

**QUEEN'S UNIVERSITY**IONIC LIQUID
LABORATORIES

QUILL

# Hybrid Thermal Runaway Propagation Prevention for Lithium-ion Batteries in EVs

**David McAreavey** 

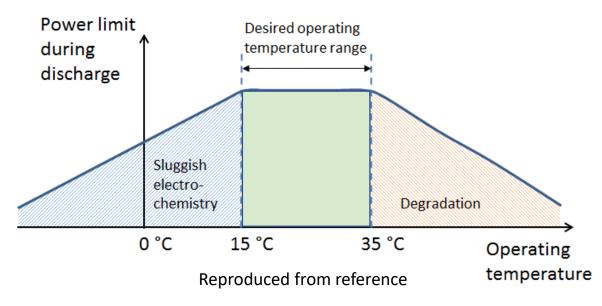
QUILL MEETING, 25/03/2024

# Battery electric vehicles (BEV)

	IC Ford F150	Electric Ford F150
Energy density	46.6 MJ/kg	0.46-0.72 MJ/kg
Energy source weight	62.6 kg (23 gallon)	816.5kg (standard range)
Vehicle weight	1845.7 kg	2948.35 kg
Battery/fuel vehicle weight percentage	3.4%	27.7%



# Project overview

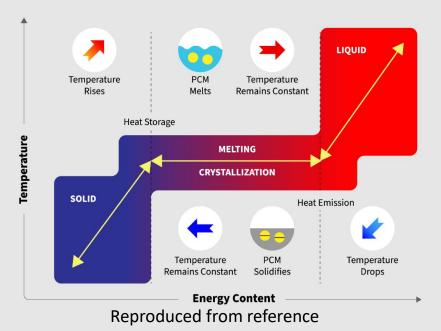


- Inadequate cooling system
- Cells at low states of health
- Cells discharged at too high a rate



Reproduced from reference

### Interstitial materials



**PCMs** 



Aerogels

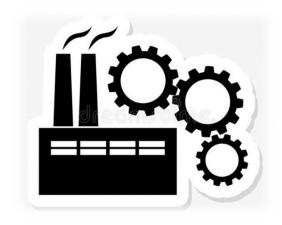


High conductivity

Metal plates

Graphite sheets

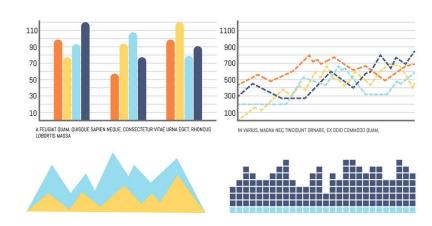
### **Industry Trends**



#### **Consumers**



#### **Past Data**



### Research



### **Industry Trends**

Energy density

Cell cost

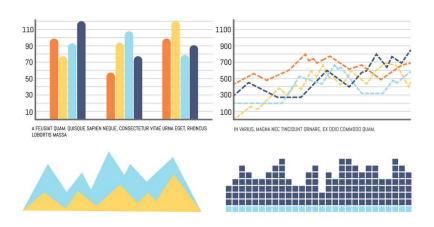
Price parity



**Consumers** 



#### **Past Data**



### Research



### **Industry Trends**

Energy density

Cell cost

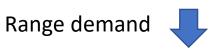
Price parity



#### **Consumers**

Consumer priorities for EV adoption, 2018 and 2020

Greater concerns are shown in orange.



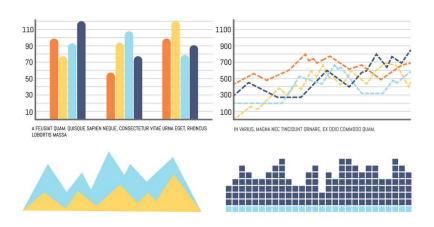
Safety concerns

			2	020 Glo	bal Auto	Consur	ner Stu	dy				
	FR	ANCE	GERN	//ANY	IT	ALY	U	IK	CH	INA	US	
In your opinion, what is the greatest concern regarding all battery-powered electric vehicles?	2018	2020	2018	2020	2018	2020	2018	2020	2018	2020	2018	2020
Driving range	31%	28%	35%	33%	4%	27%	26%	22%	25%	22%	24%	25%
Cost/price premium	32%	22%	22%	15%	19%	13%	24%	16%	9%	12%	26%	18%
Time required to charge	11%	15%	11%	14%	18%	16%	13%	16%	12%	15%	10%	14%
Lack of electric vehicle charging infrastructure	16%	22%	20%	25%	44%	32%	22%	33%	18%	20%	22%	29%
Safety concerns with battery technology	4%	11%	5%	10%	7%	10%	6%	12%	22%	31%	8%	13%
Others	6%	2%	7%	3%	8%	2%	9%	1%	14%	0%	10%	1%
Total	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Sample size	1,083	1,266	1,287	3,002	1,048	1,274	965	1,264	1,606	3,019	1,513	3,006

Source: Deloitte Global Auto Consumer Study<sup>18</sup>

Deloitte Insights | deloitte.com/insigl

#### **Past Data**







### **Industry Trends**

Energy density

Cell cost 、

Price parity



#### **Past Data**



- Inconsistent picture of the frequency of EV fires/runaway events
- Small data sets

#### **Consumers**

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#### Research



### **Industry Trends**

Energy density

Cell cost

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#### **Past Data**

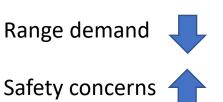


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Research Early detection · Vent gases



#### Research Phase change materials

· Paraffin wax

Cell swelling

detection

Temperature based

Rubitherm (RT15)



#### Research **Dedicated suppressants**

- Water mist
- Dry powders
- CO<sub>2</sub>



#### Research

Cell material modification

- Electrolyte
- Separator
- electrodes



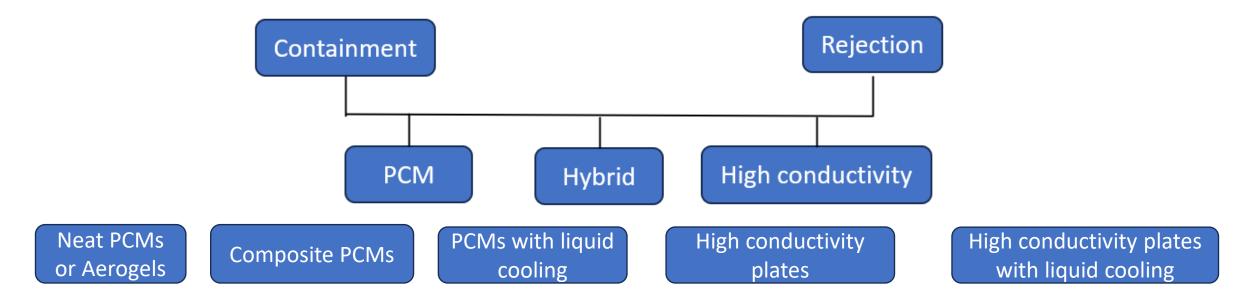
BMS -AC cooling system (refrigerant)

#### https://www.patentsencyclopedia.com/app/20100086844

- LaMonica M. MIT Technology Review . 2012. Available from: https://www.technologyreview.com
- · Koch S, Birke KP, Kuhn R. Fast thermal runaway detection for lithium-ion cells in large scale traction batteries. Batteries.
- Kshetrimayum KS, Yoon YG, Gye HR, Lee CJ. Preventing heat propagation and thermal runaway in electric vehicle battery modules using integrated PCM and micro-channel plate cooling system. Appl Therm Eng. 2019;159(May):113797. Available from: https://doi.org/10.1016/j.applthermaleng.2019.113797
- Liu Y, Duan Q, Xu J, Li H, Sun J, Wang Q. Experimental study on a novel safety strategy of lithium-ion battery integrating fire suppression and rapid cooling, J Energy Storage . 2020;28(December 2019):101185. Available from: https://doi.org/10.1016/j.est.2019.101185



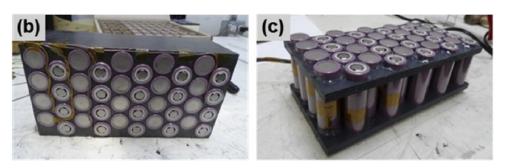
### Interstitial materials

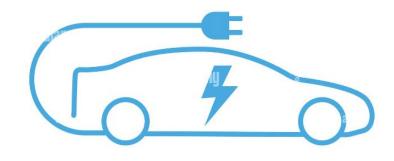


- Spectrum of interstitial materials and options.
- Optimisation of these systems for the pack design is important considering thermal conductivity and conduction paths.
- The combination of systems often shows greater success than any single approach.
- Flammability of PCMs remains a sticking point.

