Exploring Ansys LS-DYNA's Battery Modeling Capabilities

Iñaki Çaldichoury[1], Kevin Kong[1], Pierre L'Eplattenier[1] Vidyu Challa[1]

[1]Ansys

1 Introduction

Over the past decade, considerable advances have been made on battery safety models but achieving predictive accuracy across a wide range of conditions continues to be extremely difficult. From a numerical perspective, the obstacles are numerous.

Multiple physics can potentially be involved and interact with one another, electrochemistry, thermal, mechanical, fluid dynamics and so forth. The question of modeling scale also invariably arises. Is it reasonable to imagine a numerical model resolved at the micro scale being later used in a macro model such as car crash simulation?

LS-DYNA was initially approached by several actors in the automotive industry in order to develop simulation tools that would eventually allow an engineer to design a Multiphysics model for a battery pack or module that could be run as a stand-alone simulation or, later on, be included in different crash simulations at a reasonable cost. Several developments have emerged from this original ask, that are present in LS-DYNA and available to all users and engineers interested in the broad aspect of battery simulation.

In this paper, modelling techniques for the mechanical aspect of battery simulation (eg material laws), will be discussed. The BatMac module, a part of the LS-DYNA EM solver used to capture internal and external shorts will be introduced up to and including the initial heat generation, thermal expansion, and thermal runaway modelling. Validation results and workflow examples will be given. Finally, topics that are of contemporary interest to battery simulations such as busbar thermal expansion, swelling, or venting will be discussed.

2 LS-DYNA Statement of Objective

LS-DYNA is committed to its one-software approach where multiple solvers are integrated within the same code allowing for seamless communication between them and Multiphysics solves. Applied to battery crash simulations, the objective becomes being able to simulate the entire chain of events as depicted in Fig. 1. from the onset of the short (either via Thermal abuse and Mechanical abuse or both), its consequences on the battery (temperature rise, voltage and SOC drop) up to its logical conclusion (thermal runaway, swelling and venting).

The obstacles on this path of Multiphysics modelling and workflow are numerous. To increase its understanding of the process Ansys has acquired an automotive grade pouch cell on which experimental tests were conducted [1]. When referred to, this cell will be called the "Ansys test cell" for the purposes of this paper (See Fig. 2).

Challenges come from an engineering perspective (how to characterize battery material properties and experimental set up in general), others are software related (how to integrate and manipulate technologies and solving techniques under the same hood) and others stem from physics (different time scales and complex chemistry). Some simulations results are presented and discussed in [1-8]. In the rest of the paper, we'll go through the current status of the different steps described in Fig. 1 and discuss the challenges encountered as we understand them.

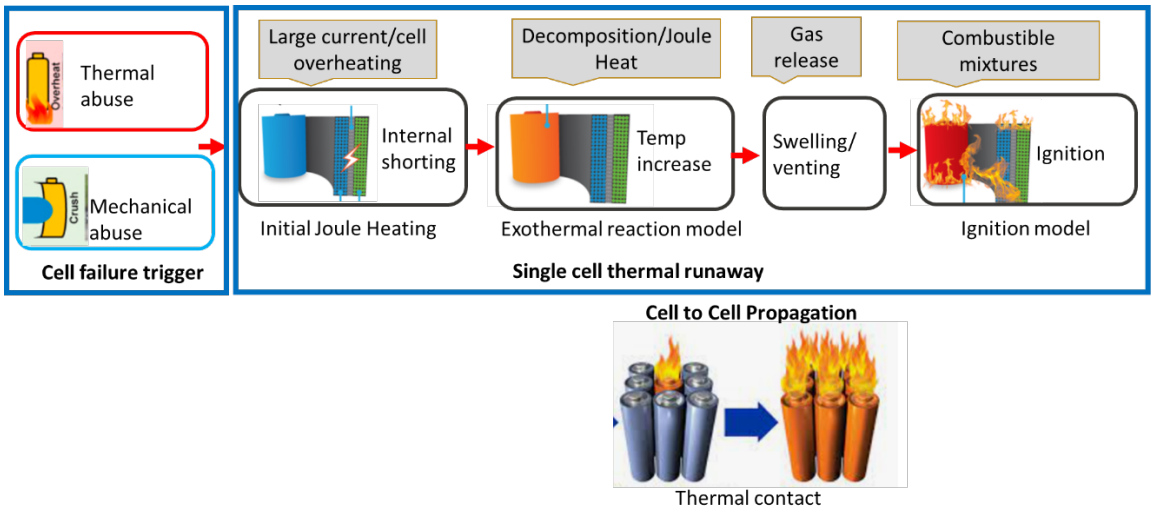

Fig. 1: Battery simulation workflow

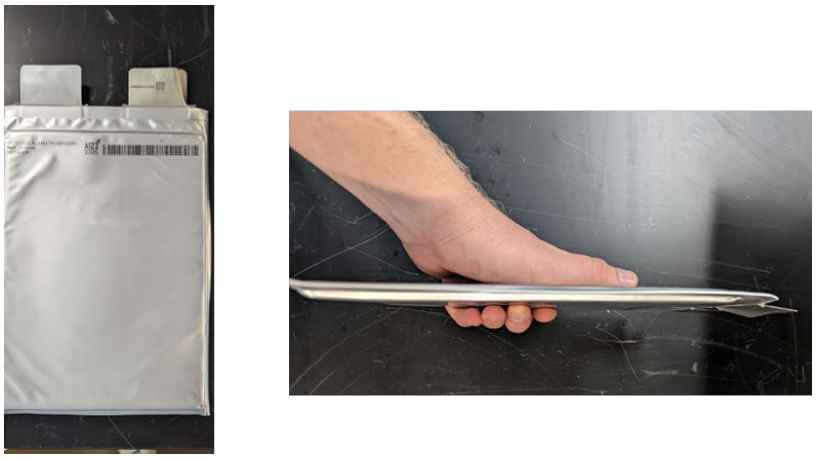

Fig. 2: Pouch cell used for the Ansys experiments (Ansys test cell)

3 Mechanical abuse

The first decision to take for the simulation engineer is whether a 'micro' approach, where all the battery layers are modelled is preferrable or whether it is more suited to use a 'macro' model where the battery cell is modeled using a single homogenous material (See Fig. 3). While both approaches can be used for subsequent Electric and thermal analysis, using a single homogenous material is the more suited approach for modelling an entire battery pack or module and is the commonly adopted route (the micro model can still have its uses to better understand local effects on a single cell).

