Thermal modeling of fire propagation in lithium-ion batteries

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ABSTRACT

The objective of the present work is to assess the risk of spreading of fire between Lithium-ion battery cells initiated by a thermal runaway. In particular it aims at developing means to predict the temperature of cells in the vicinity of an overheated cell during the first 5-7 minutes after the thermal event in a Li-ion cell that has an organic based electrolyte which is flammable. Finite-Element (FE) modelling is used to compute the heat transfer between cells. The spreading model is assessed modeling a scenario where the cells are exposed to a 15 kW propane burner. Two different models where utilized, one that considers the conjugate heat transfer between the surrounding hot gases and the battery cells while the second is a thermal model where the boundary conditions are measured in a mock-up test. The results from the two models are contrasted to experimental data where the heat release rate (HRR) is utilized as an input to the simulation. It is found that the temperature increase in a neighboring cell can be quantitatively estimated in certain cases during the early stages of the fire taking into account the anisotropic thermal conductivity of the cells using the conjugate heat transfer model. Moreover, the thermal model captures the qualitative behavior of the test results, however, the temperature increase is slower in the computational model.

KEYWORDS: lithium-ion, battery, fire, propagation, thermal model, thermal runaway

INTRODUCTION

Lithium-ion (Li-ion) batteries offer great performance in form of e.g. energy and power densities, enabling their use for a wide range of applications including the use in electrified vehicles, an application that is steadily growing. If the temperature in a Li-ion cell is increased beyond a certain threshold, a thermal runaway can occur, resulting in a rapid temperature increase and possibly other adverse effects such as, release of gas, smoke, fire and rupture/explosion. There are numerous types of abuse situations that can result in elevated temperatures inducing a thermal runaway. For example, mechanical abuse, electrical abuse and thermal abuse [1-11]. In case of a thermal runaway in a single Li-ion cell it is important to stop or at least delay its spreading to adjacent cells, since the effects from a cascading thermal runaway scenario of a complete battery pack could be devastating. Battery packs in electrified vehicles can consist of thousands of battery cells. In general, the design of a battery pack plays an important role for fire propagation, e.g. the thermal management system, mechanical support structures cell-to-cell respective module-to-module, use of fire walls and division of the battery pack into different sub-packs are important aspects.

There are relatively many simulation studies regarding general heat generation and cooling of Li-ion batteries during normal cycling (battery charge/discharge) within the battery specifications. Furthermore, Li-ion cells and battery packs with multiple-cells have been simulated during abusive conditions; by external heating in oven, short circuiting, overchargeing and deformation/crash. For example, Spotnitz et. al. [12] performed a numerical study on the influence of various heat transfer modes for the propagation cell-to-cell for a battery pack with 8 cylindrical cells of type 18650.

However, only a limited number of simulations studies of lithium-ion battery fire abuse situations are available. For example, Anderson et. al. [7] used CFD simulations with subsequent thermal modeling to study the fire resistance of a battery pack in a gasoline pool fire test according to UNECE Regulation No. 100.

A heat propagation simulation of cell-to-cell fire propagation for 5 Li-ion cells has recently been performed by Anderson et. Al [8]. That utilized recent experiments performed at SP on five EiG Li-ion 7 Ah cells where a thermal runaway was initiated in a cell using a propane burner. The resulting temperatures were monitored by thermocouples and the experiments are well suited for modelling purposes. However the predicted temperatues were found to be lower than the measured counterparts partly due to the models inability to represent the boundary in the fire test.

The present work continues this work by utilizing additional measurements of the fire load on the batteries. The aim of this work is to develop a model suitable for predicting the propagation of thermal runaways in stacked Li-ion cells. The modelling was done using the COMSOL Multiphysics software package that can model conjugate heat transfer. The software is a Finite-Element (FE) tool and in order to successfully model the experimental set-up appropriate boundary conditions are needed for reliable results. The long term goal is to be able to study protective measures mitigating the propagation of a thermal runaway event. In this paper we will extend previous work done in Anderson et al. [8] where we make use of fire abuse tests of commercial Li-ion cells where detailed measurements of the temperatures between the cells as a result of the thermal runaway response of the cells were performed. These tests may be utilized to fine tune a numerical model of the phenomena.