### Novelty

- This work wants to look at the viability of applying interstitial materials to an EV when considering:
  - Weight
  - Volume
  - Energy
- Consider the integration of a thermal runaway propagation system alongside thermal management.

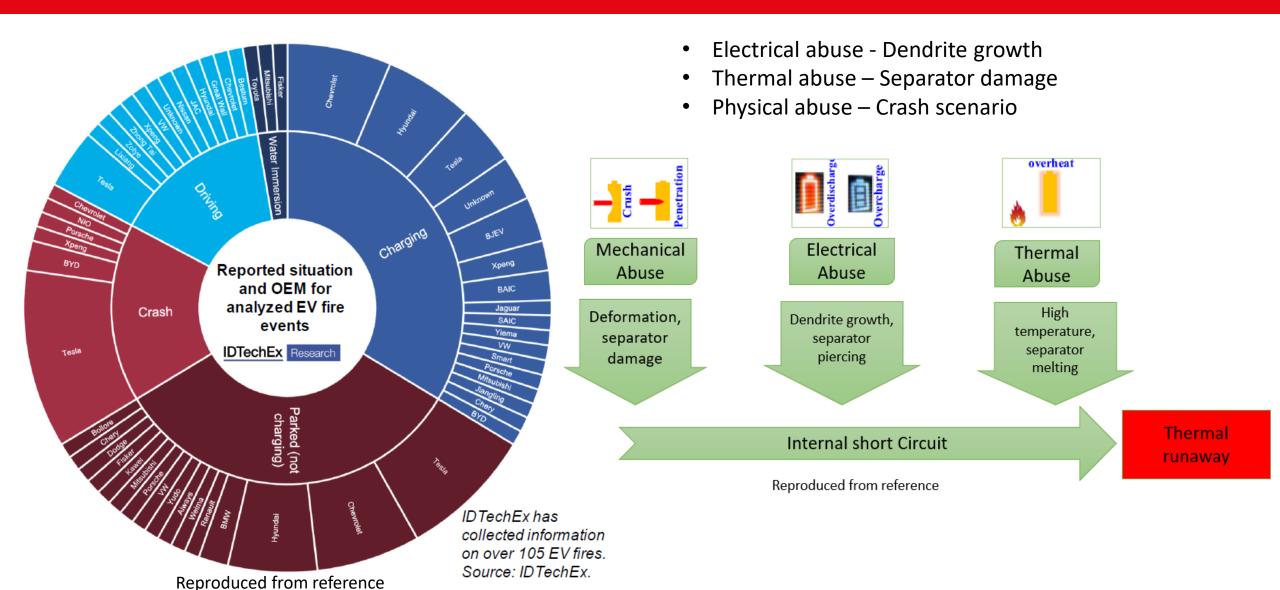




Preventing thermal runaway propagation



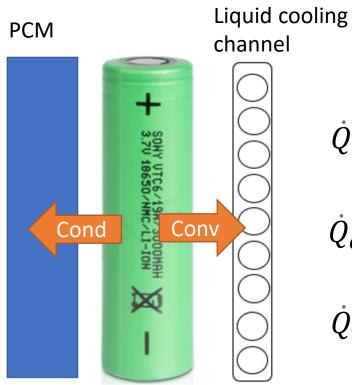
### **Initiation Scenarios**



Lai X, et al. Mechanism, modelling, detection, and prevention of the internal short circuit in lithium-ion batteries: Recent advances and perspectives. Energy Storage Mater 2021;35(October 2020):470–99. Available from: https://doi.org/10.1016/j.ensm.2020.11.026

12

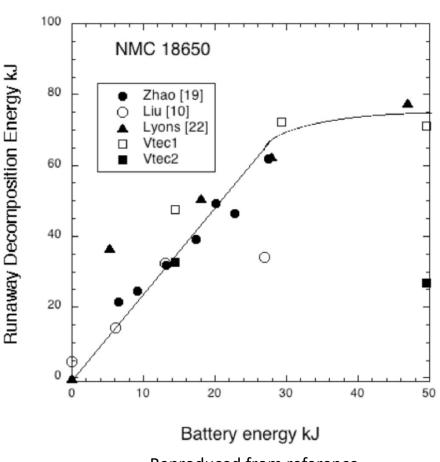
# Governing Equations of Calculations



$$\dot{Q}_{cond} = -kA \frac{dT}{dx}$$
 (W)

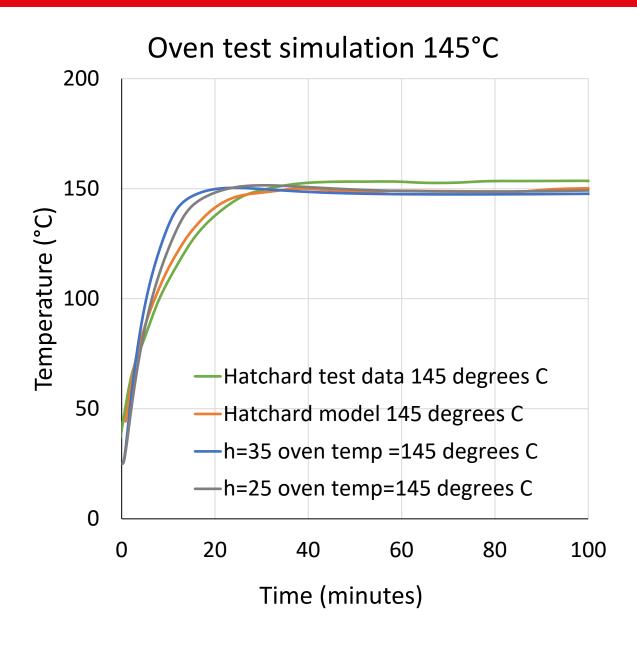
$$\dot{Q}_{conv} = hA_s(T_s - T_\infty)$$
 (W)

$$\dot{Q}_{rad} = \sigma \varepsilon A \left( T_s^4 - T_{amb}^4 \right) \text{ (W)}$$