Once the use of a homogenized model has been agreed upon, the next step becomes material characterization. *MAT_CRUSHABLE_FOAM (63) and *MAT_MODIFIED_HONEYCOMB (126) have been used. For the Ansys test cell material characterization, *MAT_CRUSHABLE_FOAM (*MAT_063) is used to calibrate the mechanical properties. Different indenter shapes were used in the Ansys experimental tests including flat, cylindrical, and spherical. Quasi-static crushes as well as fast dynamical ones were performed. Fig. 4 shows a benchmark between numerical and experimental results. Flat compression test data was used for material calibration to develop a homogenized cell through thickness stress-strain response. The material properties were then validated against other indentation load cases.

Among recent developments for battery crash, it is important to note that new options for *MAT_126 have been introduced: Poisson's effect for uncompacted status, more strain rate dependance, a combined support with *MAT_ADD_GENERALIZED_DAMAGE, an option to define failure as function of strain ratio. That latest enhancement has specifically been developed to better capture the failure

mechanisms leading to internal short circuit in Li-ion batteries under complex loadings scenarios as described in [9].

If further information on the experimental testing is desired, please contact the authors of this paper.

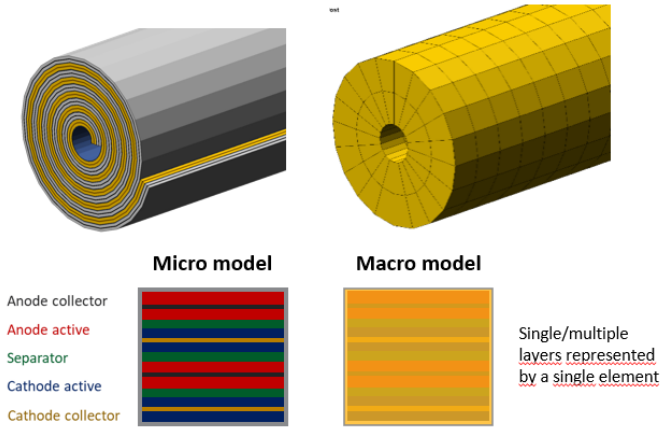

*Fig. 3: Micro versus Macro Cell modelling approaches. See *EM_RANDLES_SOLID and *EM_RANDLES_BATMAC*

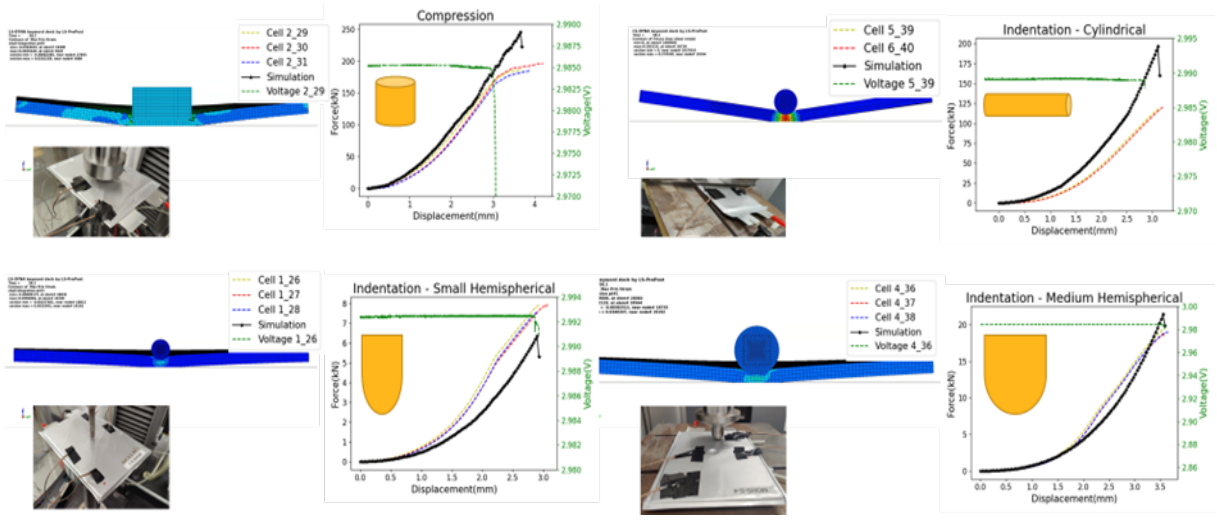

Fig. 4: Benchmark between experimental and numerical data on quasi-static crush experiments with different indenter shapes.

4 Electrical model set up

The decision whether to include the Electrical behavior and the EM solver in the simulation is two-fold. The first objective can be to study the battery module charge and discharge under different normal operating connections. For this part the complexity resides in a correct characterization of the equivalent circuit model parameters and well as establishing a workflow to easily define and identify the wirings of the cell. The second objective is to capture the onset of internal short and its consequences on the voltage drop and subsequent temperature rise. This remains a challenging aspect of building a predictive model for battery simulations.

