Journey to a New Regulatory Option

Internal Short Detection/Thermal Runaway Prevention

OICA Submission to IWG for GTR 20, Phase 2

June 2019 – IWG #18, Tokyo

Journey to a New Regulatory Option

Internal Short Detection/Thermal Runaway Prevention

- Introduce concept that detection is possible – COMPLETE
  - IWG meeting #15, Beijing (March 2018)
  - EVS1536-613
- Describe scientific basis for safe/unsafe zones and analysis methods to support development
  - Planned for IWG meeting #18, Tokyo (June 2019)
- Provide examples of how internal shorts can be detected, including potential alternative methods
  - IWG meeting #19 (late 2019)
- Describe acceptable risk concepts and levels – How good does detect/prevent need to be?
  - By mid 2020
- Demonstrate successful detection and benefit when detection occurs
  - Mid 2020
- Develop conceptual regulatory framework
  - Late 2020
- Write draft regulatory language

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KEY MESSAGE:
Under some circumstances, cell internal shorts are detectable. This detection may provide opportunity to take action prior to thermal runaway, thereby completely preventing thermal runaway propagation.

Detection of Cell Internal Shorts

Excerpts from EVS1536-613, March 2018

- Careful cell design (chemistry, configuration) and manufacturing process steps will minimize risk that a severe internal short circuit event can occur.
- Many internal shorts can be detected both during manufacture and in usage
- Internal short behavior can often be measured and understood
- There have been <u>no</u> known incidents of internal short circuits resulting in cell thermal runaway

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KEY MESSAGE:
Proven scientific principles can be used to explain thermal runaway behavior, including how it is possible to have an internal short without thermal runaway.

Description of a scientific basis for safe and unsafe zones with respect to thermal runaway and thermal propagation

including: an example of application of an analysis method to support development

Essentials of scientific basis: Background

Thermal runaway is not a problem that is unique to batteries. For example, thermal runaway is a well-known phenomenon in different areas of chemical engineering.

Several concepts have been developed to deal with the situation, e.g.

- classical **Semënov theory**, named after Nikolai N. Semënov, Nobel prize 1956, see e.g.

  [1] D. Steinbach: Safety assessment for chemical processes. Weinheim(VCH) 1999

- classical **Frank-Kamenetskii theory** for dust explosions

etc.

These theories are also used in up-to-date scientific literature on lithium-ion batteries, e.g.

[2] Q. Wang, P. Ping, X. Zhao, G. Chu, J. Sun, C. Chen, J. Power Sources **208,** 210 (2012)

[3] P. Huang, H. Chen, A. Verma, Q. Wang, P. Mukherjee, J. Sun, J. Hazardous Materials **369**, 268 (2019)

Essentials of scientific basis (2): How to treat thermal runaway

The basic idea of the Semënov theory is to compare the balance of heat that is generated and heat that is removed from a system (e.g. by cooling, dissipation, heat-consuming reactions and processes etc.).