RESULTS FROM THE FIRE TESTS

Commercial Li-ion (EiG ePLB-F007A 7 Ah) pouch cells were exposed to a 15kW propane burner that initiated a thermal runaway event in the cell closest to the burner. During the tests heat release rates and temperatures, measured by thermocouples between the cells, were measured. The resulting HRRs have been published as well as one preliminary study on modeling one of the tests [6,8]. The tested EiG cell had a lithium-iron phosphate, $LiFePO_4$, cathode and a carbon based anode. Each of the tests consisted of five cells tightly packed together with steel wires, see Figure 1 (left). Also in Figure 1 (right), the mock-up used in to determine the impact from the burner can be seen and is described in detail below.

Figure 1. Fire test on EiG 7 Ah LFP pouch cells (left) and measurement of the impact on a mock-up (right).

The cell terminals (tabs) were cut-off prior to the tests for all but the middle cell. In the tests the thermal runaway was initiated by a LPG burner of approximately 15 kW placed underneath the packed cells, see Figure 1. Several tests with varying state of charge was done yielding cases with varying reactivity. The HRRs are presented in Figure 2, however in this paper we will focus on modeling the case with 75% state of charge (SOC) indicated by a dashed line, previously the case with 100% SOC was used.

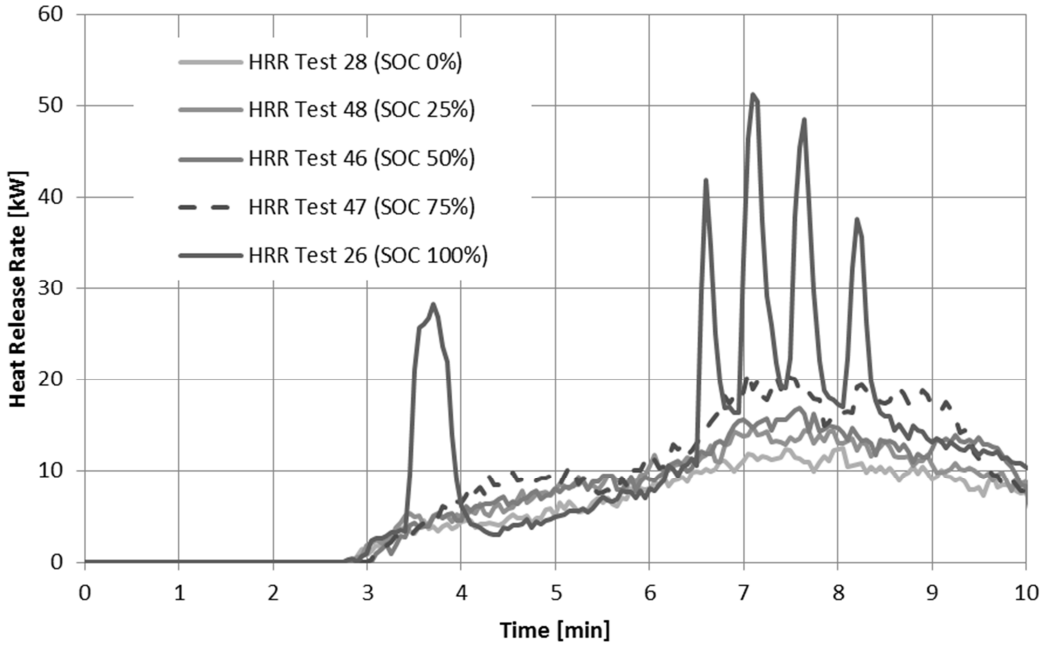

Figure 2. The heat release rate of the EiG 7 Ah LFP pouch cells where the heat from the burner is subtracted.

Additional quantities of interest was measured in each test such as cell voltage of the mid cell however this is out of the scope of the present work. We noted that the measured voltage breakdowns occurred earlier for increasing SOC values, in accordance with faster thermal response for increasing SOC shown by temperature and HRR measurements. During the test temperatures between some of the cells were carefully monitored in four positions, see Figure 3.