4.1 Set-up of the cell Randles parameters.

Randles circuits are typically used as Equivalent circuit models (or ECMs) to model the electrochemistry behavior of the battery. The advantages of such an approach are that it adds a reasonable computation

cost while retaining good accuracy in normal as well as abuse conditions and is now a well-established approach for battery electro-thermal simulations. When applied to the homogenized cell material modelling approach, the so-called Battery Macro or “BatMac model” needs to be called by the EM solver (See Fig. 3).

The Randles parameters of the Randles Circuits Model, which are used to represent the cell’s electrical properties, can be obtained from capacity test and Hybrid Pulse Power Characterization (HPPC) test on one cell, as described in detail in [10].

Fig. 5 shows the electrical components of the Randles Circuit Model and the contribution of each component to the cell voltage response as the cell gets charged and discharged. An example of the model prediction on the Ansys test cell’s voltage response under the HPPC tests is also shown.

Considering that the HPPC test data is collected at several SOCs and the test is repeated at multiple temperatures, we felt a need to automate the process of extracting the Randles circuit parameters from the HPPC test data. Ansys has developed a workflow using pythonic APIs of several of its tools to fully automate the cell characterization process. The curve fitting required to extract the Randles parameters is built into this workflow. Fig. 6 shows the web interface that can be used to easily extract the Randles parameters from the test data. The extracted R0, R10 and C10 parameters are written out as *DEFINE_CURVE and *DEFINE_TABLE_2D so that it can be easily used in the input file for EM_RANDLES_BATMAC models.

To know more on accessing this app, please with your Ansys point of contact.

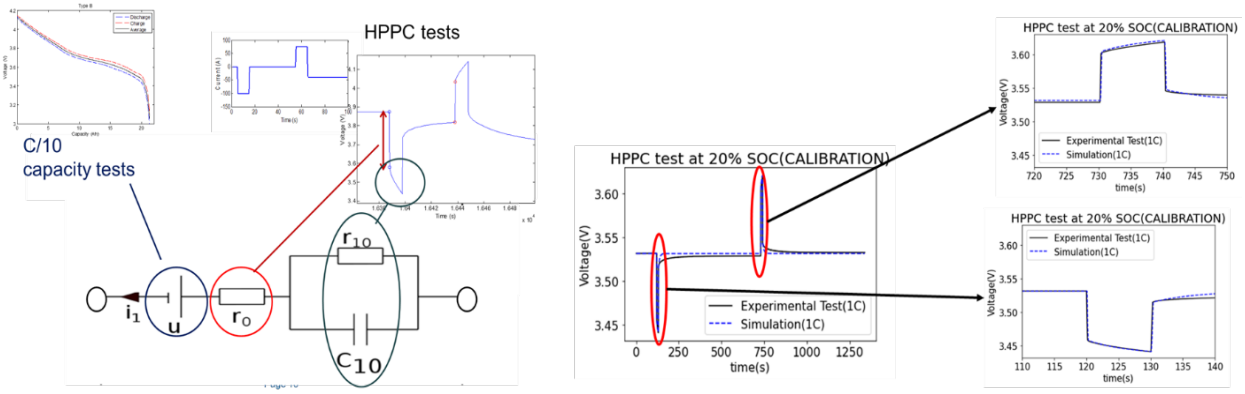

Fig. 5: Setup of the Randles parameters given HPPC test results, with the comparison of the HPPC voltages between experiment and simulation on the Ansys test cell.

Fig. 6: Sample Curve fit generated by the Cell Characterization App

4.2 Wiring & Connectors

A module consists of many different cells wired together with connections between tabs. Here the challenge becomes a visualization and organizational one on how to properly and correctly identify the keywords (*EM_ISOPOTENTIAL and *EM_ISOPOTENTIAL_CONNECT) that make those connections on a battery module or pack (See Fig. 7).

LSPrePost is currently developing an interface capable of identifying and setting up these connections in a more user-friendly way and allow scaling and copying cell definitions in order to more easily jump from single Cell model to complete battery pack. Fig. 8 and Fig. 9 offer snapshots of this interface. Naturally since this capability is in the process of being developed and can benefit all LS-DYNA users, constructive feedback and requests are welcomed by the authors of this paper as well as the LSPrePost development team.

In parallel, our Oasys partners are also developing a tool trying to address the challenges in battery modelling (See Fig. 10). To know more, please check the link at [11].