If heat generated in the system **<** heat removed from the system

=> **thermal runaway will not take place**

From basic physical chemistry it is known that

- the generated heat will often follow an Arrhenius-type behavior

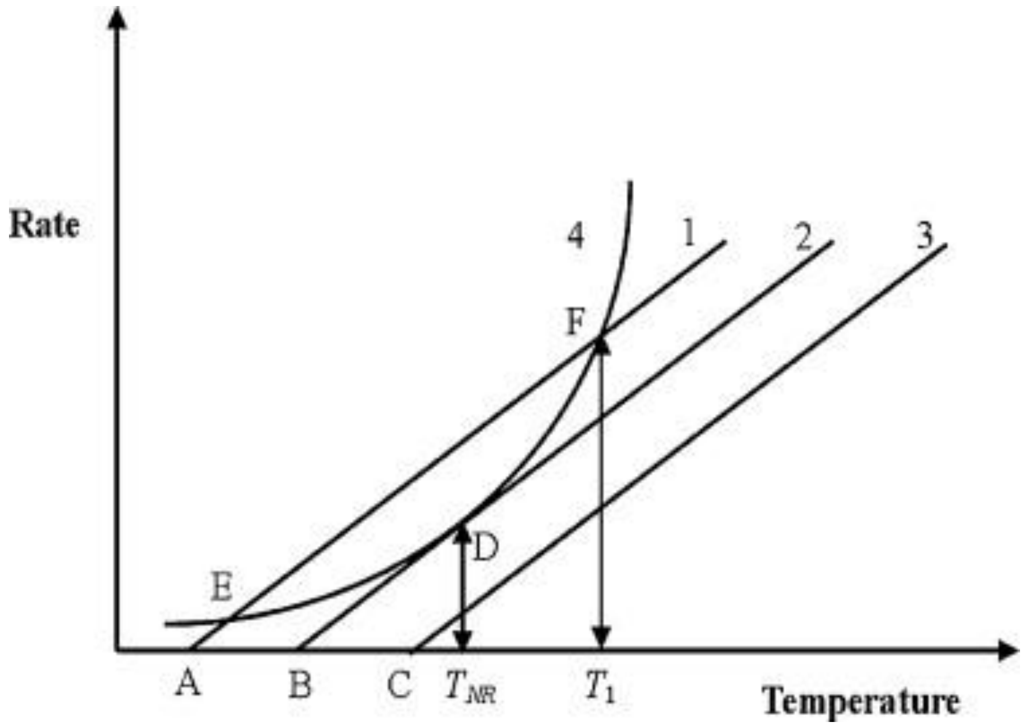
  $\dot{Q} = \Delta H \cdot k_0 \cdot \exp(-E_a/RT)$ i.e. exponential

- the removed heat will often follow the Fourier laws of heat dissipation

  $\dot{Q} = U \cdot A \cdot \Delta T$ i.e. linear

Essentials of scientific basis (3): graphic illustration

This leads to the following kind of plots (so-called Semënov plots, here taken from [2]):

