FireFOAM to Model inside Battery Thermal Disorder Propagation

B. TRUCHOT, G. MARLAIR, A. LECOCQ

10th FM Global Open Source CFD Fire Modeling Workshop , Norwood MA on May 30 - 31, 2018.

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Some words about the context

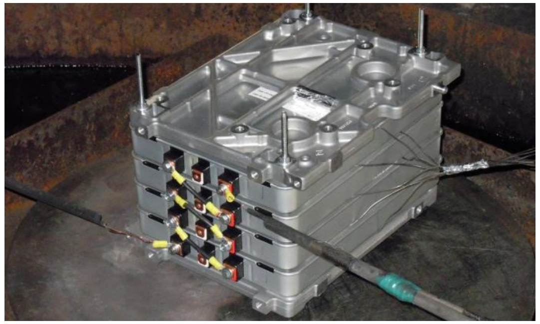
Energy storage is becoming a critical issue

- For stationary applications (renewable generation plants, electric grids, …)
- For various mobile applications (cars, electronic devices, …)
- Current Lithium Ion Batteries (LIBs) are more & more used

For all cases, autonomy is a key

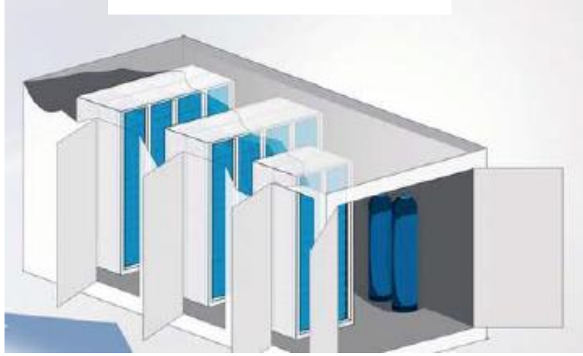
- Energy density is increasing ➔ compacity increases
- Battery size is more and more important
- Safety is still highly important

From the individual cells



Through the module

To the battery pack



Safety management for LIBs

Safety is commonly addressed using experiments

- Individual cell behavior depending on the chemistry
  - Crash, stability, impact, overcharge, …
  - Gas production, HRR and other measurements
- Lots of data are available regarding battery testing

The current very large batteries require an innovative approach

- With very large experimental facilities … up to a certain limit (20 MW in INERIS)
- Using numerical modelling

From physical phenomena to CFD

Several steps to be modelled

1. Ignition in one cell
   - Several complex physical phenomena
   - Depending on the ignition source (internal short-circuit, overcharge, …)
2. Gas release and ignition
   - Mixture of several flammable gases (EC / DMC / …)
3. Temperature rise in the surrounding
   - Combustion of the emitted gases
   - Strong interaction with the air flow and battery structure opening
4. Other cells runaway
   - Assuming other cells will be ignited by thermal runaway
   - Evaluation of the internal temperature
5. Neighbor cells burning
   - Similar to the initial burning cell