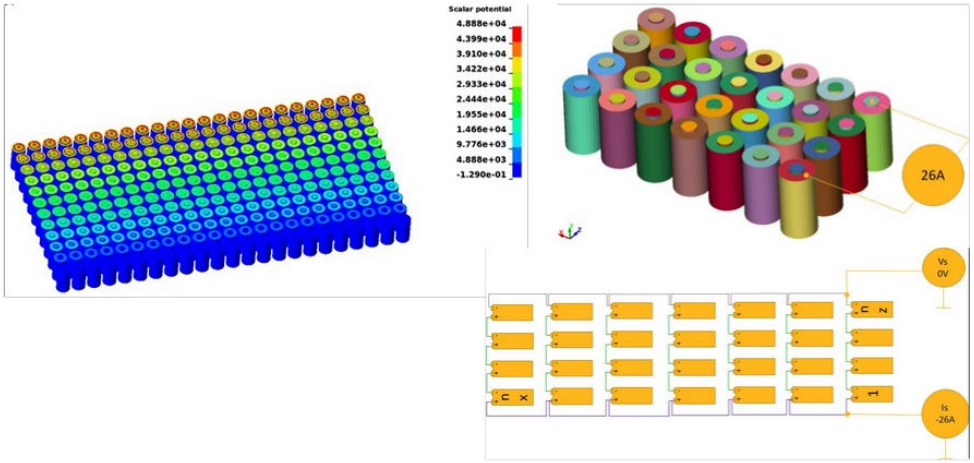

Fig. 7: Examples of a battery pack and its multiple connections

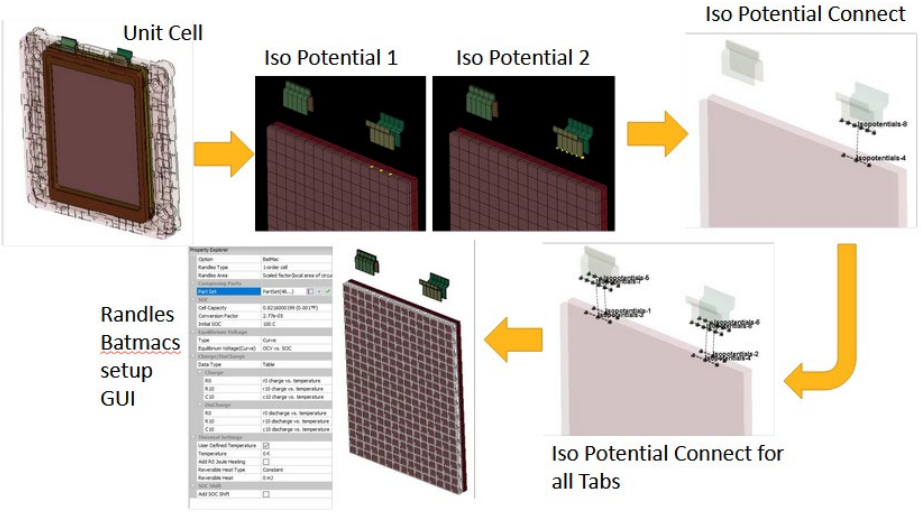

Fig. 8: LSPrePost : Setting up and visualising tab to cell connections

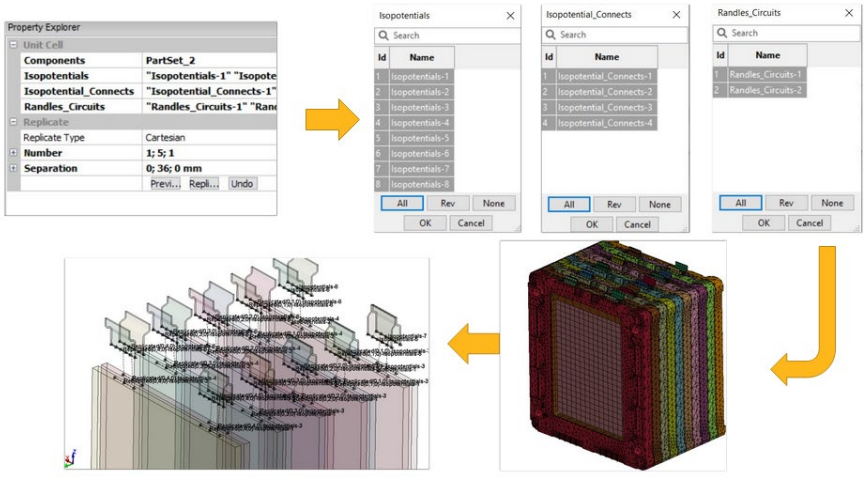

Fig. 9: LSPrePost: From a Cell to a Module - Duplicating and scaling tool

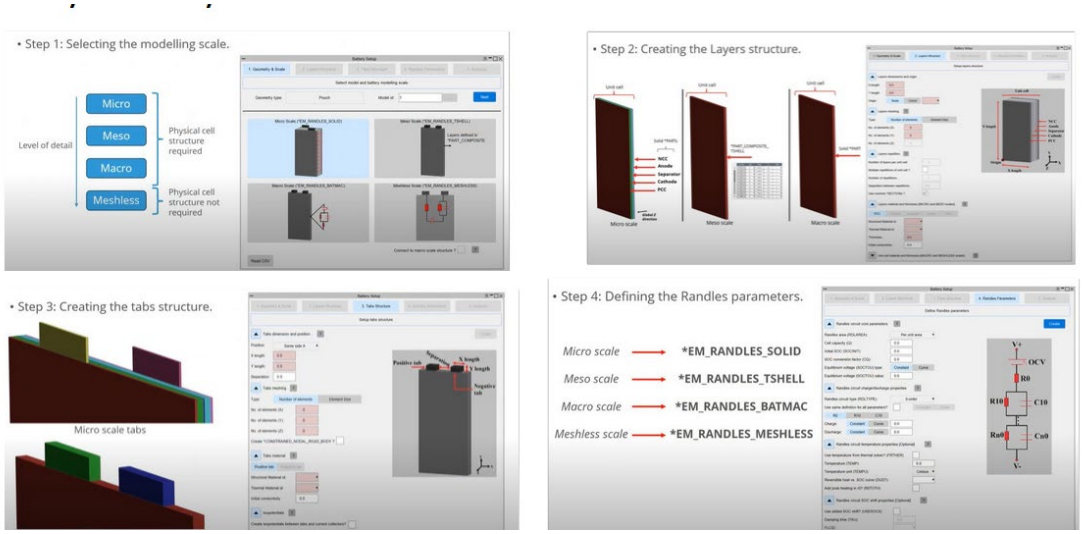

Fig. 10: Oasys Battery Tool

4.3 Internal Short

Numerically, when an internal short is triggered at a certain location, the Randles circuit will be replaced by an internal short resistance value that will cause the battery cell to self-discharge and the higher localized current will trigger a temperature rise in the cell.