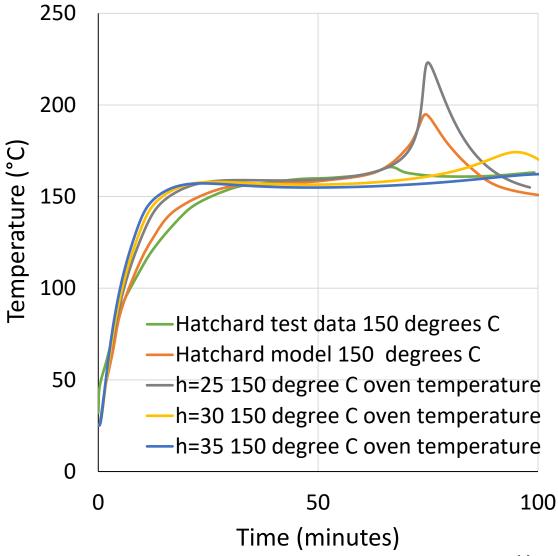


Reproduced from reference

### Oven tests 2D MATLAB

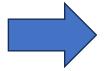


#### Oven test simulation 150°C

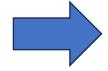


### Model development

#### Excel



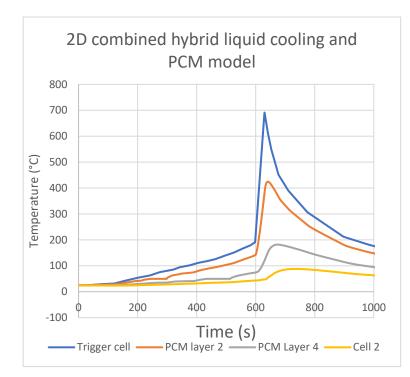
#### **MATLAB**



#### **COMSOL**

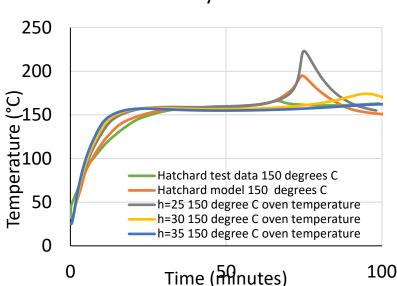
Simplified 2D model

Difficulty in calculating with small enough time steps and dealing with thermal gradients.



More developed 2D kinetics model

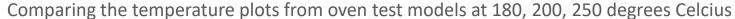
- Improvements calculating with a small time interval and dealing with thermal gradients.
- Still some problems with instability, some safeguards installed in early versions.

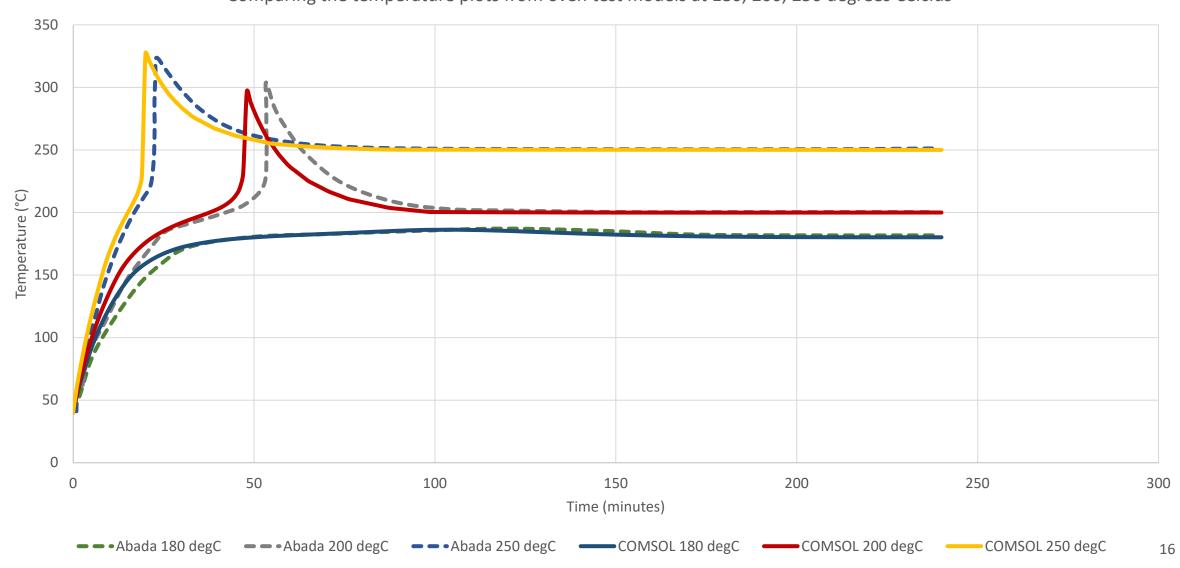


3D model, resolving shell, lumped jelly roll and active material and mandrel.

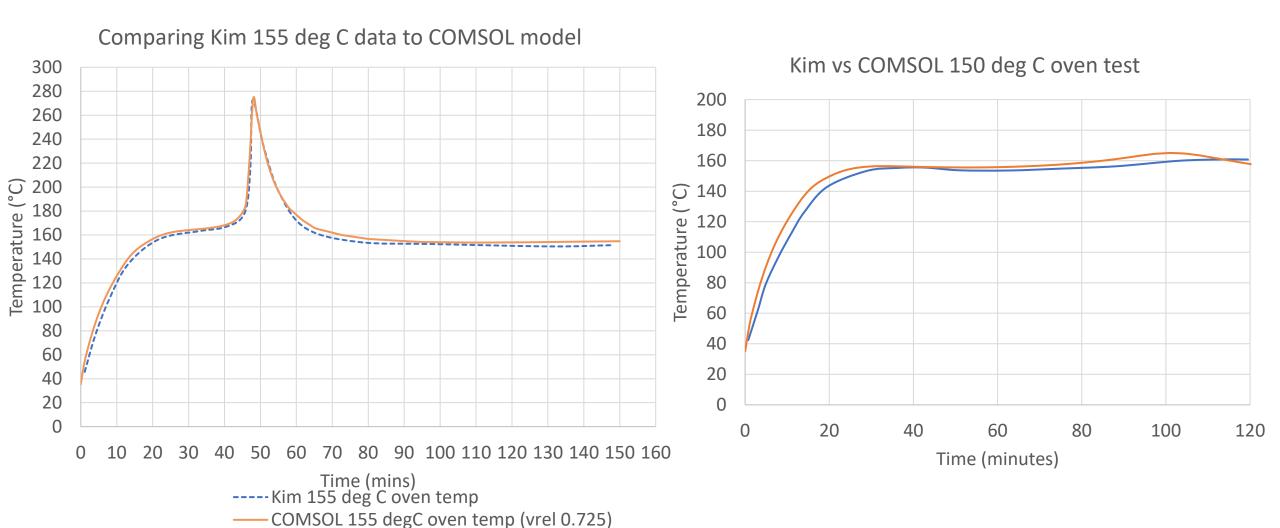
Further improvements with steep gradients and accuracy of the simulations.