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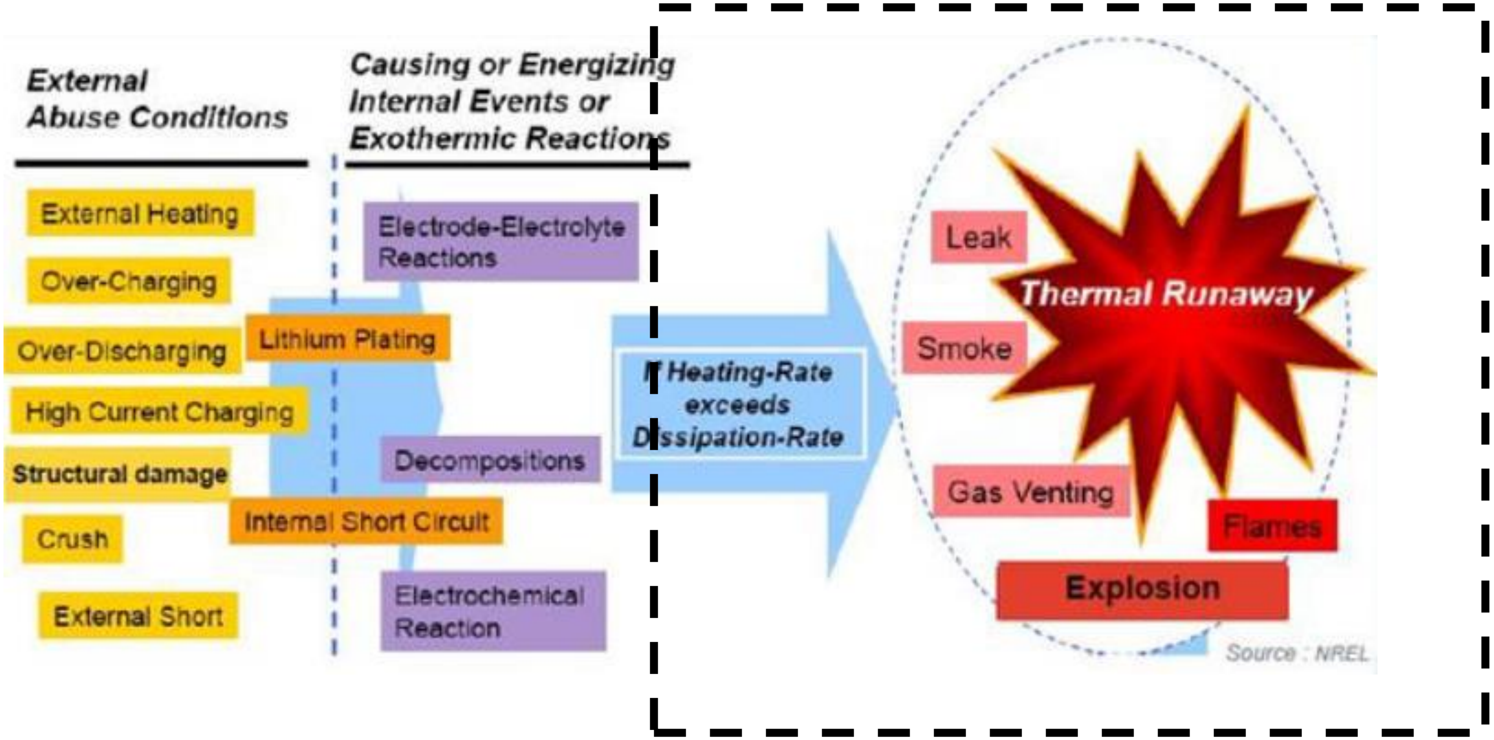
Ignition of a LIB cell

As usual, ignition is very complex

- Cell ignition depends on the source
  - Short-circuit, overcharging, structural damages, …
  - Clearly impossible to consider each kind of possible sources
- Hopefully, during the propagation process
  - Ignition mechanism is based on thermal effect



Source : NREL

Ignition in FireFOAM

Ignition is a phenomenon governed by inner cell behavior

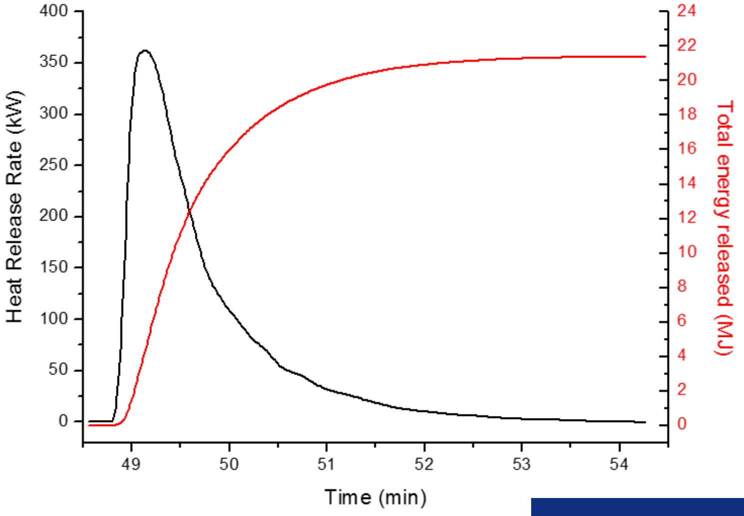
➔ We decided not to model phenomena inside the cell

Ignition is considered to occur at a given time

- The HRR from the first cell is fixed thanks to experimental data

This requires

- An experiment at cell scale with HRR measurement
- An experimental control of the failure mode