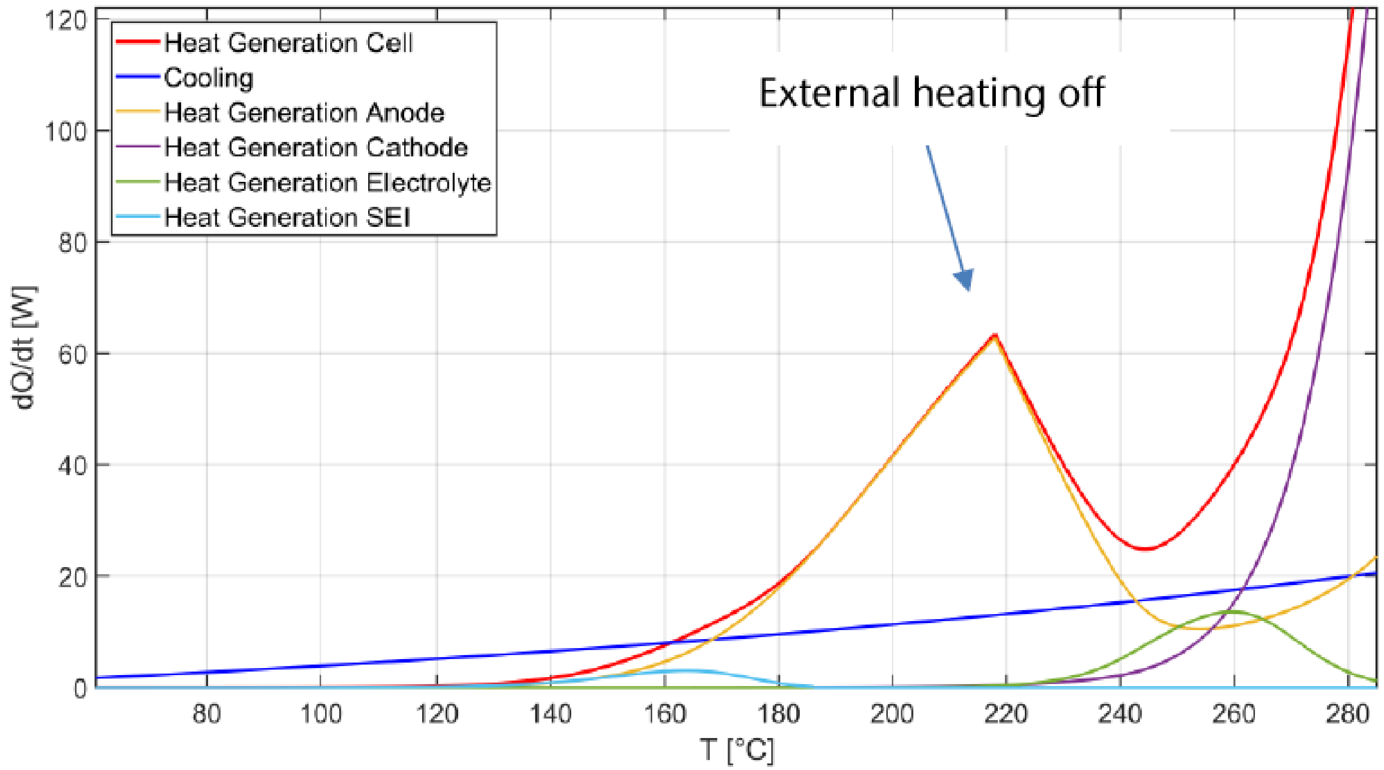


linear: heat removal

exponential: heat generation

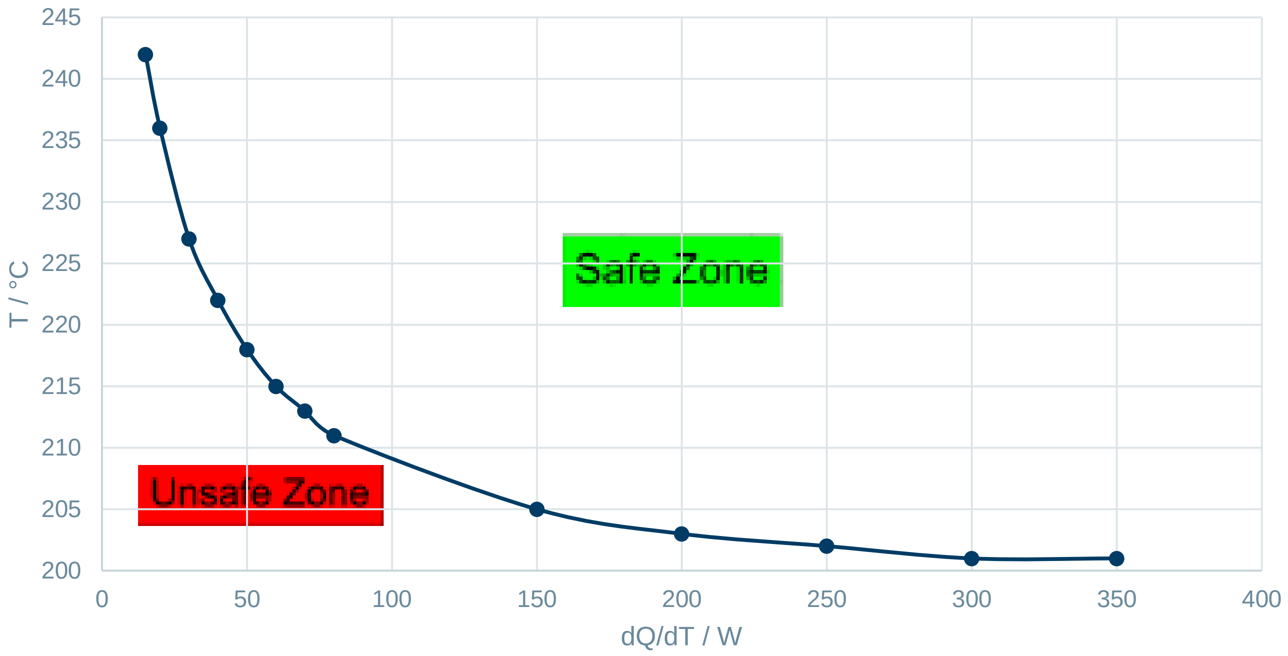
When the straight line is above the parabola, no TR can take place!