# Validation of LFP against oven model



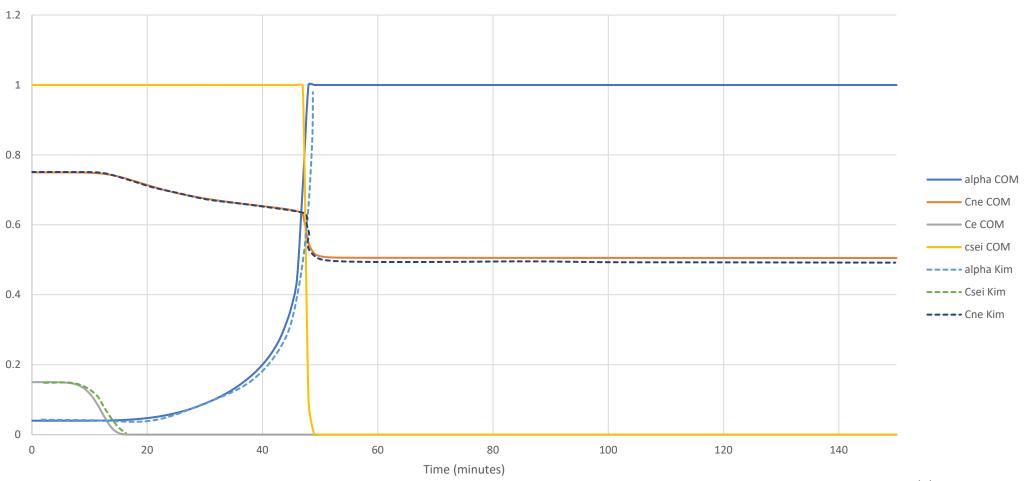


### LCO oven test model



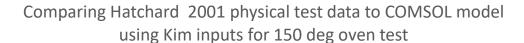
# Comparison of conversion metrics

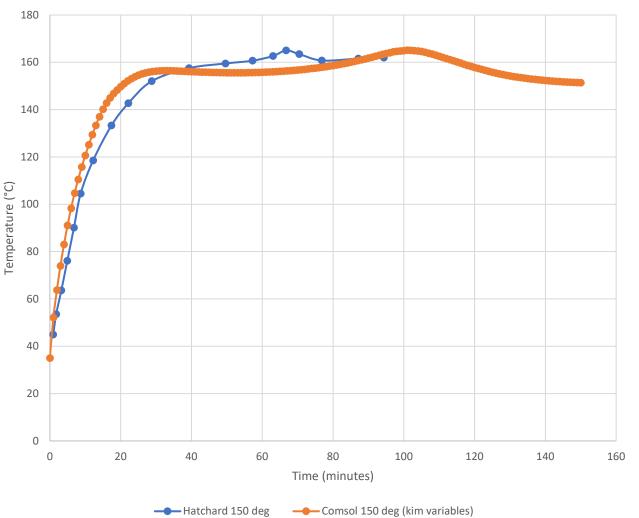




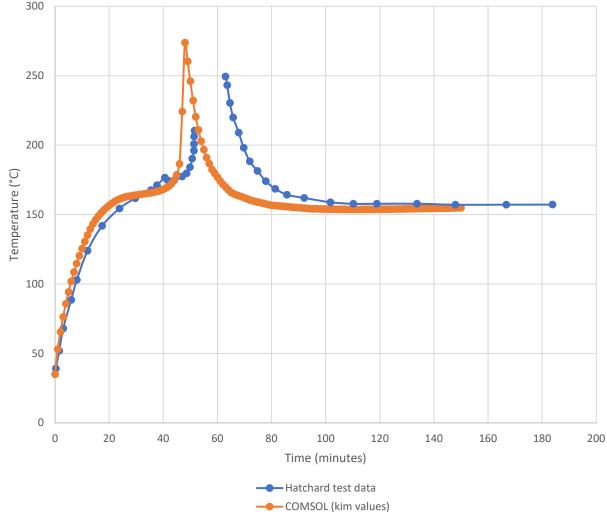
Alpha – conversion degree of positive electrode Cne – reaction of intercalated lithium at anode Ce – proportion of electrolyte remaining Csei – sei decomposition

# Comparison with test data

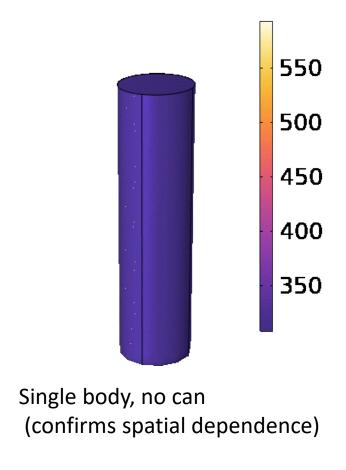


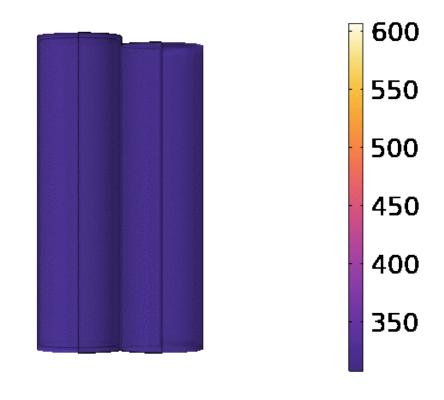


### Comparing Hatchard 2001 physical test data to COMSOL model using Kim inputs for 155 deg oven test



### Animations

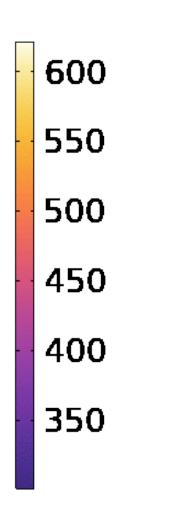




Two cells, multi body, conduction

### **Animations**







Control volume convection, radiation

Control volume, flowing air, convection, radiation

### Project direction

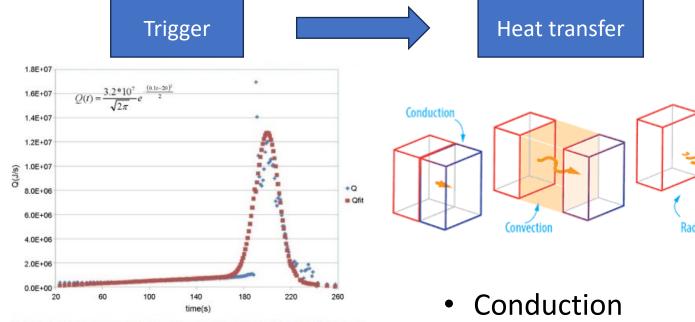


Fig. 3. Rate of heat generation per unit time based on measurements by ARC for Type 18,650 high power cells. An alternative cooling system to enhance the safety of Li-ion battery packs