The *EM_RANDLES_SHORT keyword allows the user to trigger a local internal short as a function of mechanical parameters such as strain or stress, or thermal parameters such as temperature (e.g., internal short induced because of separator melt). Parameter identification including mechanical/thermal threshold to induce internal shorts as well as calibrate the short resistance are highly test data dependent. The short activation threshold can be identified based on failure strain/stress as simulated in the finite element model.

Fig. 11 shows the benchmark of the voltage drop during an internal short on the Ansys test cell under two different impactor profiles.

Currently, the calibration process involves measuring the voltage drop occurring during an internal short and using its magnitude and rate of change to retrofit the short resistance value. Temperature probes are often also present in the experimental testing but due to their limited number and other experimental set up constraints, they also offer only a limited view of the process occurring.

Although decent results can be achieved, these limitations in our data collection techniques and our indirect retrofitting currently result in a collective bottleneck in the establishment of a fully predictive model. Further research and collaborations on this topic are encouraged.

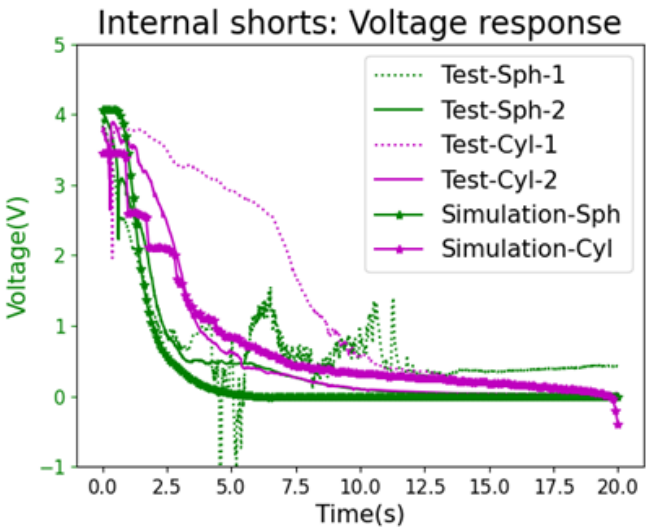

Fig. 11: Benchmark between test results and numerical simulation showing the voltage drop after the onset of the internal short. The green lines correspond to a spherical indentation and the pink ones to a cylindrical indentation.

5 The Thermal analysis

At this stage, the LS-DYNA thermal solver will be used. Similarly to the EM solver, it is an implicit solver automatically included in LS-DYNA and the two solvers can be coupled to run electro-thermal analysis. A classic application that comes to mind is to study the structural expansion due to heat of key components such as busbars. Current is imposed, Joule heating is generated that triggers heat and thermal expansion. The ICFD solver can also optionally be used to take the cooling channels into account (See Fig. 12).

For battery module charges and discharge simulations under adverse or normal operating conditions, the principle is similar. The heat generated by the Randles circuits is automatically transferred to the thermal solver as well as the heat generated by the short resistance (if present). For the cell thermal conductivity characterization, the material properties for the current collectors can be used as rough guidelines but the best approach is again to do some experimental testing with temperature probes on different sides of the battery cell to study heat diffusion.

One note is that a single surface thermal contact was developed and is now available. The need arose specifically in thermal battery applications to help the user with model set up in battery pack or module cases where individual thermal contacts per cell would otherwise be required.

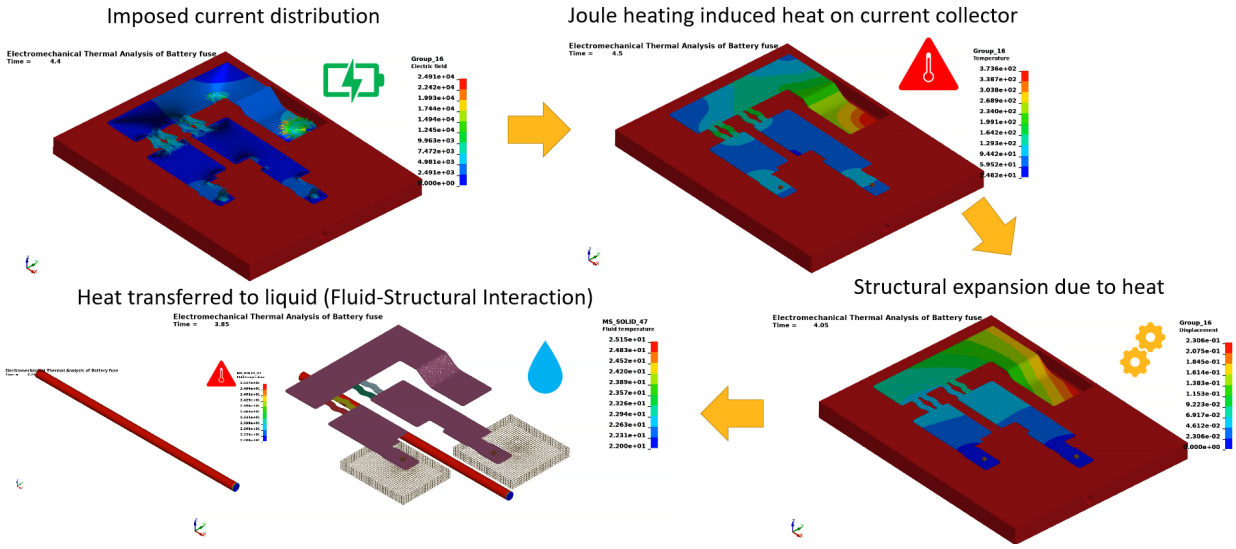

Fig. 12: Busbar thermal expansion analysis in battery model.