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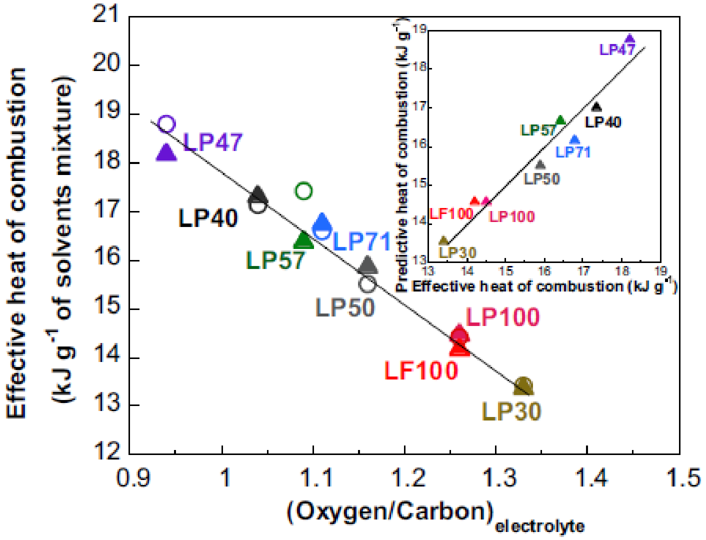
With the key issue of chemical reactions

Electrolyte is composed of several chemicals



- Mixtures of
  - ethylene carbonate (EC) – $C_3H_4O_3$
  - dimethyl carbonate (DMC) – $C_3H_6O_3$
  - ethyl methyl carbonate (EMC) – $C_4H_8O_3$
  - diethyl carbonate (DEC) – $C_5H_{10}O_3$
  - … + Lithium salt ($LiPF_6$)
- Individual mixture test at lab scale (FPA) using CDG and OC calorimetry

Definition of the chemical reaction to be used

- LP50 case : EC/EMC (1/1, wt/wt) + 12,2%wt of LiPF6, neglected

$$1.14\ C_3H_4O_3 + 0.96\ C_4H_8O_3 + 7.16\ (O_2 + 3{,}72\ N_2) \rightarrow 7.3\ CO_2 + 6.12\ H_2O + 26.6\ N_2$$

- Average value: $\Delta Hc \approx 16$ kJ/g
- A simplified reaction used as a first approach

$$C_3H_4O_3 + 5/2\ (O_2 + 3.72\ N_2) \rightarrow 3\ CO_2 + 2\ H_2O + 9.3\ N_2$$

Then a model can be built

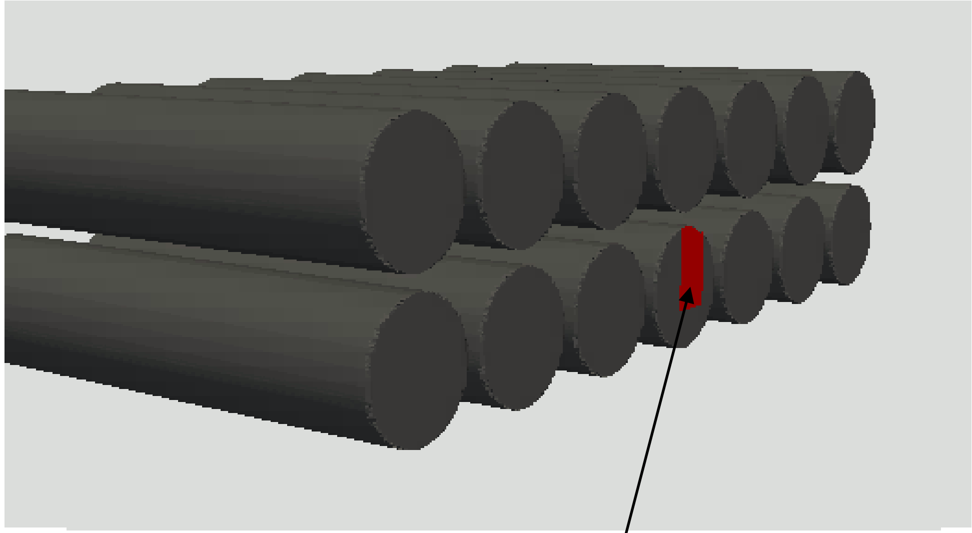
Considering the cell geometry

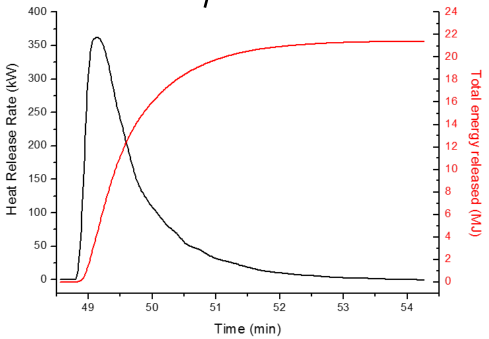
- **Cylinder**; Pouch; Prismatic

With a gas injection boundary condition

- Gas flow designed to reproduce the measured HRR
- Based on the chemical reaction and the ΔHc