### Trigger profile

- Calorimetry
- Bell curve

#### **Validation**

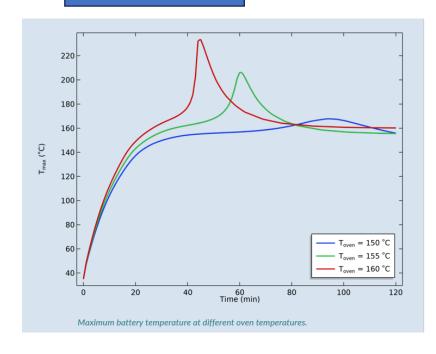
 Directly from test data

- Convection
- Radiation

### **Validated**

From low power cartridge physical test

#### Cell response



Chemical kinetics

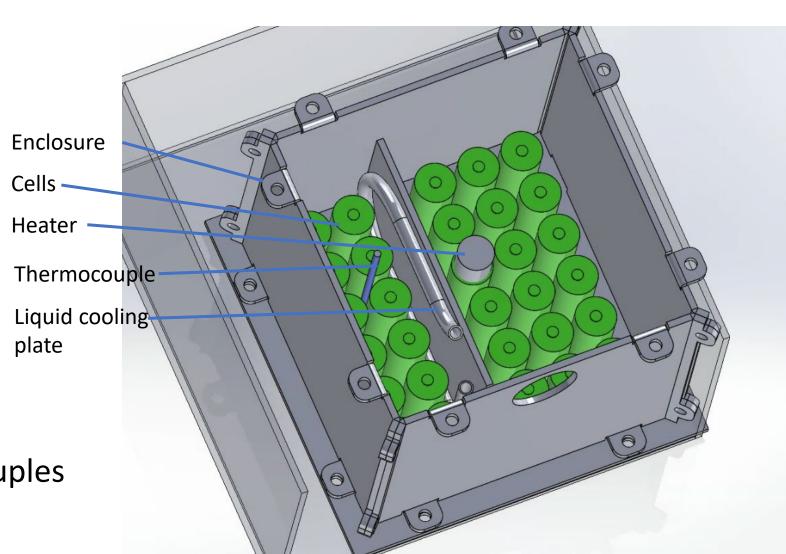
#### **Validated**

From oven tests

### Rig Design

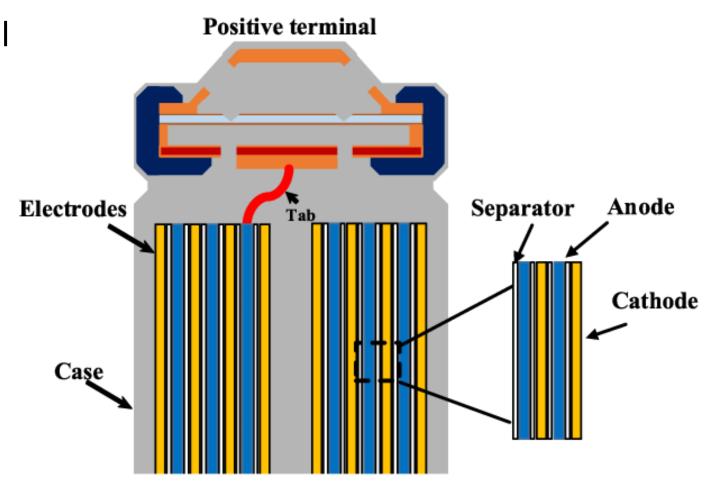
### Rig purpose

- Low power testing- COMSOL validation
- Rig for final full physical test
- Containing mock cells
- Liquid cooling
- Stainless steel enclosure
- Instrumented with thermocouples



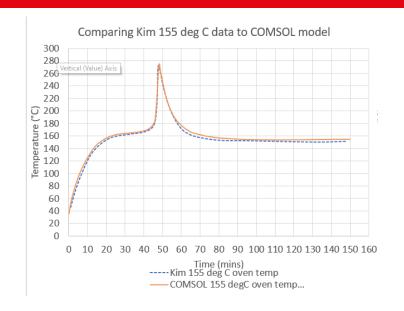
### Mock cell

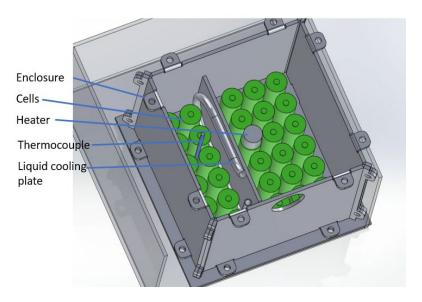
- What to consider for this mock cel
- Components
  - Can
  - Jellyroll
  - Mandrel
- Properties
  - Anisotropic thermal conductivity
  - Heat capacity
  - Dimensions
  - Cell density



### Summary

- 3D COMOSL model with chemical kinetics validated
- Full scale COMSOL model under development
  - Conduction
  - Radiation
  - Liquid cooling
  - Chemical kinetics
- Rig to validate full scale model mid development
- Cell analogue mid development.





### Future work

Present

Develop cell analogue

Produce rig

Validate COMSOL Simulation

Conduct novel simulations

November year 3

Final physical test/validation (time permitting)

- Run a range of low power tests
   Variables
- Multiple trigger profiles
- Flow rates
- Interstitial materials
- Sensitivity analysis
- Weight optimisation
- Volume optimisation
- Environmental affects

# Acknowledgements

#### Supervisors:

- Dr. Glover
- Dr. Istrate
- Prof. Nockemann

### Funding:

Department for the Economy (DfE DTP)



### Runaway reactions

$$q_{sei} = H_{sei} W_c R_{sei}$$

$$R_{sei}(T,C_{sei}) = A_{sei} \exp{(\frac{-E_{a,sei}}{RT})} C_{sei}^{M_{sei}}$$

$$q_{ne} = H_{ne}W_cR_{ne}$$

$$R_{ne}(T, C_{ne}, t_{sei}) = A_{ne} C_{ne}^{m_{ne}} \exp\left(\frac{-E_{a,ne}}{RT} - \frac{t_{sei}}{t_{sei0}}\right)$$

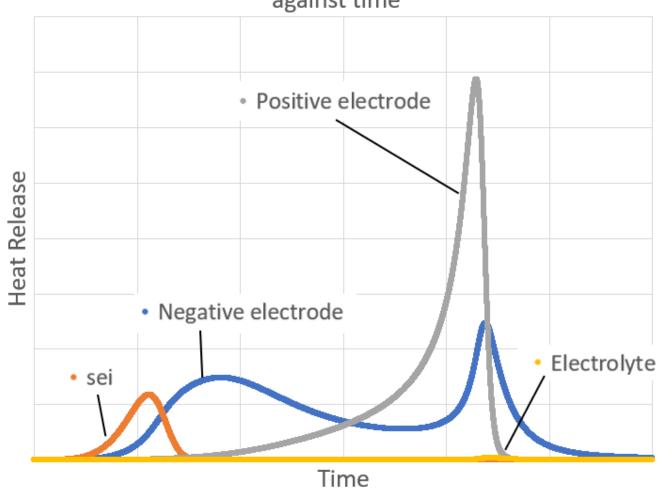
$$q_{pe} = H_{pe} W_p R_{pe}$$

$$R_{pe}(T,\alpha) = A_{pe}\alpha^{m_{pe}}(1-\alpha)^{m_{pe}}\exp(\frac{-E_{a,pe}}{RT})$$

$$q_e = H_e W_e R_e$$

$$R_e(T, C_e) = A_e \exp{(\frac{-E_{a,e}}{RT})} C_e^{m_e}$$

# Heat release in Joules across four components against time



### **Industry Trends**





#### Consumers

- Tightly packed with increasing energy density
- Cell to pack and cell to car technology
- Liquid or air cooling employed

### **Policy**

Price parity of electrified vehicles are on the horizon

### Introduction Consumer demand

### Consumer priorities for EV adoption, 2018 and 2020

Greater concerns are shown in orange.

Energy density

Cell cost

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Source: Deloitte Global Auto Consumer Study<sup>18</sup>

### **Past Data**

### **Industry**

#### Tesla Vehicle Safety Report



- 2012-2021 approximately one Tesla fire for every 210 million miles travelled
- 2012-2018 approximately one Tesla fire for every 170 million miles travelled
- NFPA shows in the US there
   is a vehicle fire for every 19
   million miles travelled

Vehicle fires a	ttended by th	e London Fire Brigade
	Electric	Internal combustion
Fires in London 2019	54	1,898
Vehicles in London	27,000	2.56 million
Incident rate	0.194%	0.075%

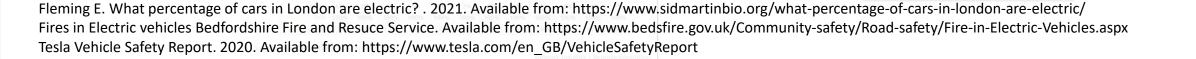
**Policy** 





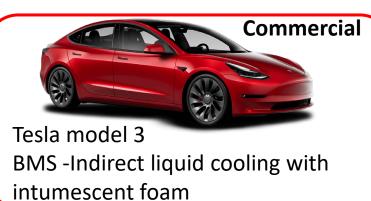


Difficult to draw reliable statistically significant conclusions from this data.