Application 1: influence of different processes during thermal runaway



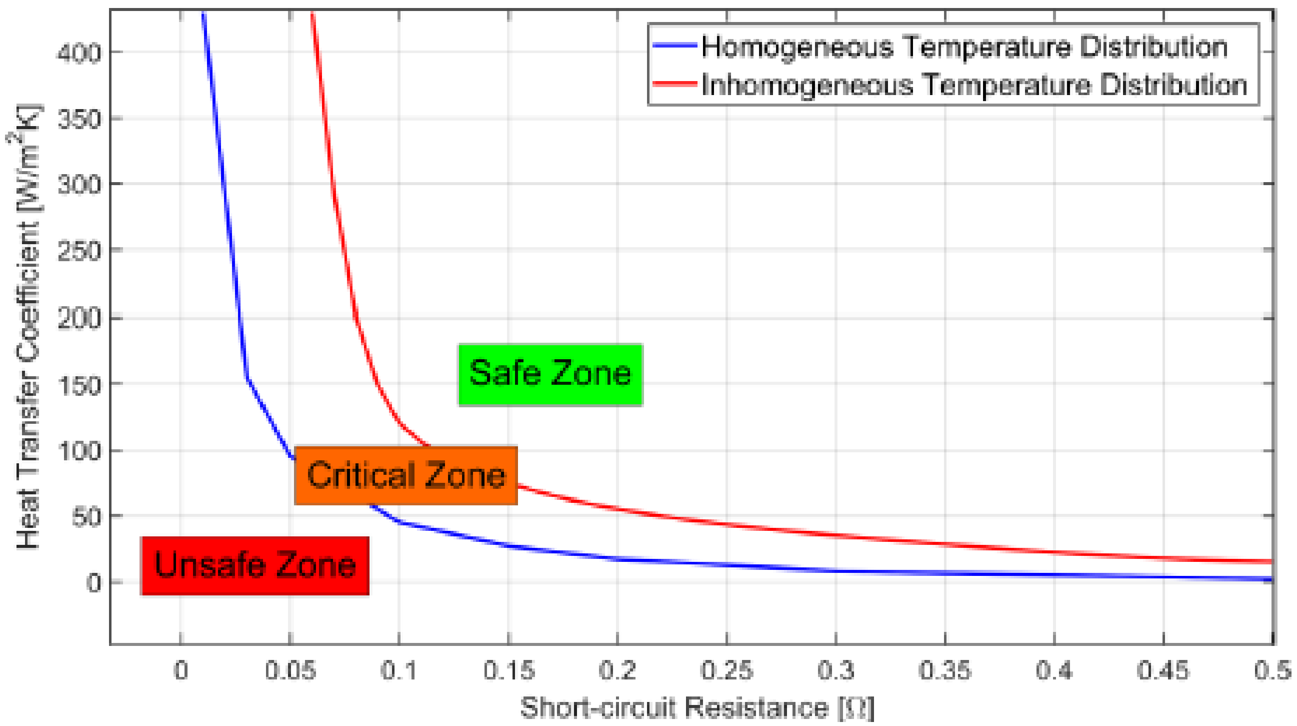
Simulation results of Thermal Runaway initiated by external heating shown as Semenov Plot.

Application 2: safe and unsafe zones



Critical temperatures at different cooling rates

Application 3: the appearance of an intermediate zone



Analysis of different short-circuit resistances on the effect on the critical heat transfer coefficient in cases of homogeneous and inhomogeneous temperature conduction

Temperature inhomogeneity (as unavoidable in a battery) lead to the appearance of an intermediate zone.

Conclusions

1) The results of the simulation study show that realistic thermal runaway situations can be modelled by literature-known techniques. A further ACEA research study has shown that a variety of modelling methods exists also for module and system levels.

2) The results show that safe zones exist where thermal runaways cannot occur. So far, the GTR 20 discussions don‘t really reflect how to treat these systems if GTR 20 keeps the goal the create a „universal“ thermal propagation test based on a suitable trigger method.

3) However, it is not realistic and would be an overburdening of EVs if we require them to be designed in a way that they are always in the safe zone (also ICE vehicles can burn, i.e. they are not required to stay always in the zone). The results show that there is an intermediate, i.e. a critical zone, where an internal heating-up can occur but where measures can be taken to prevent it from becoming a real danger for passengers.

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KEY MESSAGE:
State of the art analytical methods can be used to simulate certain aspects of thermal runaway and thermal runaway propagation. Results from such simulations can be used to understand these behaviors and illustrate the potential value of and methods for detection of internal shorts.

