circuit device (ISCD) implanted inside, used for triggering thermal runaway at low temperatures.
The simplified lumped model was then coupled with a 2D thermal FEM for investigating the pack design. The simplification consists of implementing an efficiency factor term in the energy equation which accounts for the energy leaving with the gas and solids;
3. An electrochemical model for investigating the discharging process of prismatic large-cell battery packs designed by the project partner company Banke A/S. The cells were charged at different ambient temperatures, and the capability of phase change materials to protect the cells was investigated. Moreover, the influence of including the fluid flow equations was analyzed. A 1D electrochemical model was developed by using the mass, charge and energy conservation equations for a single cell and coupled with a 2D thermal model.

By comparing the pressure, the temperature, the vapor quality and mass loss, the results from the venting model showed good agreement with analytical calculation, within a deviation of 3.5%. When compared against the experimental data, it was found that the model predicted the amount of energy measured experimentally for different states of charge, within a deviation of 1.75%. The venting model is the only model available in the open literature for analyzing in detail all the stages of thermal runaway in a cylindrical cell.

The results from the simplified thermal runaway model showed that by fitting an efficiency factor for modeling the battery cells with an internal short circuit device, the maximum temperature predicted by the model matches the maximum temperature measured experimentally. By using the simplified model and coupling it with a 2D model of the battery pack, the model showed good agreement with the experimental data, with a slight difference (from 5 to 10 degC) in the peak temperatures. The simplified model is the only model available in the open literature for modeling the internal short circuit device developed by NASA and its partners.

The third electrochemical model was initially validated experimentally, and good agreement with experimental data was found. The results showed that by having phase change materials around the battery cells in a pack, and discharging the cells at extreme ambient temperatures, no significant improvements are achieved. It was found that at low ambient temperature, having air is better than phase change materials. . .