Considering the chemical product and reaction





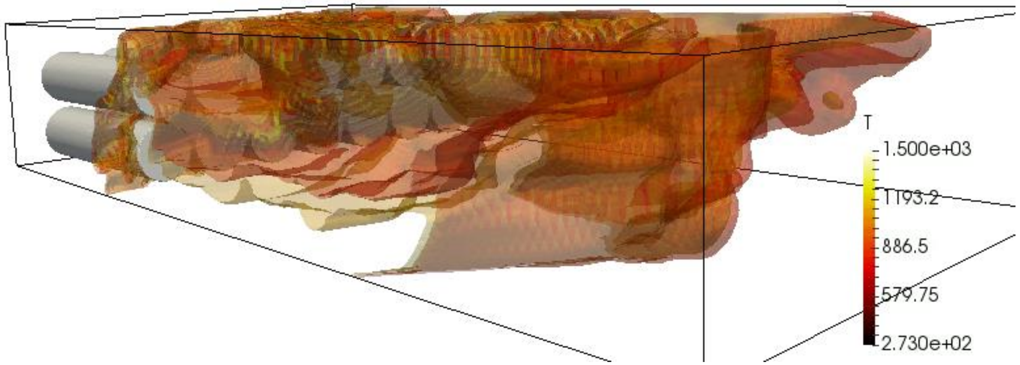
A first comparison

Fire behavior comparison in an open field, unfortunately

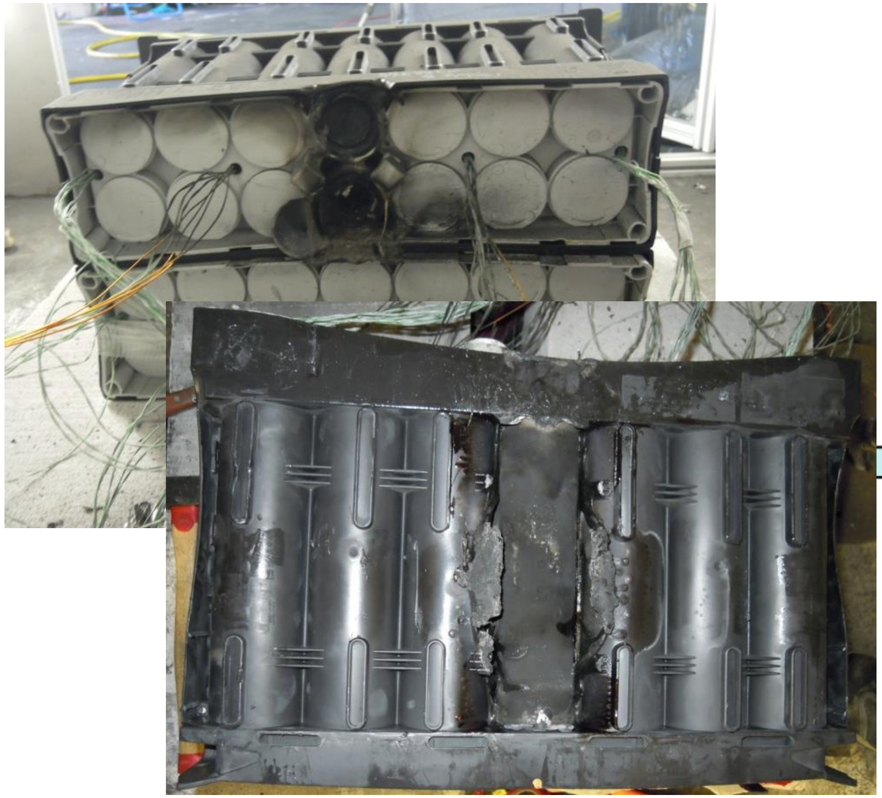
- Battery tests are not designed for CFD code validation