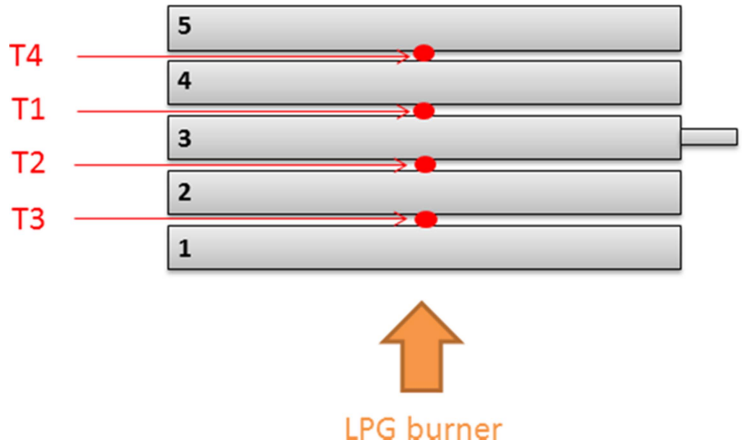

Figure 3. The placement of thermocouples in the live fire test.

In the previous paper by Anderson et al [8] it was identified that a well defined fire source is needed in order to more accurately describe the evolution of the temperatures between the cells. For modeling purposes one test with a

mock-up was performed where the impact of the burned was assessed. To achieve this the mock-up shown in Figure 1 was constructed of promatect clad with custom made plate thermometers. Although the moisture level in promatect is very low it was dried for around 48 h further reducing the moisture content. The plate thermometers were approximately 40 mm x 100 mm in size to fit on the side of the mock-up. The objective of the mock-up test is to estimate the fire source's impact on each side of the mock-up by measuring the adiabatic surface temperature (AST). The AST is an artificial effective temperature that replaces the gas and radiation temperature that describe the local conditions around the test object. It is defined as the temperature of a surface that cannot absorb any heat. However, due to the limitations of the physical extensions of the object the size of the plate thermometers were smaller than usual indicating that they may experience somewhat different convection radiation equlibrium since the estimation of the AST becomes more sensitive with smaller devices.

THE SET-UP OF NUMERICAL SIMULATIONS

The modeling was performed in two stages; the first stage covered the fluid-structure interaction in a conjugate heat transfer model; the second stage was a thermal model where the boundary conditions were taken from measurements. Common in both models was to use the measured HRR produced in the thermal runaway event. The models were built in the multi-physics software COMSOL suitable for studying heat transfer problems. In the models the five battery cells have been implemented where bulk values of the density, specific heat and thermal conductivity are specified. Below we present the particulars of the models.

The conjugate heat transfer model

The software solves the heat transport taking into account heat conduction and radiation as well as solving for the Navier-Stokes equations to assess the convection around the cells coming from the fluid movement of air around the cells. The software is a Finite-Element (FE) code and the Reynolds number is assumed to be small, such that turbulent fluctuations can be neglected. The model consists of around 10000 elements in order to have sufficient convergence and accuracy. The solution time of the model is about 10 minutes on an ordinary personal computer. A simplified 2D geometrical model was constructed for this work. In the model, the battery cells are in the same ambient conditions (T0) as the surroundings of that particular test and the cells are assumed to always be in perfect contact to each other. The ambient conditions give the boundary conditions for the thermal exchange between the cells and the surroundings by conduction, convection and radiation. The 15 kW heat of the propane burner was assumed as a boundary heat source placed directly beneath the first battery cell. The measured heat release rate was used as input in the model for the thermal energy which was deposited homogenously into the bottom cell. The heat generated by the propane burner was taken into account, however, the extra buoyancy of the exhaust gases from the burner was omitted since numerical instabilities occurred.

The thermal model

Similarly to the conjugate heat transfer model the thermal model was built in COMSOL. The test specimen was modelled in 3D with half the amount of cells compared to the other model. The thermal model is considerably faster with runtimes of a few minutes. The boundary conditions were estimated by assuming a heat flow in to the specimen determined by the AST (T_{AST}) in the following manner,

$$\dot{q}'' = h(T_{AST} - T).$$

Here the heat flow is determined per unit of time and area where h is the heat transfer coefficient. The heat transfer coefficient is taken from Eurocode standard [13] to be h = 25 W/(m^2 K). No assumption was necessary for the propane burner since this is included in the AST. Otherwise the model had a similar set-up as the conjugate heat transfer model.