### Commercial and Research







#### Research

Phase change materials

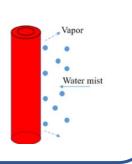
- Paraffin wax
- Rubitherm (RT15)



#### Research

**Dedicated suppressants** 

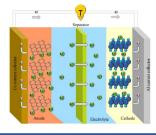
- Water mist
- Dry powders
- CO<sub>2</sub>



#### Research

Cell material modification

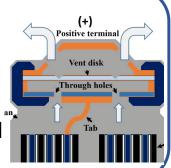
- Electrolyte
- Separator
- electrodes



#### Research

Early detection

- Vent gases
- Cell swelling
- Temperature based detection



- https://www.patentsencyclopedia.com/app/20100086844
- LaMonica M. MIT Technology Review . 2012. Available from: https://www.technologyreview.com
- Koch S, Birke KP, Kuhn R. Fast thermal runaway detection for lithium-ion cells in large scale traction batteries. Batteries. 2018;4(2):1–11.
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- Liu Y, Duan Q, Xu J, Li H, Sun J, Wang Q. Experimental study on a novel safety strategy of lithium-ion battery integrating fire suppression and rapid cooling. J Energy Storage . 2020;28(December 2019):101185. Available from: https://doi.org/10.1016/j.est.2019.101185

# Future work/ areas for investigation

Model based design Accumulator pack layout Module walls Multiple PCMs 26650, 18650 (cell trends) Novel parameters **Environmental effects** Non uniform PCM Directional calorimetry Staggered cells vs in line Thermal management Areas for Physical testing investigation Correlation of model results to physical testing Characterisation of PCMs at QUB (flammability) Define required parameters of an ideal PCM (spider plot)

Present

Model development

Design of **Experiments** 

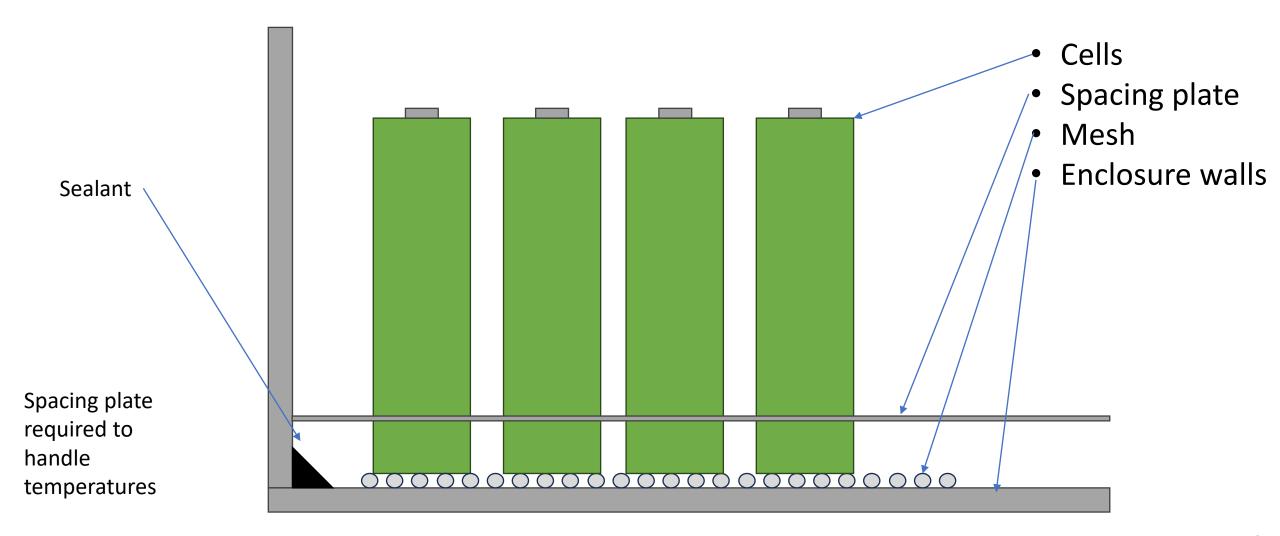
Validation

Software driven viable parametric change

Final physical test/validation (time permitting)

October year 3

# Enclosure design



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**Energy density** 

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#### Consumers

#### Consumer priorities for EV adoption, 2018 and 2020

Greater concerns are shown in orange.

• Range demand

Safety concerns



			2	020 Glo	bal Auto	Consur	ner Stud	ly				
	FR	ANCE	GERN	/ANY	IT/	ALY	U	K	CH	INA	US	
In your opinion, what is the greatest concern regarding all battery-powered electric vehicles?	2018	2020	2018	2020	2018	2020	2018	2020	2018	2020	2018	2020
Driving range	31%	28%	35%	33%	4%	27%	26%	22%	25%	22%	24%	25%
Cost/price premium	32%	22%	22%	15%	19%	13%	24%	16%	9%	12%	26%	18%
Time required to charge	11%	15%	11%	14%	18%	16%	13%	16%	12%	15%	10%	14%
Lack of electric vehicle charging infrastructure	16%	22%	20%	25%	44%	32%	22%	33%	18%	20%	22%	29%
Safety concerns with battery technology	4%	11%	5%	10%	7%	10%	6%	12%	22%	31%	8%	13%
Others	6%	2%	7%	3%	8%	2%	9%	1%	14%	0%	10%	1%
Total	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Sample size	1,083	1,266	1,287	3,002	1,048	1,274	965	1,264	1,606	3,019	1,513	3,006

Source: Deloitte Global Auto Consumer Study<sup>16</sup>

Research Phase change materials Paraffin wax Rubitherm (RT15) Research Early detection · Vent gases · Cell swelling Temperature based detection

BMS -Air cooled battery pack

#### Research



#### Research Dedicated suppressants

- · Water mist
- Dry powders
- CO<sub>2</sub>

  - LaMonica M. MIT Technology Review [Internet], 2012. Available from: https://www.technologyreview.com Koch S, Birke KP, Kuhn R. Fast thermal runaway detection for lithium-ion cells in large scale traction batteries. Batteries.
  - Kshetrimayum KS, Yoon YG, Gye HR, Lee CJ. Preventing heat propagation and thermal runaway in electric vehicle battery modules using integrated PCM and micro-channel plate cooling system. Appl Therm Eng [Internet]. 2019;159(May):113797. Available from: https://doi.org/10.1016/j.applthermaleng.2019.113797

Research

Electrolyte

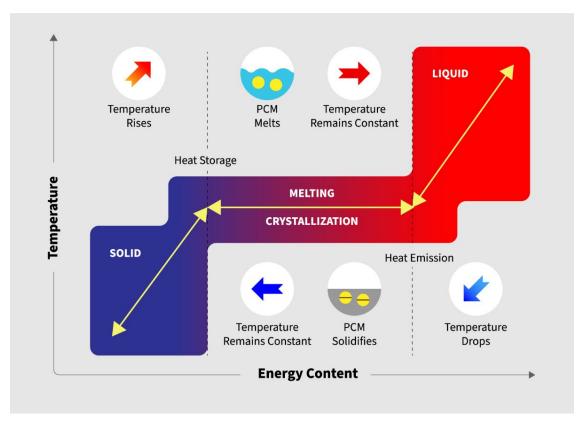
Separator

electrodes

Cell material modification

Liu Y, Duan Q, Xu J, Li H, Sun J, Wang Q. Experimental study on a novel safety strategy of lithium-ion battery in egrating fire suppression and rapid cooling. J Energy Storage [Internet]. 2020;28(December 2019):101185. Available from: https://doi.org/10.1016/j.est.2019.101185