Modelling as a tool to predict Li ion battery thermal propagation safety performance

A literature survey of state of the art principles and commercial software

Introduction

Background

- Modelling and simulation are frequently used engineering tools for product development and system performance characterization in the automotive industry
  - Evaluate design requirements and limits
  - Cost-effective approach to investigating a large number of possible scenarios
  - Identify “worst case conditions” for further performance verification

Objective

- Feasibility study of current state-of-the-art simulation methods for thermal propagation within automotive traction batteries
- Focus on battery pack/system modeling
- HORIBA-MIRA performed the study on commission from ACEA TF-EVS

Battery modelling – general review

- Three scales suggested
  - ➢ Material level – Microscopic length scale – Elementary processes such as charge transfer, Li diffusion through the active material particles and electrolyte or particle deformation are described
  - ➢ Cell level – Mesoscopic length scale – Transport, thermodynamic, thermal, mechanical and kinetic phenomena to describe cell performance. For efficiencies sake, microscale physical models are in reduced form at this length scale
  - ➢ Pack level – Macroscopic length scale – Cells are undifferentiated with their behavior averaged, to address integration issues
- Two types of models:
  - Empirical – no physiochemical information – Equivalent Circuit Models (ECM)
  - Analytical – electrochemical, thermal and/or multi-physics principles

CAEBAT program

- The Computer Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT) project was launched by US DOE 2010
  - NREL lead
  - 5 national labs, 7 industry partners, 4 research institutes

  https://www.nrel.gov/news/features/2017/computer-aided-design-speeds-development-of-safe-affordable-and-efficient-batteries.html
- Objective to develop cutting edge battery simulation tools
- Program developed a flexible model to help with the prediction of battery behaviors at larger scales under a wider variety of performance and abuse conditions
- Program model basis for 3 commercial software developments
  - ANSYS
  - Siemens
  - Gamma Technologies

CAEBAT program

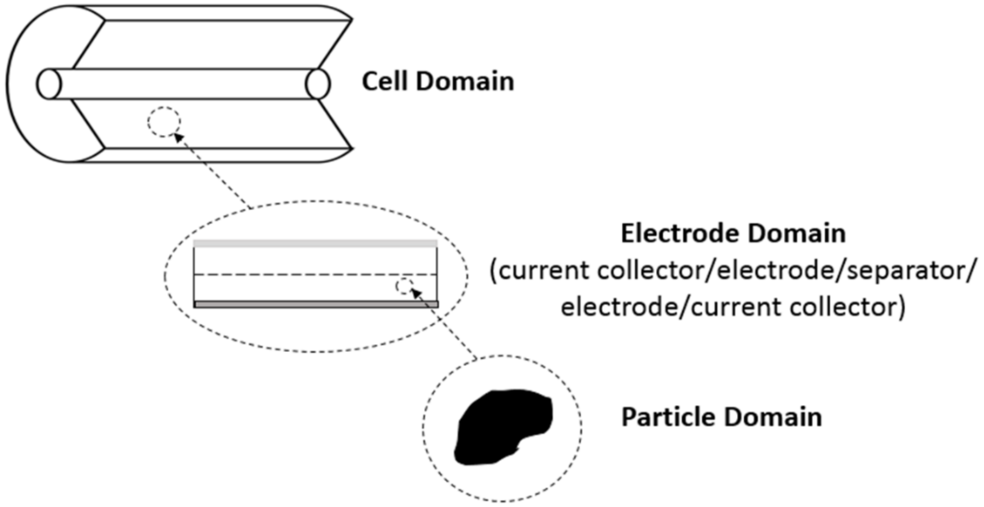
- CAEBAT-I (2011): Multi-Scale Multi-Domain (MSMD) model
  - Modular multi-physics framework
  - Software tools for cell and battery design

  http://jes.ecsdl.org/content/158/8/A955
- CAEBAT-II (2016): GH-MSMD model - Centered on safety performance
  - Couple MSMD electrochemical, thermal and chemical models with LS Dyna Mechanical crash package

  http://jes.ecsdl.org/content/164/6/A1076.full
- CAEBAT-III (ongoing): Effect of microstructure to understand impact of material formulation and manufacturing control

MSMD model features

- Applicable to large format prismatic cell formats and battery packs
  - ➢ Addresses interplay of physics on varied scales
    - ✓ Non-uniformity of the electric potential along the current collectors in cell composites
    - ✓ Non-uniformity of the temperature throughout the cell volume
- The model has a hierarchical structure in that solution variables defined in a lower hierarchy domain have finer spatial resolution than those solved in a higher hierarchical domain
  - ➢ Independent coordinate system is used in each domain to spatially discretize the variables solved in that domain
  - ➢ Decoupled geometries but coupled physics
  - ➢ Flexible model in that multiple sub-model options, with arbitrary physical and computational complexities, can be implemented in a domain independently from the choice of models and solver schemes used in the other domains.