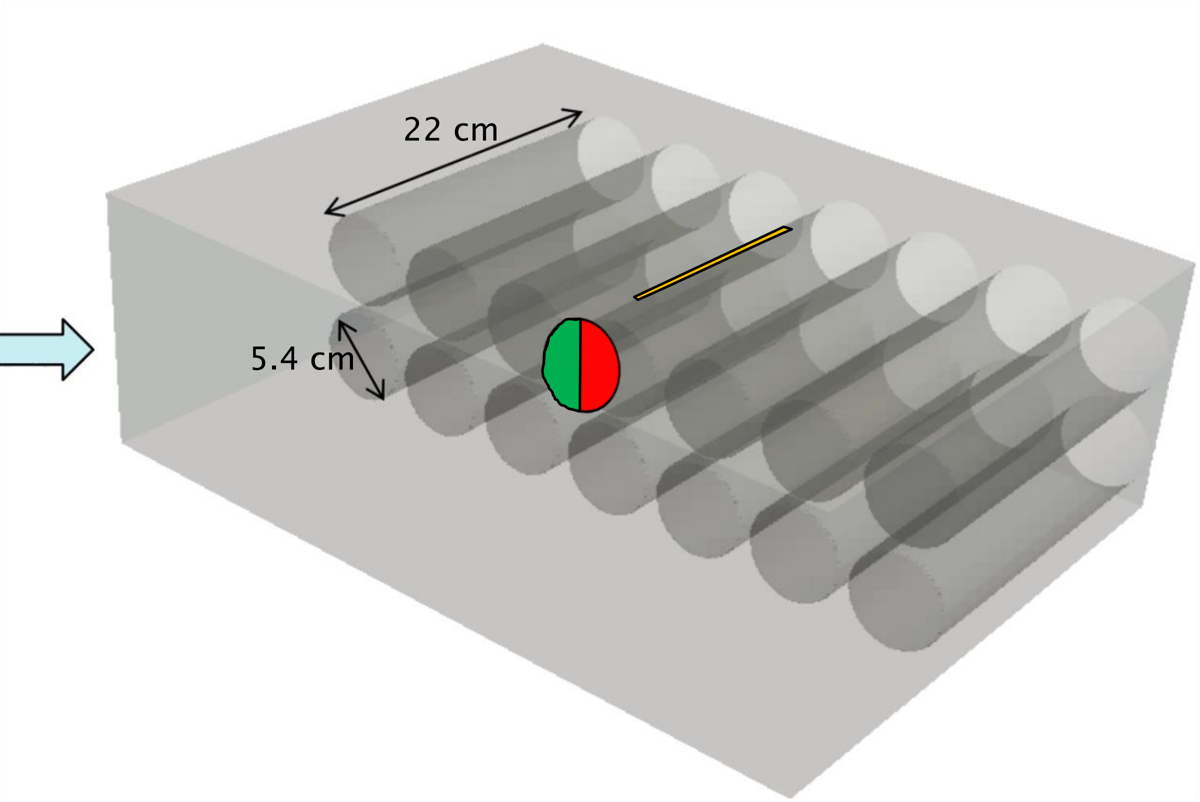
The flame is 3 times longer than the cell and as large as the module

- Flame length is quite correct
- Temperature is in the correct order of magnitude
- But how is representative the boundary condition?



But inside a module the flame geometry is complex

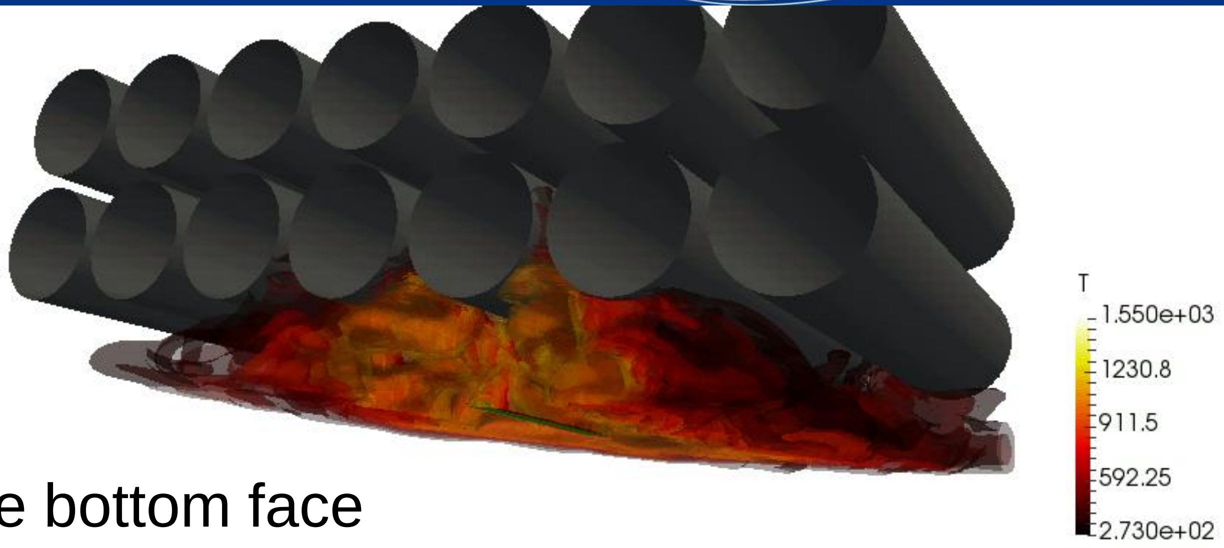




The cell opening mode is crucial

- The whole back face
- A part of the back face
- An opening along the external surface