Bulk material data

The physical structure of the pouch cells is complex with a repeatable layering of anode and cathode material. The total numbers of layers is of the order of 150 layers. The thermal properties of the materials vary significantly in terms of thermal conductivity, density and specific heat along and across the cell due to the layered structure. To be

able to accurately compute the temperatures in the 5-cell-pack realistic values of the thermal properties are needed in combination with a well-defined fire source in terms of the measured heat release rate. This complex structure of the cell makes detailed modeling impractical however for our purposes bulk values of the thermal properties are enough to capture the essential propagative features. In the present study these values are estimated from literature values by Spotnitz and Franklin, Fan et al., Wu et al and Chacko et al, [12], [14] –[16]. Ideally, careful measurements of these quantities at elevated temperatures are needed but generally difficult to obtain. The heat conductivity coefficient, k, was varied in the simulations since the multi-layered structure of the battery cell allows for this value to be highly anisotropic. Table 1 shows the thermal material properties of the cells used in the thermal simulations.

Table 1. Values of the thermal properties of the cell used for the simulations.

Notation used in this paper	Density ρ [kg/m^3]	Specific heat C_p [J/(kg K)]	Thermal conductivity k [W/(m K)]
Anisotropic k=13	1895	700	k_x = 13 and k_z = 0.4
Anisotropic k=27	1895	700	k_x = 27 and k_z = 0.8

RESULTS FROM THE NUMERICAL SIMULATIONS

In this section we will present the numerical results found using the developed models. We have chosen the test with 75% SOC as a representative case in the test series for corroborating the simulations. In this test four time series with temperature data, T1-T4, were recorded. In Figure 4, the results by comparing the experimental data with the simulations using isotropic (a) and anisotropic (b) thermal conductivity are presented using the conjugate heat transfer model. It is found that T1 and T2 of the middle cell can be modeled as described previously [8], but the temperatures are lower than the experimentally measured values. However, T3 at the top of the initiating (bottom) cell that undergoes thermal runaway deviates quite early.

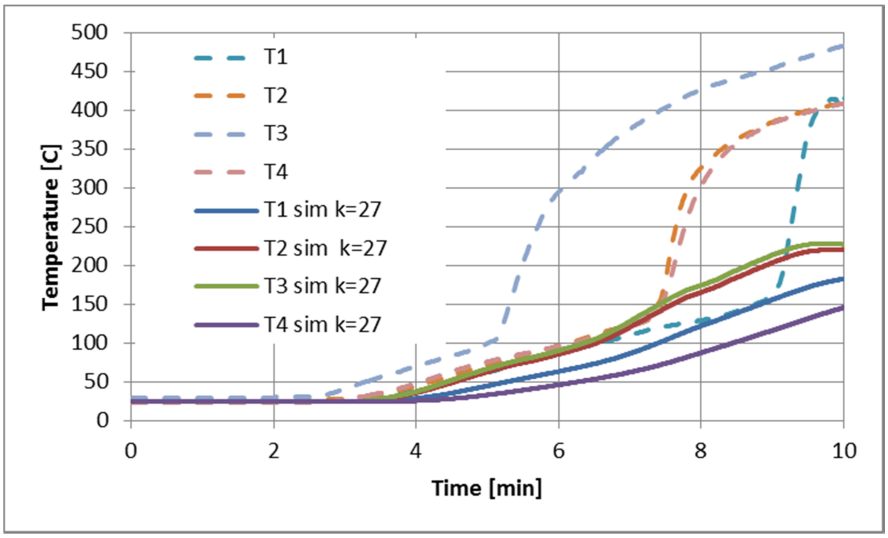

Figure 4. Comparison between test results and simulated temperatures at 75% SOC using the conjugate heat transfer model. A comparison of temperatures T1, T2, T3 and T4 found in the experiment and the simulation assuming anisotropic heat conductivity k=27 (kx =27 W/(m K) and kz = 0.8 W/(m K)).

In Figure 5, the same test is modelled using the thermal model with the AST used as boundary conditions however the same HRR is used. We find also in this case that the model yield lower temperatures compared to the experimental values. Interestingly, a higher value of the heat conductivity would yield lower temperatures through the whole test specimen.