5.1 Thermal runaway modelling

Thermal runaway is the process by which the battery's temperature, after a slow and continuous rise, will dramatically increase over a brief period resulting in swelling, venting and potential ignition. Physically, it is understood as an Arrhenius law type behavior that translates into an additional heat source term in the thermal heat equation that exponentially rises as temperature goes up until all reactive material is consumed.

To illustrate the NREL's 1 and 4 equations models [12] have been implemented in LS-DYNA, through the *LOAD_HEAT_EXOTHERMIC_REACTION card. Fig. 13 shows an application example where a small battery pack goes into thermal runaway following a localized internal short in one of the cells.

To aid the simulation engineer in cases where the EM solver is present, another way to set up the exothermal reaction is offered through the *EM_RANDLES_EXOTHERMIC_REACTION card. Similarly to the short resistance card, this feature allows the user complete control via a *DEFINE_FUNCTION of the additional heat source added to the thermal solver. The heat addition can be triggered, and the amount controlled by the user via retrofitting experimental results. The define function also returns the total accumulated exothermal energy (via the variable H_ex, H_ex=H_ex+dt*H_p with H_p the power given by the define function at the previous step) which can be used by the user to turn off the exothermal heat once a certain energy threshold has been reached. The temperature difference between pre-thermal runaway and thermal runaway would inform users of the amount of heat/power that is required to simulate the temperature rise. The temperature drop after thermal runaway can be modeled using convection boundary condition to release heat. This process calibrates the cell's capability to exhibit a thermal runaway event provided the temperature threshold is met. This card was used on Ansys test cell and the comparisons between experimental and numerical temperatures are given in Fig. 14.

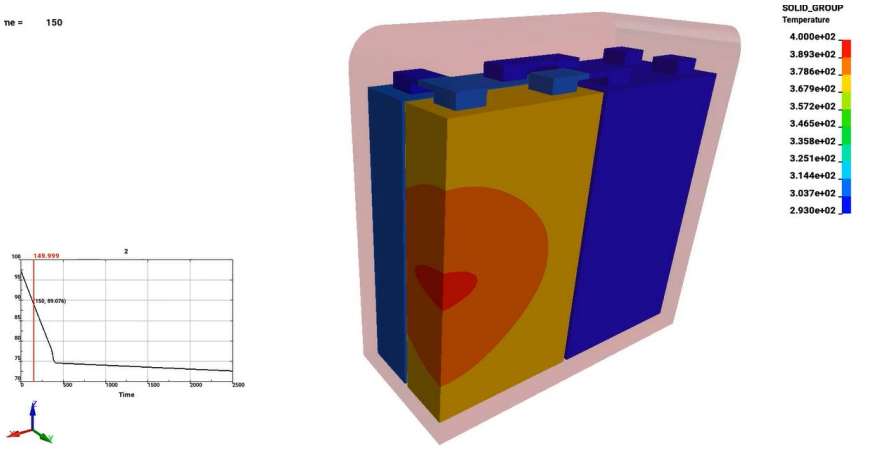

Fig. 13: Local short causing SOC drop and temperature rise in battery pack, leading to a thermal runaway (modelling using the 4 Eq. model approach)

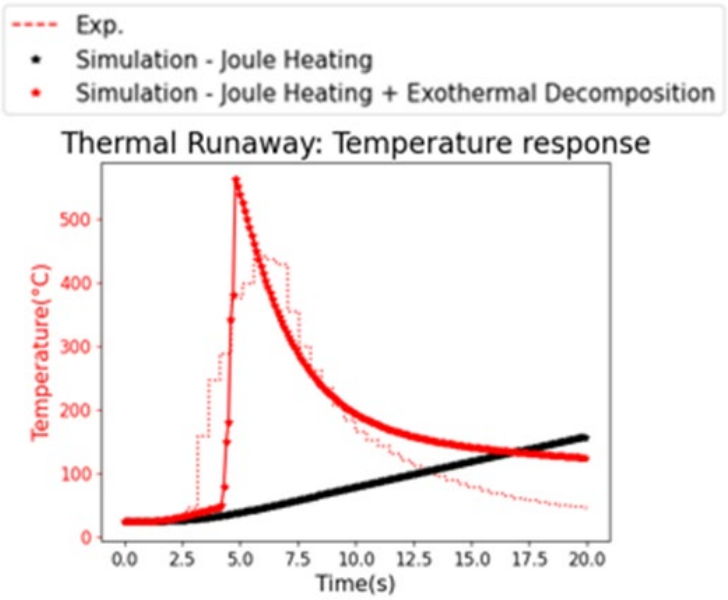

Fig. 14: Benchmark of temperature rapid rise and slow drop caused by an internal short between experimental (light red), numerical results with only the joule heating due to the internal short (dotted black), and the numerical results with joule heating +exothermal reaction (dotted red)

6 Venting and Swelling

After a catastrophic event has occurred such as thermal runaway or excessive heating or deformation, venting will usually be triggered by the battery cell with gases escaping. This can cause swelling of the pouch as well as undesired heat transfer between cells. To study this part, some gas modelling technique is required.

6.1 The CPM approach

For gas venting, we must turn to the LS-DYNA solvers that are traditionally used by the automotive industry for airbag deployment. Among those, the CPM approach has gained the widest usage due to its practicality and reasonable computation cost (see *AIRBAG_PARTICLE). The method is unique in that it is not based on continuum physics, but on a macro homogenization of kinetic gas theory.