# Phase change materials - PCM



Logic state = 1

SET

Crystallization

RESET

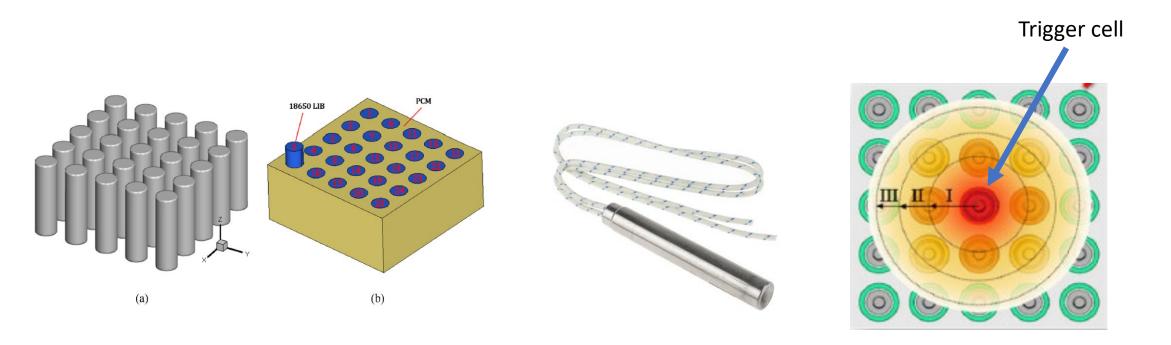
Reproduced from reference

Reproduced from reference

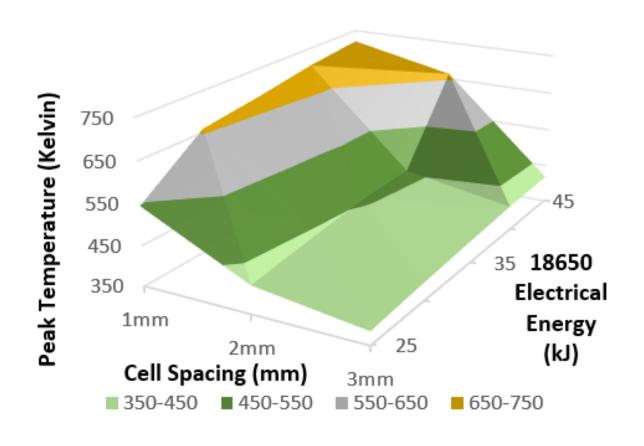
	Cp J/kgK	K radial W/mK	K axial W/mK	Density kg/m3	Cell chemistry	Source
Hatchard 2001	830	0.34		2580	18650 LiCoO2	Thermal model of cylindrical and prismatic Lithium-Ion cells
Abada 2018	1100	0.7	140	2231	18650 LFP	Combined experimental and modelling approaches of the thermal runaway of fresh and aged lithium-ion batteries
Jia				2580	18650 LCO	Thermal runaway propagation behaviour within 18650 lithiumion battery packs: A modelling study
Coleman2016	1200	0.633	48	2222		Reducing cell-to-cell spacing for large format lithium ion battery modules with aluminium or PCM heat sinks under failure conditions
Zhang	1143	5	1	2800	18650 Samsung 33G	Non-uniform phase change material strategy for directional mitigation of battery thermal runaway propagation
Yuan	1143	5	1	<del>2800</del>	18650 Samsung 33G	Inhibition effect of different interstitial materials on thermal runaway propagation in the cylindrical lithium-ion battery module
N.Spinner (Analytical)	972+-92	0.55+-0.23	21.9+-1.7		LiCoO2	Analytical, Numerical and Experimental Determination of Thermophysical Properties of Commercial 18650 LiCoO2 Lithium-Ion Battery
Nieto 2014	<del>1076</del>	<del>1.36</del>	<del>29.4</del>	<del>2382</del>	NMC Pouch	Novel thermal management system design methodology for power lithium-ion battery
S.J Drake 2013	1720+-86	0.2+-0.01	30.4+-1.5	2362	18650 LFP	Measurement of anisotropic thermophysical properties of cylindrical Li-ion cells
Gumussu 2017	814-2400	0.219	28.05	2939	Panasonic NCR18650B	3-D CFD modeling and experimental testing of thermal behavior of a Li-Ion battery
Sabbah 2008	900	3	30	2663	18650 high power	Active (air-cooled) vs. passive (phase change material) thermal management of high power lithium-ion packs: Limitation of temperature rise and uniformity of temperature distribution
Jiang 2023		2.4	14.07	3020		Axial and radial thermal conductivity measurement of 18,650 Lithium-ion battery
Average	1123.57 (830-1200)	1.005 (0.2-5)	44.62 (30-140)	2599.7 (2200-2800)		

# Experimental

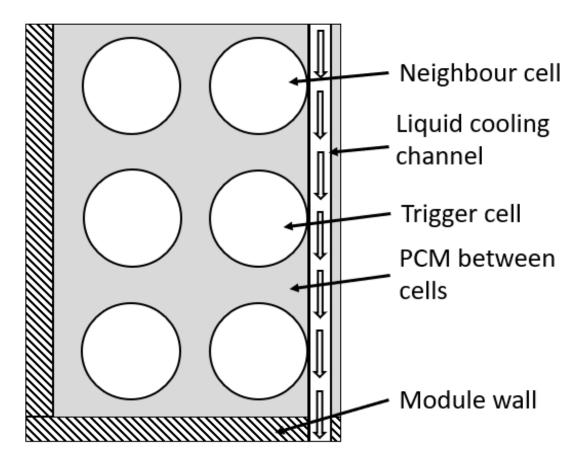
- Strict safety concerns with provoking a module of cells.
- Cartridge heater as a cell analogue that can be controlled.
- Using thermal profiles from literature.
- Thermocouples to record temperature profiles.



# Combined model outputs – Cell spacing

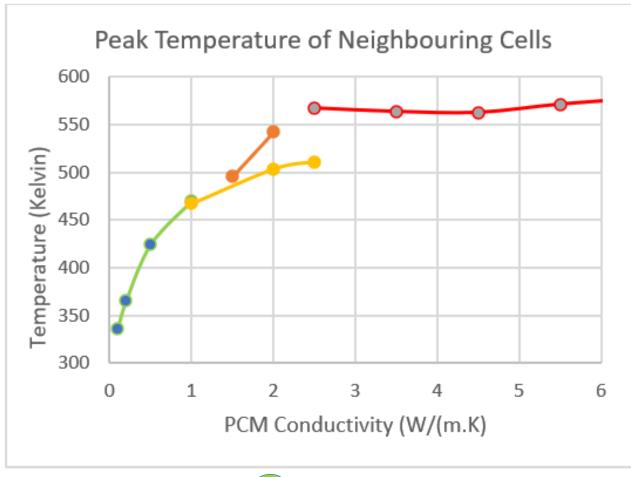


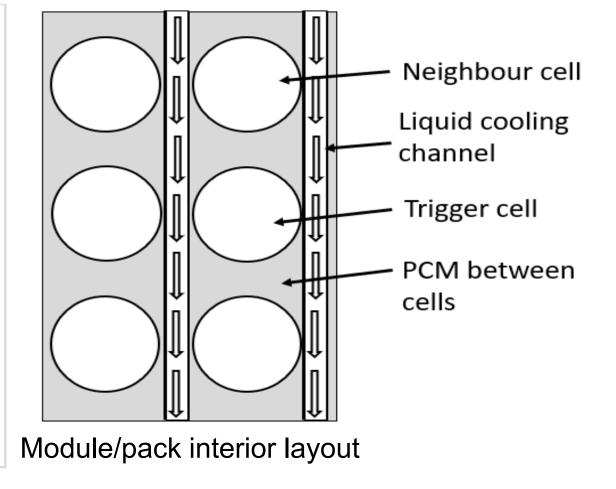
PCM paraffin (RT42) K=0.2W/mK Flash point 459K