Spotnits ARC approach

- New modeling approach for estimating thermal abuse tolerance of LIB packs presented 2006
  - Cell exothermal behavior described by Accelerated Rate Calorimetry (ARC) measurements
  - Energy balance solved at pack level

Key modelling observations

- Arrhenius equations commonly used to describe the chemical reaction kinetics of thermal runaway
  - Parameters needed as input can be obtained from through Accelerating Rate Calorimetry (ARC), Differential Scanning Calorimetry (DSC), Vent Size Package 2 and C80 Micro-Calorimeter testing
- 3D Convective flow and heat transfer is a key aspect of battery modelling including thermal runaway and thermal propagation
- 3D electrical bus bar connector conductive pathways should be included in battery models as they can be an important heat transfer path especially during thermal propagation modelling
- Current modelling approaches assume the structural integrity of the cell and its contents remains unchanged by a thermal runaway event.
- Sooting of cells and surrounding components (cells, case, electrical tabs etc) undergoing thermal runaway increases the surface radiation surface emissivity values (black body) and is likely to be an important effect

Conclusions

- Thermal propagation studies at module or battery level emerging in scientific reports and commercial modelling tools are available
  - CAEBAT one of the most ambitious modelling efforts and is the basis of several software packages
  - Flexible model to help with the prediction of battery behaviours at larger scales under a wider variety of performance and abuse conditions
  - Modelling in multiple scales speed up computational time
- Sensitivity studies of critical modelling parameters show that thermal propagation can be slowed down and some times prevented by
  - Increasing the thermal runaway temperature
  - Reducing total energy release during thermal runaway
- 3D CFD approaches incorporating analytical electrochemical and empirical electrical ECM models appear to be a mainstream research area
- Battery thermal modelling and in particular thermal runaway simulation, is a complex, non-trivial and specialized area requiring expert knowledge in many disciplines, backed up with extensive testing for input data as well as to correlate and tune the modelling approaches

Back-Up

Description of a scientific basis for safe and unsafe zones with respect to thermal runaway and thermal propagation

including: an example of application of an analysis method to support development

Annex 1

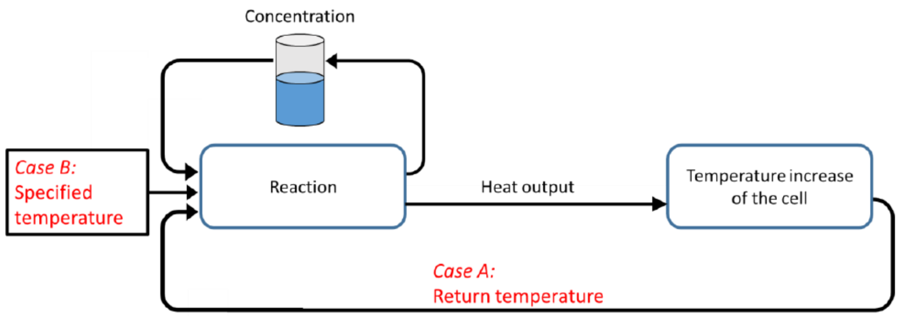
List of parameters used in the simulation model

starting point: parameters often used in the literature, i.e.:

Symbol	Value	Physical description
m	$0{,}05\ kg$	Mass of cell
c_p	$830\ J/(kgK)$	Heat capacity
α	$7{,}17\ \mathrm{W}/(m^2K)$	Heat transfer coefficient
A	$0{,}0042\ m^2$	Surface
T_{amb}	$298\ K$	Ambient temperature
ρ	$2700\ kg/m^3$	Density
V_c	$1{,}654 \cdot 10^{-5}\ m^3$	Volume
V_{jr}	$1{,}3832 \cdot 10^{-5}\ m^3$	Jellyroll volume
$\dot{Q}_h$	$50\ W$	Heating power
R	$8{,}314\ J/(mol\ K)$	Gas constant
W_C	$610{,}4\ kg/m^3$	Specific carbon content in jellyroll
W_{NMC}	$1221\ kg/m^3$	Specific NMC content in jellyroll
W_e	$406.9\ kg/m^3$	Specific electrolyte content in jellyroll
H_C	$1{,}174 \cdot 10^6\ J/kg$	Anode-Electrolyte heat release
H_{SEI}	$2{,}57 \cdot 10^5\ J/kg$	SEI-Decomposition heat release
H_{NMC}	$3{,}14 \cdot 10^5\ J/kg$	Cathode-Electrolyte heat release
H_e	$1{,}55 \cdot 10^5\ J/kg$	Electrolyte-Decomposition heat release

List of chemical reactions used in the simulation model

starting point: a Matlab/Simulink model with reactions often used in the literature



used literature for the chemical reactions:

L. Zhang, M. Xu, P. Zhao, and X. Wang, "A Computational Study on the Critical Ignition Energy and Chemical Kinetic Feature for Li-Ion Battery Thermal Runaway: WCX World Congress Experience," 2018.

P. T. Coman, E. C. Darcy, C. T. Veje, and R. E. White, "Modelling Li-Ion Cell Thermal Runaway Triggered by an Internal Short Circuit Device Using an Efficiency Factor and Arrhenius Formulations," *J. Electrochem. Soc.*, vol. 164, no. 4, A587-A593, 2017.

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Annex 2

Information of commercial software packages

Commercial/industrial software packages

Main packages:

- COMSOL - Multiphysics + CFD Module + Batteries & Fuel Cell Module
- ANSYS - Fluent
- SIEMENS - Battery Design Studio & Star-CCM+
- Gamma Technologies – GTSuite + Autolion1D, AutoLionGT, AutoLion3D, AutoLionST (Acquired from EC Power)
- ThermoAnalytics Incorporated – TAITherm + Battery Module

Note: Software information and summary of main strengths and weaknesses is found on the following slides.

Company	Software Products	Type
COMSOL	Multiphysics	Main multiphysics simulation package
	CFD Module	CFD solver add on module
	Batteries & Fuel Cell Module	Battery & Fuel cell add on module
	Heat Transfer Module	Heat transfer including 3D surface to surface radiation

Strengths
Coupled wide ranging multiphysics environment
Very detailed electrode and cell modelling abilities
1D electrical ECM models (empirical)
1D electrochemistry models (Physics based Newman P2D, reduced order SPM), 3D cell model coupled to 1D electrochemistry model
Cell level ISC modelling (particles/fibres/filaments) with exothermic decomposition reactions to model TR
Detailed hetrogeneous porous electrode model (more involved than homogeneous Newman model)
Butler-Volmer & Tefal equations for predefined kinetics
Simplified 1D SPM formulation for electrode electrochemistry
Lumped battery model
Modelling of aging mechanisms due to structural, thermal and chemical effects - including SEI layer growth modelling
Intercalation (internal particle diffusion) modeling

Weaknesses
Many add on modules required for module/pack level simulation (cost)
Scalability to Module/Pack Level TR? (long simulation time/high numerical expense?)
Detailed CFD meshing required of solids and fluid regions
No NREL MSMD framework?
Required parameter inputs (the more physics the more parameters required)
Newman P2D model requires the most user inputs and is numerically expensive (most accurate) for module/pack level
3D air/liquid flow only accounted for via CFD module use
Level of CPU core parallelisation?

Company	Software Products	Type
ANSYS	Fluent	CFD solver with battery module included

Strengths

CFD solver gives a naturally 3D and time dependent thermal and flow environment

Single Potential empirical battery model - for single cells

- NTGK electrochemical model (simple)
- Geometry of current collector/electrodes/seperator are fully resolved

Dual Potential MSMD battery model - NREL MSMD framework (& faster GH-MSMD) - volume mesh of the cell not constrained by the microstructure (jellyroll)

Detailed 3D meshing of the cell microstructure (components) not required with MSMD framework

DP-MSMD model - 3 Electrochemical submodels

- NTGK (simple empirical model, with overpotential and entropic heat sources)
- Electrical ECM (empirical)
- Newman P2D (physical model)