It has been successfully applied in battery modelling and swelling applications. The modelling approach used is as follows: gas particles are generated and accumulated within the cell, particle accumulation

within the cell causes the cell to expand, once a burst criterion is reached the gas particles from the cell model are released to the surrounding volume i.e the pouch.

The required input to simulate the cell swelling and venting would be gas information including gas mass flow rate and gas temperature time history which can be difficult to obtain (same as in airbag modelling). The gas information is measured during the test in a pressure vessel and multiple temperature probes are located within the vessel to measure the gas temperature as the cell vents. The swelling force is also measured from the clamp plates where the cell sits in between.

Fig. 15 shows an experimental test setup conducted internally that was used as an example to illustrate the feasibility of the workflow. Fig. 16 shows the benchmark between the experiment and simulation. The simulation captures the general trend of the experimental cell swelling force data. The temperature and the pressure data for the first 5 seconds are in good agreement with the model making the CPM approach a viable candidate for battery swelling and venting modelling.

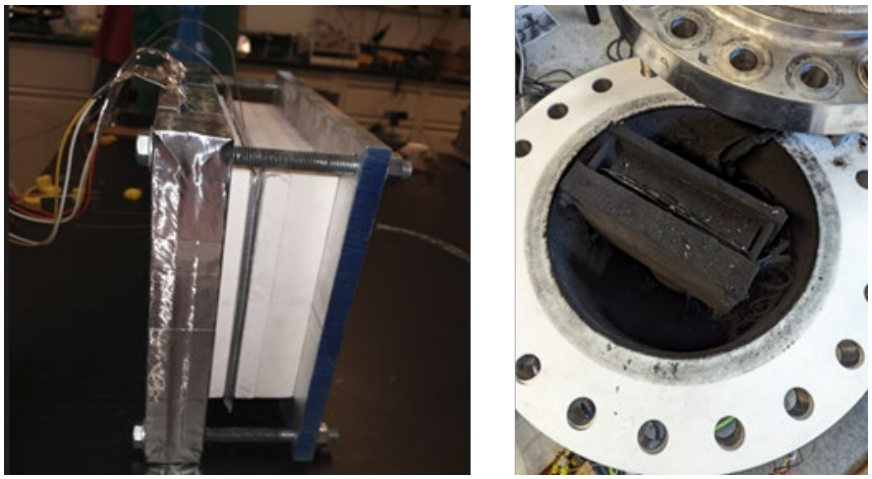

Fig. 15: Experimental setup used to measure the gas emission of the cell during thermal runaway.

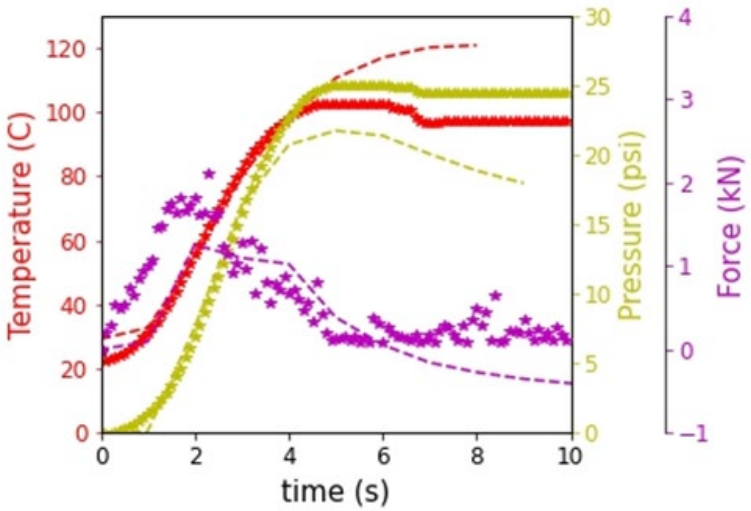

Fig. 16: Experimental (dashed) vs numerical (dotted) gas pressure (yellow), force (purple), and temperature (red) vs time.

6.2 The CPG approach

As described above, the CPM approach relies on kinetic gas theory which is a fast and efficient approach but can require a lot of model calibration and does not allow to study local effects such as local heat spots or gas flow patterns. An alternative approach would the to use a compressible flow approach that

solves the complete Navier Stokes set of equations as well as gas transport. A similar conclusion was reached in Airbag modelling [13].

For this reason, the Continuum-based Particle Gas (CPG) approach was introduced in LS-DYNA [13]. CPG is an innovative particle-based numerical method which relies on continuum physics principles. Like CPM, CPG is a particle-based approach that eliminates the need for meshing the airbag's internal volume (See Fig. 17). However, CPG adopts continuum theory and resolves the compressible Navier-Stokes equations (momentum+continuity+energy) coupled with an ideal gas equation of state which brings it closer to traditional compressible fluid solvers.

For battery venting and swelling applications, the advantages would be a more accurate tracking of gas species transportation as well as heat transfer. An application would be cells venting (similarly to CPM, the mass flow of the different venting gas species needs to be known, as well as the temperature of the gas being expelled which can be challenging to obtain) in a pouch with the pouch swelling and heating. Fig. 18 shows an example of a battery simulation using CPG.