Module/pack periphery layout

# Thermal conductivity impact





No propagation expected

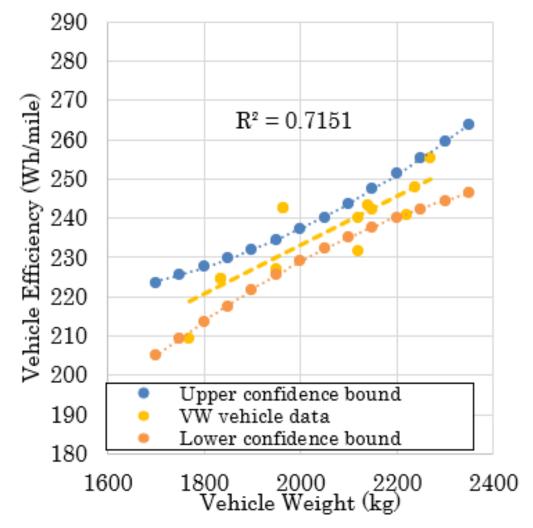
Propagation expected

Transition region

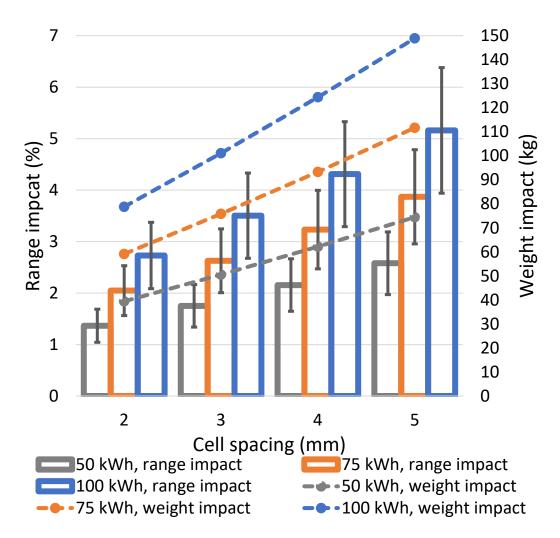
No kinetics heating

### Weight impact

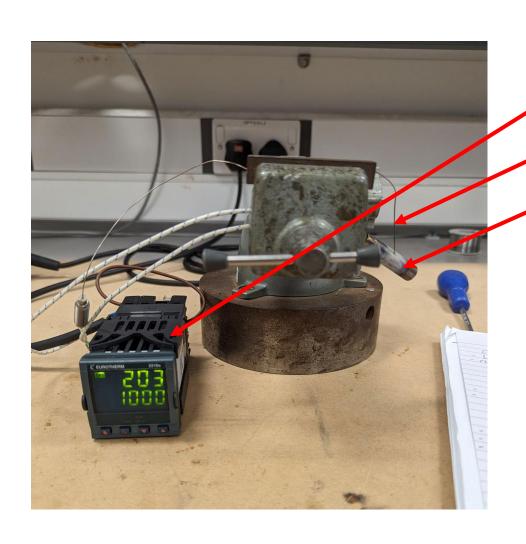
EV efficiency against vehicle weight (MEB platform)



Range and weight impact of cell spacing to accommodate PCM



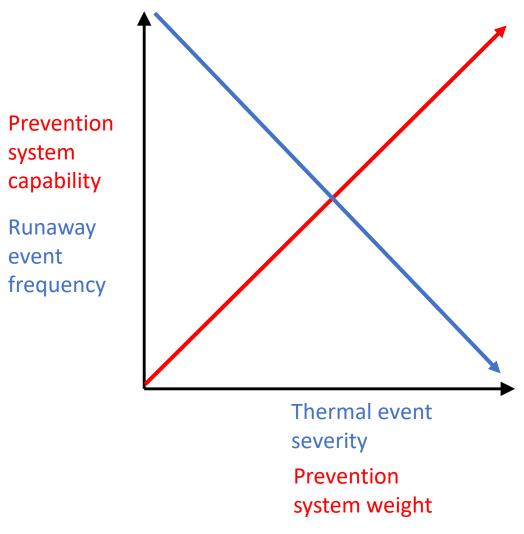
# Heating loop



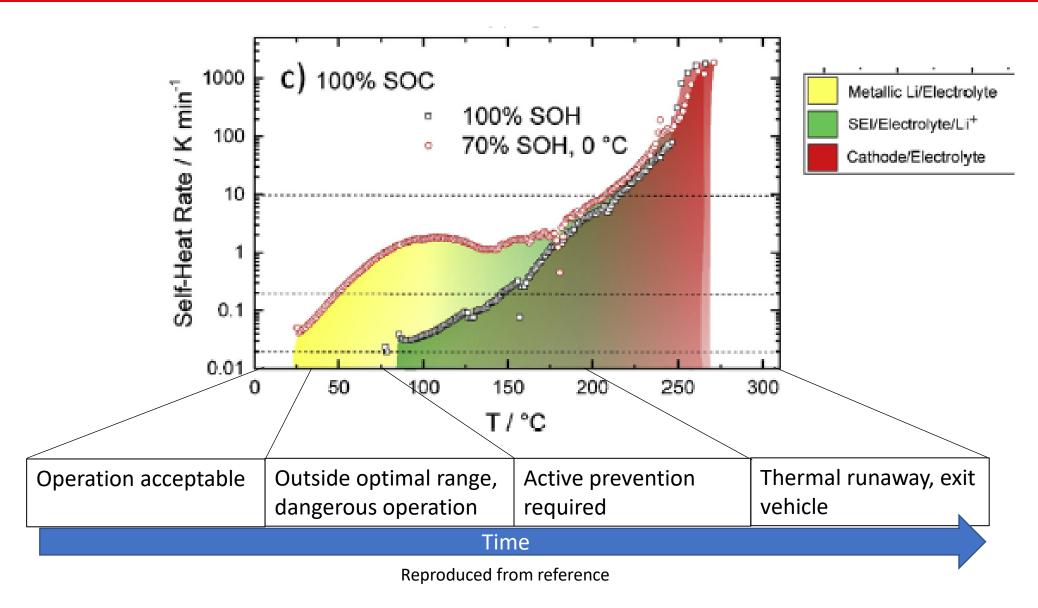
- PID controller
- Thermocouple
- Heater

- PID good for 1000 degrees
- 200W test heater in this case

# Project objectives



### Time Sensitivity



Pro	ject Plan												ESTIPASS	QUEEN' UNIVER BELFAST	
NA/D	Table	Year 1				Year 2					Ye	Year 4			
WP	Task	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1
Lit. review	1a. Complete literature review													complete	
	Model development														
	2a. Use refined model to develop a novel set up														
Modelling	2b. Refine design across range of parameters														
	2c. Run refined design as part of a drive cycle														

Validation complete

2d. Model refinement Physical testing

testing

Investigation

Validation

3a. Design and develop of test rig and DOE. 4a. Sensitivity analysis of key

parameters within practical scope

4a. Validate results with physical

4b. Refine if required

Proj	Project Plan  Outen's University Belfast														
	Took	Year 1				Year 2					Ye	Year 4			
WP	Task	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1
Lit. review	1a. Complete literature review													complet ature re	
	Model development														
	2a. Convert refined model to novel set up														
Modelling	2b. Refine design across range of parameters														
	2c. Run refined design as part of a drive cycle														

Validation

complete

APR<sub>2</sub>

Viva



2d. Model refinement

4a. Validate results with physical

4b. Refine if required

5a. Write thesis

Physical

testing

Validation

Thesis

DOE.

testing

- 3a. Design and develop of test rig and

**IR** 

Diff

APR1