

CRANFIELD UNIVERSITY

MANLIO VALERIO MORGANTI

THERMAL-MANAGEMENT ORIENTED,
MULTI-DOMAIN BATTERY MODELLING AND
EXPERIMENTAL VALIDATION

SCHOOL OF AEROSPACE, TRANSPORT AND
MANUFACTURING
Automotive Engineering

PhD

Academic Year: 2019–2020

Supervisor: Dr S. Longo, Prof M. Tirovic
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requirements for the degree of PhD.

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Abstract

A cross-domain battery simulation methodology, that could allow, a more streamlined design process, was needed. Acausal, object-oriented, multi-domain modelling strategies are becoming more and more common, beside traditional co-simulation methods, since they avoid the development of several different models for each causality type and leaving therefore flexibility to the user. A multi-domain, re-scalable, battery model and a re-configurable battery-module test-rig are introduced in this thesis. The chosen approach allows the final user to generate different module and pack layouts from a single cell model. Materials were fully characterised, then initial conditions were defined, boundary conditions outlined and ultimately the strategy was tested against different scenarios. It is therefore possible to generate arrays of more cell models connected with each other, resulting in a module model. Such an approach achieved higher accuracy than a lumped element model with computational cost being lower than finite element models. The error in simulated voltage estimation was low and the model could handle the transient with a reduced error in temperature. In order to validate such models a test-rig, capable of hosting different battery layouts was implemented. Extensive hardware characterisation, including sensor uncertainty analysis was carried out on the experimental layout. The model of a battery module was successfully implemented. When comparing with experimental data, the discrepancies in the case of the module were larger than in the case of single cell, but the outcome was still laying in the interval of confidence. The temperature profile has been predicted well for cell and module at reduced computational costs. The case studies proved the effectiveness of cooling which was accurately captured by the models developed. Moreover, it was demonstrated that indirect liquid cooling based on removable heat cold plates can be very effective in keeping the battery module within safety operational temperatures during fast charging.

Keywords

Battery; Lithium-ion; thermal modelling; rescalable; test rig.

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List of Abbreviations

BTMS	Battery Thermal Management System
DASSL	Differential Algebraic System SoLver
DEC	Di-Ethyl Carbonate
DMC	Di-Methyl Carbonate
EC	Ethyl Carbonate
ECM	Equivalent Circuit Model
EIA	United States Energy Information Administration
EV	Electric Vehicle
HEV	Hybrid Electric Vehicle
HIL	Hardware In the Loop
ICE	Internal Combustion Engine
NMC	Nickel-Manganese-Cadmium (battery cells)
OCV	Open Circuit Voltage [V]
PCM	Phase-Change Material
PHEV	Plug-in Hybrid Electric Vehicle
SOC	State Of Charge [%]

Nomenclature

Latin letters

A	Surface area [m^2], ageing coefficient (with subscript)
b	Translation coefficient
C	Capacitance [F]
c	Concentration [$mol \cdot m^{-3}$]
c_p	Specific heat [$W \cdot kg^{-1} \cdot K^{-1}$]
C_t	Capacity [Ah]
D	Diffusion coefficient, hydraulic diameter [m]
E	Energy [J], Nernst potential (with subscript)
e	Error
F	Faraday's constant [$F \cdot mol^{-1}$]
h	Convective heat transfer coefficient [$W \cdot m^{-2} \cdot K^{-1}$]
i	Current densit [$A \cdot m^{-2}$]
j	Pore-wall flux across interface
k	Frictional coefficient, thermal conductivity coefficient [$W \cdot m \cdot K^{-1}$]
L	Length [m], cell thickness [m]
m	Mass [kg]
N_{cyc}	Number of cycles
N_M	Permeability

N_p	Number of calendar years
p	Pressure [Pa]
Q, q	Energy dissipated as heat [J]
r	Radius [m], radial coordinate [m]
T	Temperature [K]
t	Time [s]
t^0	Ion conductivity
U	Potential, voltage [V]
u, v, w	Velocity terms [$m \cdot s^{-1}$]
V	Voltage [V]
z	Charge number

Greek letters

α	Transfer coefficient
δ	Debye's length
ε	Dielectric constant
θ	Dimensionless concentration; angular coordinate
κ	Electrolyte conductivity
μ	Chemical potential
ν	Number of ions
ρ	Density [$kg \cdot m^{-3}$]
σ	Solid matrix conductivity
ϕ	Percentage of liquid phase [%]
ψ	Porosity [%]
ω	Rotational speed [$rad \cdot s^{-1}$]

Subscripts

<i>amb</i>	Ambient
<i>be</i>	Bulk element
<i>cc</i>	Current collector
<i>e</i>	Phase change
<i>electrolyte, el</i>	Electrolyte
<i>elem</i>	Element
<i>f</i>	Fluid
<i>j</i>	Ohmic
<i>Li</i>	Lithium
<i>ne</i>	Nearby element
<i>r</i>	Reaction
<i>s</i>	Solid
<i>sol</i>	Solvent
<i>0, o</i>	Initial

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“Verbum inquireribus, magnum opus Verbum est.”

(St. Augustine)

“La geografia della fame è una leggenda [...] Ho lottato anch’io contro l’idea fissa che esisteva nel mio Paese: che l’Italia fosse condannata ad essere povera [...]”

(Enrico Mattei)

“Por mais que você programe sua vida, a qualquer momento tudo pode mudar.”

(Ayrton Senna)

“Dominus providebit”

D.O.M.