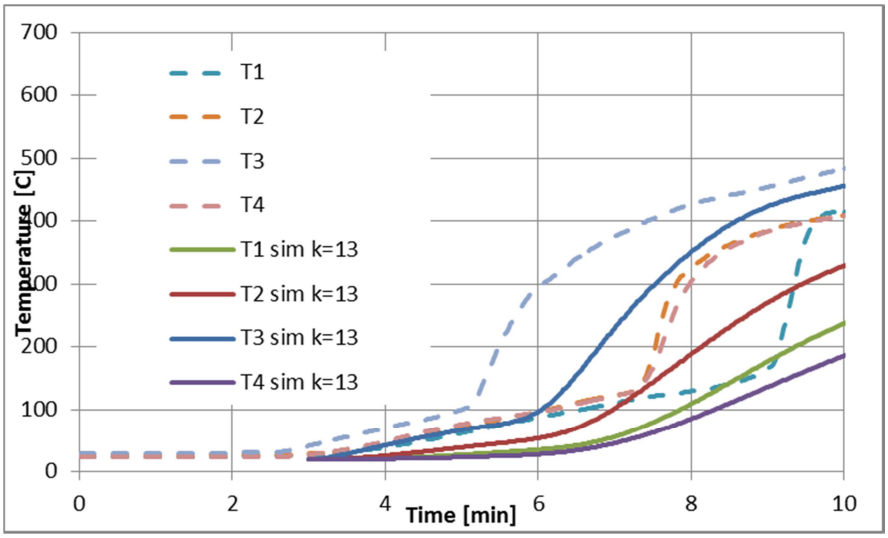

Figure 5. Comparison between test results and simulated temperatures at 75% SOC using the thermal model. A comparison of temperatures T1, T2, T3 and T4 found in the experiment and the simulation assuming anisotropic heat conductivity k=13 (kx =13 W/(m K) and kz = 0.4 W/(m K)).

However, the qualitative behavior is considerably better in the thermal model and it is very likely that using values corresponding to a lower thermal inertia would give a much better correspondence with the experimental results. In particular, the value for the specific heat and density may decrease considerably as the reactions progress. We note that in the experiment the measured temperature closest to the top is elevated, T4 is close to T2, indicating a significant amount of heat coming in from the top surface.

DISCUSSION

This paper presents an attempt to predict the progress of a thermal runaway/fire in a cell to neighboring cell by simulating the temperature development on neighboring cells in the same lines as in our previous work, Anderson et al. [8]. Simulations and experiments have been conducted for varying SOC, this paper focuses on the case with 75% SOC as an example of results.

Modeling battery cells in such harsh conditions as that of a fire is a rather difficult task due to the lack of knowledge of the precise local conditions around the test object. This gives an uncertainty in the boundary conditions to be used. Another difficulty is the lack of knowledge of the material data. In order to have a reliable model the precise temperature dependency of the heat conductivity, specific heat and density are needed.

Using the conjugate heat transfer model we find that the model captures the first minutes of the test however as the runaway event progresses large deviations are found, this is partly due to that the thermal exposure in that case is only assumed to be underneath the cells and not around the entire object. In the thermal model a good qualitative match between the test and model is found however the thermal inertia in the model seems to be larger compared to the actual cell case. The thermal model uses the measured AST values as input however it is uncertain how representative this measurement is as in the real case the boundaries are not smooth/edges are sharp creating a complex convective heat transfer. Furthermore, radiative losses at the top surface are likely since the flames are rather thin resulting in a different boundary.

The simulations are in reasonable agreement with the experimental result up to the point where the thermal runaway is initiated but still the simulations under-predict the temperature in the neighboring cell somewhat in all cases.

However the model can be further developed by:

1. A two stage simulation using the methodology in Anderson et al [7] is likely to be a more proper representation of the turbulent driven convective heat transfer process.
2. Investigate in more detail different boundary conditions. Since the dimensions of the battery pack is rather small the influence of the boundary is important and can be a source for uncertainties. Both geometry at the edges and different forced convection boundaries should be investigated.
3. Simulating different contacts between the cells using a thin contact element with variable thermal resistance should be investigated.
4. More adequate values of the thermal properties data including temperature variation.

With these improvements there is great potential for the simulations to be able to better predict the temperature development in a neighboring cell. A conservative model of the propagation is desirable to be on the safe side in the predictions.

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