With consequently strong fire differences

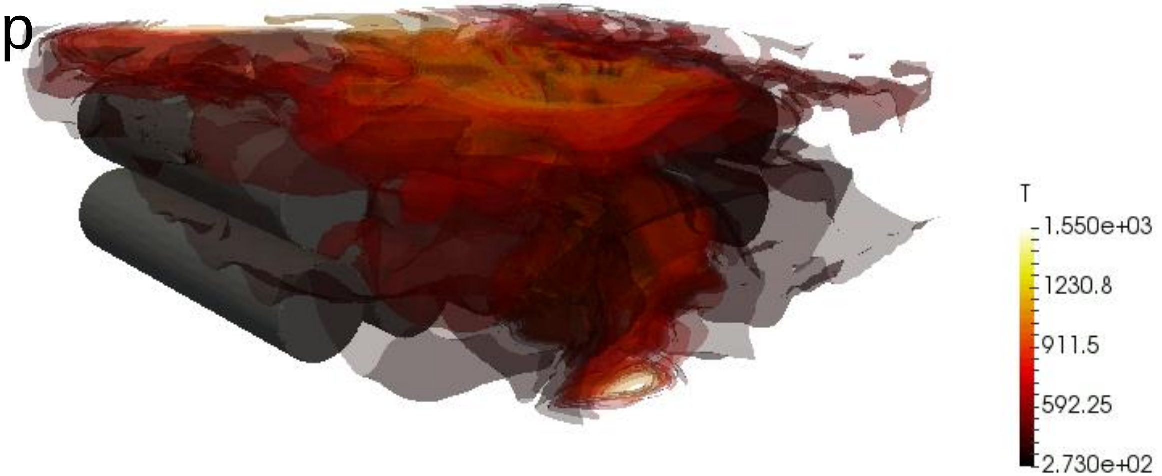


Slice for underneath cells

- Fire impinges several cells at the bottom
- Cells are mainly heated by the bottom face

Open at the back of one cell

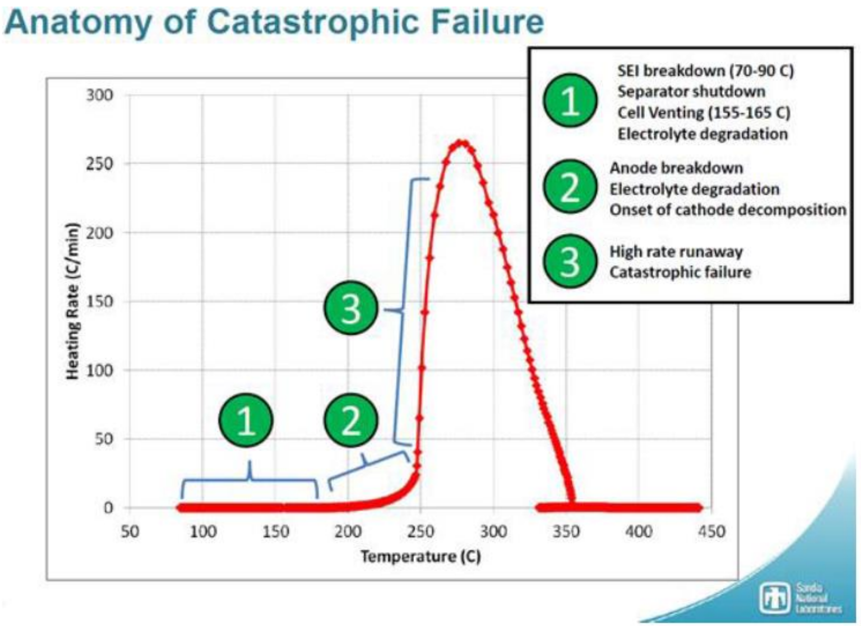
- Fire impinges the back of the module
- Surrounding cells are heated at their back
- Some cells are heated by the top



Cell to cell propagation model

Requirement of dedicated boundary conditions

- To consider the heating of the surrounding cells
- To evaluate their ignition delay