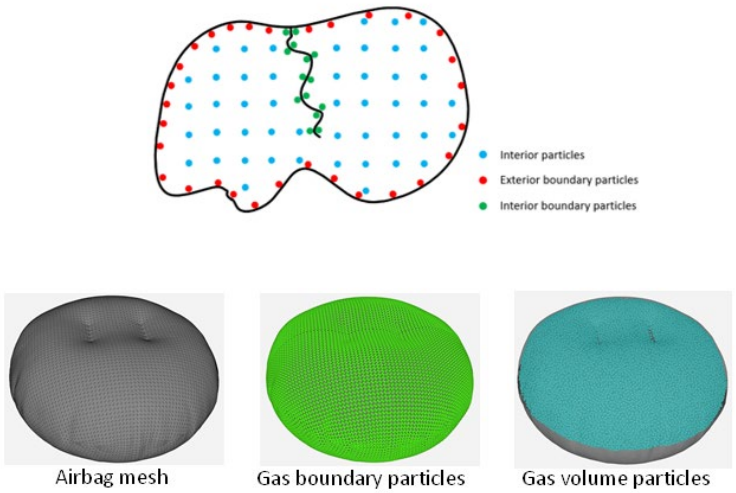

Fig. 17: CPG Discretization

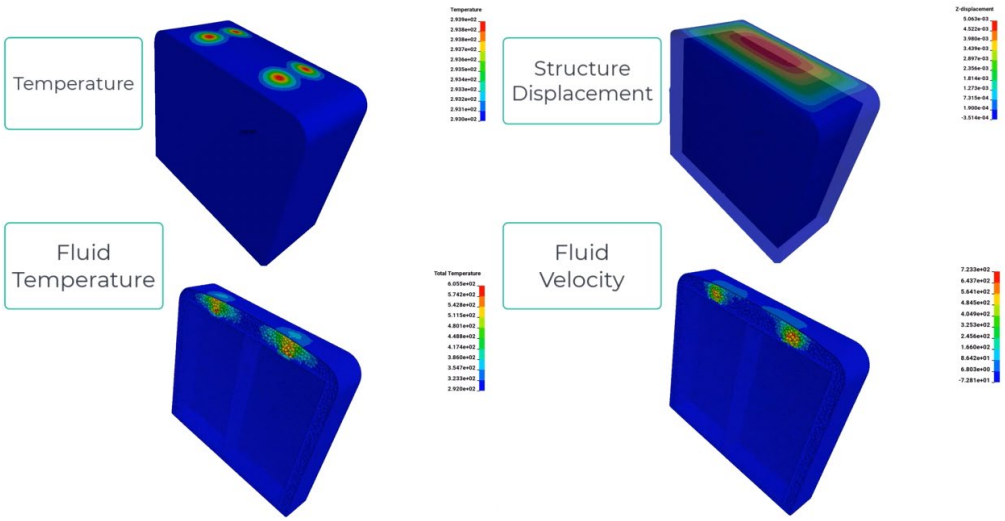

Fig. 18: CPG battery pack venting simulation. Vents are expelling hot gases causing the pouch to expand, deform and heat up.

7 Main take aways

We can broadly regroup the steps discussed in this paper into three broad categories. The initial onset of the short, which is usually a very brief event (ms, up to seconds), followed by a long EM+thermal event, where the battery slowly discharges and heats up (this can take minutes or hours) and finally, the venting event which is again relatively brief and catastrophic (a few seconds). The question becomes how to connect and link those events together.

During the battery crash event, as we have seen the correct material characterization is key to getting good and predictive deformations and developments are active in this area with collaborations with various research groups. From a numerical perspective, it is possible to couple those simulations directly with the EM and thermal and there are various techniques to handle the transition of time scales (usually involving freezing the mechanics so the timestep of the mechanical solve can be drastically increased). The main challenge at this juncture is characterizing the short resistance upon which the voltage drop, and heating will be entirely dependent. The current approach is an indirect one (retrofitting experimental voltage drop measurements to numerical simulations) and it is still an open question whether a better system could be designed.

If this short resistance hurdle is passed, the coupled electric-thermal analysis should handle the solution in good fashion, the main challenge at this stage becomes a pre-processing one, when switching from a single cell to a complete battery pack. Several tools are currently under development to handle and display the data input in keywords to avoid user errors. At the end of the thermal analysis comes the thermal runaway where again, we run into the lack of material data problem. It is generally understood that a thermal runaway will follow an exponential growth law but the parameters defining this law are often unknown. Two schools of thought are being pursued. The first one is by trying to properly define and fit parameters into Arrhenius type equations as evidenced by the implementation of the 1 Eq and 4 Eq models in the thermal solver, the other is by adopting a more engineering practical approach by user calibration based on some total available energy cut off criteria. Perhaps the exact representation of the thermal runaway is not always needed and in practical applications, it will be enlightening enough to get the information of when it happens and to have an idea of what max temp it reaches, without the need to precisely capture the path it took to get there. This information may be useful in deciding to trigger the last part of the process i.e the venting and subsequent swelling.

For now, venting simulations have been run as stand-alone problems. Two methods show promise. The CPM, traditionally used in Airbag simulations as well as the newly introduced CPG which is based on traditional compressible flow solve with the objective of addressing some limits inherent to the CPM. In both cases however, the key component will be having an accurate picture of the mass flow rate of the different gas species expelled as their temperature. For this, good experimental data is required. As a next step, it is envisioned that some temperature data from the previous EM-thermal analysis could be carried over to the CPM/CPG simulations as input (for a vent trigger or to decide on which gas gets expelled at what temperature).

8 Final Conclusion

As discussed in the Statement of Objective, battery simulations under duress are a vast topic with different steps, solvers and physics that each bring their own challenges, both as stand alone solves and when bringing them together. Software progress reflects this mosaic as developments happen in many directions. Even so, LS-DYNA retains an advantageous position in the fact that part of the model (mesh, keyword settings etc) can be retained and easily transferred from one simulation to another either in sequential solves or simultaneous Multiphysics analysis.

Collaboration and feedback with research groups are encouraged to improve our simulation tools and our general engineering and scientific understanding.

9 Literature

[1] Name, Abbreviation of first name: "publication", issue, year, pages