External & ISC short models (DP-MSMD)

Highly parallelised CFD solver (run on 1000's of CPU cores)

2 Semi-Empirical TR abuse models - 1 eqn & 4 eqn kinetics decomposition models (SEI/-ve electrode-electrolyte/+ve electrode-electrolyte reactions/Electrolyte)

Surface to Surface radiation model along with conduction modelling

Air/liquid flow and convective expicitly solved with the Navier Stokes equations

Fully coupled flow/thermal/electrochemistry

Weaknesses

NTGK model cannot accurately capture cell dynamic (inertial) response

Newman P2D model requires the most user inputs and is numerically expensive (most accurate) for module/pack level

Transient run time of days likely

Parallel solver licences cost extra

No aging model

No detailed cell designer

Company	Software Products	Type
SIEMENS	Battery Design Studio (BDS)	Battery cell design tool (jelly roll design)
	STAR-CCM+	CFD solver

Strengths

BDS - Comprehensive cell designer used to create and investigate single cell designs, including the jellyroll electrode design.

STAR-CCM+

4 Electrochemical models

- NTG model (empirical)
- Electrical ECM model (empirical)
- Newman P2D, includes aging model (SEI growth)
- 3D Microstructural electrochemistry model
    - Explicit 3D representation of non-homogeneous components in the electrode layer (different particle shapes and distributions)

Air/liquid flow and convective expicitly solved with the Navier Stokes equations

Surface to Surface radiation model along with conduction modelling

Fully coupled flow/thermal/electrochemistry

Weaknesses

NTG model cannot accurately capture cell dynamic (inertial) response

Newman P2D model requires the most user inputs and is numerically expensive (most accurate) for module/pack level

Transient run time of days likely

Add on cost

Parallel solver licences cost extra

TR abuse reaction modelling?

Company	Software Products	Type
Gamma Technologies	GT-Suite	Multiphysics system level package
	AutoLion1D	1D LIB cell design/evaluation tool
	AutoLionGT	Autolion battery models in 1D GT-Suite system
	AutoLion3D (AutoLion acquired from EC Power)	3D thermal/electrochemistry module

Strengths

GT-Suite - Excels at system level 1D modelling (flow and thermal)

AutoLion1D

- 1D material scale to cell level electrochemistry evaluation under different duty cycles, aging models (calender and cycle)
- Large database of existing chemistries

Autolion3D

- 3D CAD and mesh 3D cells/modules
- Cell level (3D thermal + 3D cell electrochemistry) and pack level (3D thermal + 1D electrochemistry model)
- TR modelling (ISC, external shorts, nail penetration)

AutoLionGT

- Allows GT-Suite to have a comprehensive electrochemical materials database of AutoLion battery models
- Prediction of vehicle range performance
- Aging models (SEI layer growth, lithium plating)
- Pack level modelling (1D)

Electrical ECM model (empirical) and Electrochemistry battery models (Newman physics based P2D)

BMS assessment

Weaknesses

Autolion3D - For CFD flow and heat transfer needs 3rd party CFD solver (run entirely inside CFD solver) - Added cost

Autolion3D - Runs only in a third party CFD solver?

Costs of modules

Company	Software Products	Type
ThermoAnalytics Incorporated	TAITherm Battery Module CoTherm	Thermal Analysis package

Strengths
3D Surface to Surface Radiation (including diurnal solar) and 3D multilayer conduction nail ISC external short 3 Battery electrochemical models (all empirical) - NTG ECM model (0D lumped electrical model) - NTG Distributed Model (cell mesh duplicated to represent thermal and electrical domains) - single cell analysis - NREL ECM model (0D lumped electrical model, includes filter circuits for better transient prediction + current limiting device option) NREL TR model NREL life cycle and aging model Focused on Cell/Module/Pack level analysis Speed advantage compared to CFD or 3D FEA methods (due to no analytical electrochemical model and no 3D flow solver)

Weaknesses
0D/1D Convection heat transfer No 3D flow solver/3D convection - Requires CoTherm to 2 way couple with a CFD flow solver (more complexity/longer run times) Battery & CoTherm Modules - Add on costs Not highly parallel No Newman P2D electrochemical physical model