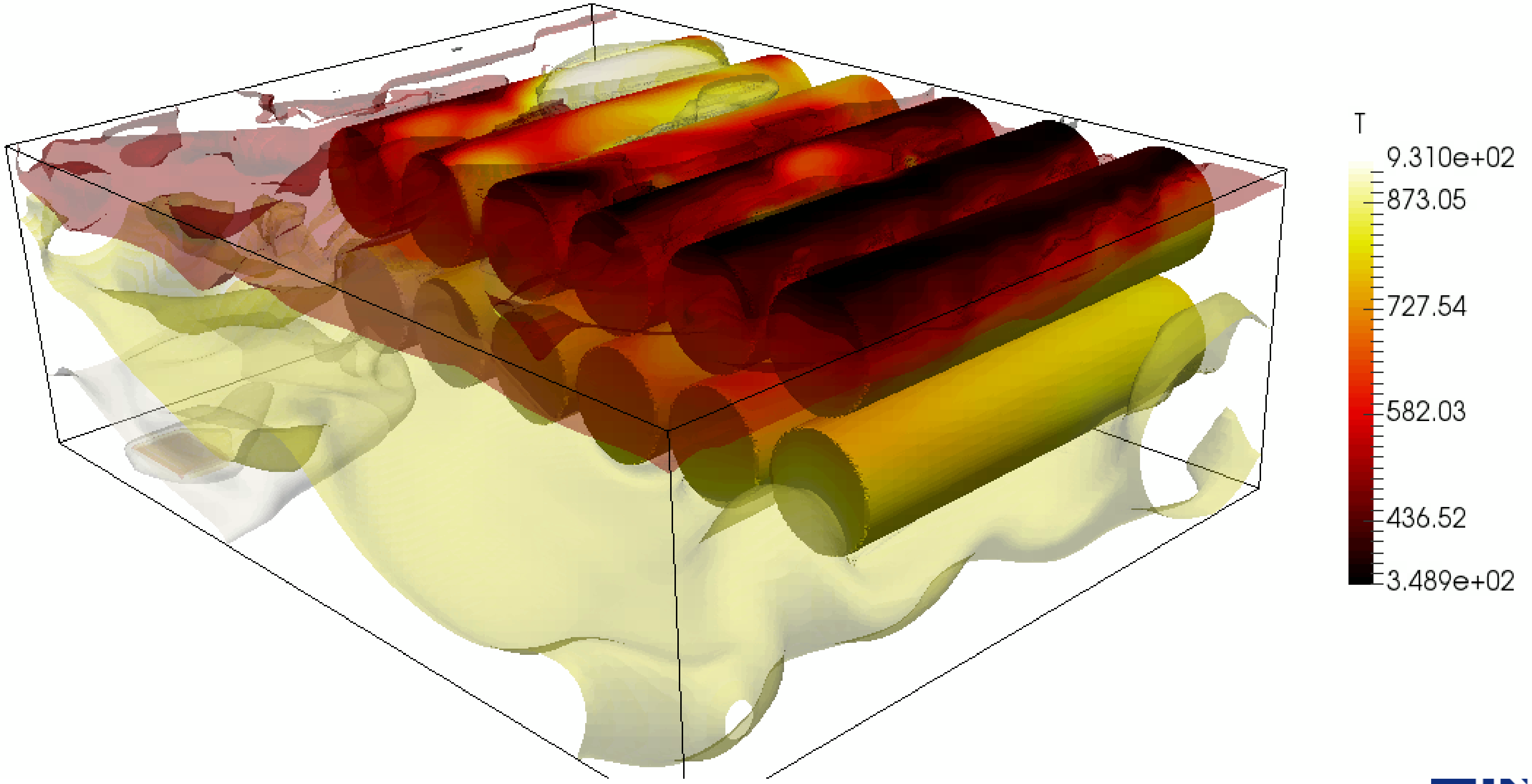
Such an approach requires first

- To take into account the geometry of the battery
- To consider the geometry of the fire ➔ the opening mode of the cell
- To have a correct prediction of the HRR and, consequently, of the temperature

The first step: Energy given to the cell

Based on the temperature distribution

- Evolution on the cells surface along time
- Enables computation of the inner cell temperature



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Thanks to a dedicated boundary condition

A very simple approach

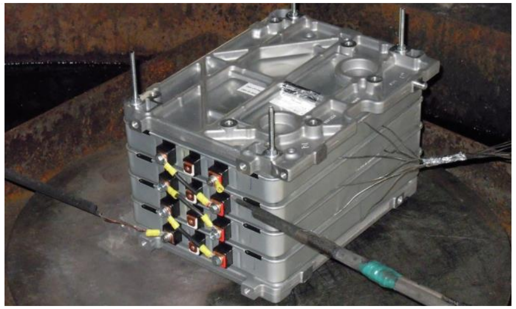
- When the temperature reaches 155°C ➔ cell turns into fire
- Simple to model but does not consider the specific cell volume

The considered approach

- Energy received by the cell is used to heat the electrolyte ($mC_p\Delta T$)
- When the inner cell temperature reaches 155°C ➔ cell turns to fire
- Does not consider the electro-chemical parameters

  ➔ To be introduced later
- Initial temperature is a critical parameter (20°C, 50°C, 80°C ?)

But non only



Cells are located into a module

Modules are placed into the LIB

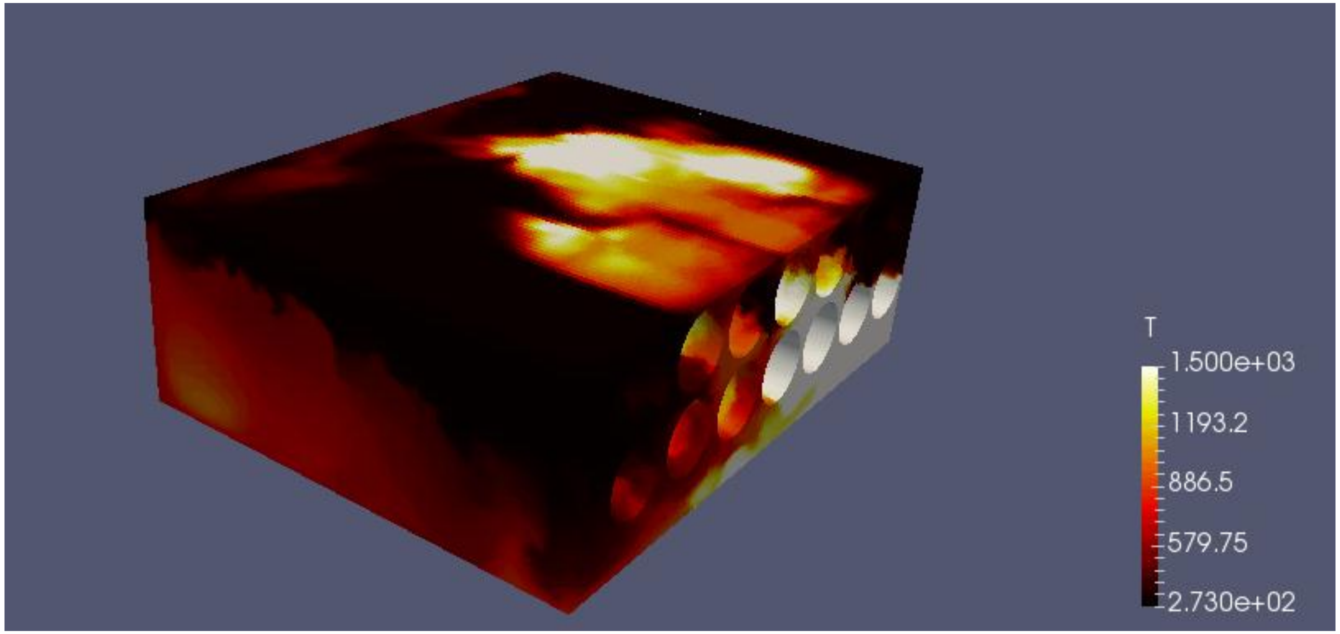
Fire ventilation is a fundamental issue

- The initial available oxygen
- The vent behavior
  - Opening based on T and P
- The cell structure breakage
  - Criteria requirement

Opening criteria based on surface temperature

Several steps

- Surface temperature computation
- Evaluation of the inner material temperature increase considering thermo-physical properties and thickness
- When the structure resistance reached 30% of the initial value, structure to be open (BC modification)



Current and future work

Achieved

- First evaluation of the FireFOAM capability
  - Geometry, chemistry, …
- Evaluation of the input hypothesis
  - Nature of the cell opening, HRR, …

To be done

- Confinement opening because of the temperature rise
- Module to module propagation
- Thermal protection influence evaluation

Acknowledgments

This project is receiving funding from the EU Comission under the H2020 grant agreement # 769900 under the name DEMOBASE

Coordinated by: SAFT - Name : DESPREZ Philippe

Project name : Design and Modelling for improved Battery Safety and Efficiency

- Project partners :

- SAFT SAS
- ACCUREC-RECYCLING GMBH
- FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V.
- INSTITUT NATIONAL DE L'ENVIRONNEMENT ET DES RISQUES INERIS
- INFINEON TECHNOLOGIES AG
- MODELON AB
- IFP Energies nouvelles
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