List of publications

Journal papers

- Morganti, M.V., Longo, S., Tirovic, M., Blaise, C.Y. and Forostovsky, G., 2019. Multi-scale, electro-thermal model of NMC battery cell. *IEEE Transactions on Vehicular Technology*, 68 (11), pp.10594-10606. doi: 10.1109/TVT.2019.2943052

Conference papers

- M. V. Morganti, S. Longo, R. M. Shah bin Raja Ahsan (2018, October), A flexible, re-configurable electro-thermal battery cell model. FISITA World Automotive Congress, Chennai (India) 2nd-5th October 2018.
- M. V. Morganti, S. Longo, M. Tirovic, D. J. Auger, & R. M. Shah bin Raja Ahsan (2018, May). Modular Battery Cell Model for Thermal Management Modelling. In *Vehicle and Automotive Engineering* (pp. 87-102). Springer, Cham., doi: 10.1007/978-3-319-75677-6_8
- M. V. Morganti, S. Longo, and R. M. Shah (2017), Development of a HIL rig for vehicle thermal management systems design and optimisation, IMechE Vehicle Thermal Management Systems (VTMS) Conference 13, London 17th-18th May 2017, ISBN: 978-151087386-5

Chapter 1

Introduction

This chapter provides some introductory remarks. The market shift towards battery vehicles is analysed and explained. The concepts of efficiency and energy storage are introduced, then batteries are defined and introduced, outlining their major issues. Finally gaps in the research, aims and objectives are stated and explained.

1.1 The context

Battery-powered vehicles are reshaping both private and public transport, enabling the cut of oil-based fuels and infrastructure costs [1, 2]. Such vehicles are causing a paradigm shift in design from an internal-combustion-engine-centred system, to a battery-centred system. Lithium-ion batteries have become the preferred type, having a low memory effect within an appropriate temperature, voltage and current range, low self-discharge effect when not in use and high energy-to-weight ratio [3].

1.1.1 The automotive industry in the world of today

China and USA are the World's two largest markets for vehicles. These two countries also represent approximately one third of world oil consumption. Both countries rely on import for nearly a half of their oil need. The Chinese market experienced an average growth by 29% per year in the last few years. Approximately 50% of the Chinese oil consumption and two thirds of the oil consumed in the USA are used for vehicle powertrains [2]. In such a context, it is evident that both countries depend on foreign oil imports for their transportation. This has a massive impact on the international affairs of both countries. The plan of the US Energy Department is to cut oil imports by at least 15% within 2040, ideally even becoming a net oil exporter by that date. The latter scenario, however, according to the 2017 Annual Energy Outlook, released by the EIA, is unlikely to happen [4]. Proven that alternatives to oil are found for power generation, powertrain electrification could cut oil imports of the two countries dramatically. Since USA and China are the two largest vehicle markets in the world, electrification of powertrains there would force all other countries on the same route. There are of course drawbacks. In China 75% of electricity is obtained from coal combustion [2]. Of course an increase in the demand for electricity could eventually cause a growth in polluting emissions by China. On the other hand, the US Department of Energy has estimated a major increase in energy production from dry gas and a slight increase in nuclear and renewable energy production throughout the next two decades. This will ultimately result in a decrease in emissions in the USA [4].

Let us also look at another important region: Europe. In the Old World, the view on the problem is different, but it has similar effects on the vehicle market. The European Commission has outlined energy efficiency as a target for transport industry. The European Union has required a 20% cut in vehicle energy consumption by 2020. In addition,

the new regulations on homologation drive cycles, will force many manufacturers to discontinue some engines, most prominently small Diesel engines and large petrol engines. In fact many of these engines will not be able to comply to the new limits in NO_x emissions [5, 6]. The convenience of powertrain electrification, given this scenario, is clearly evident. In such a situation, HEVs, PHEVs and EVs will experience a massive growth in their market share, especially in USA and China.

1.2 Energy storage systems in automotive

Any object in the universe complies with the first law of thermodynamics [7]. Any machine or device needs therefore a supply of energy to perform an action. There are several ways of supplying energy, depending on the nature of the device.

In the specific case of vehicles, energy can either be provided continuously by an external power supply or, stored on an onboard device which is provided periodically with an energy source [8, 9].

1.2.1 Efficiency as a burning issue

Efficiency is the most important focus of engineering. Let us assume we have a power source. Not all the consumed power will be used to perform the required task. Efficiency can be defined as the power used to perform the task divided by the power provided by the source, which we could call input power, and is usually defined as a percentage [10, 11]:

$$\text{efficiency} = \frac{\text{power used to perform the task}}{\text{input power from source}} . \quad (1.1)$$

Considering a vehicle as a specific device, only a certain proportion of the input power will be used for propulsion. The remaining part of the power is dissipated either to the external environment, or by each component to the surrounding components either thermally or mechanically.

The vehicle is a complex system in which many physical and chemical processes occur, each of which involves one or more vehicle components. Any mechanical or physical process between adjacent components will result in a change in kinetic energy of the involved components. Since friction occurs and since the components cannot be isolated totally from the external environment, some kinetic energy is lost as heat. This is the origin of heat transfer processes in powertrains. Heat transfer absorbs a very high percentage of the power provided by the input power. When the power source is fossil fuel, losses due to heat transfer can reach up to 70%, as it can be seen in Figure 1.1 [12]. When the power source is an electrochemical storage (e.g. a battery), losses due to heat dissipation can reach up to 10% in the storage device only, along with a further 10% lost from other vehicle components.

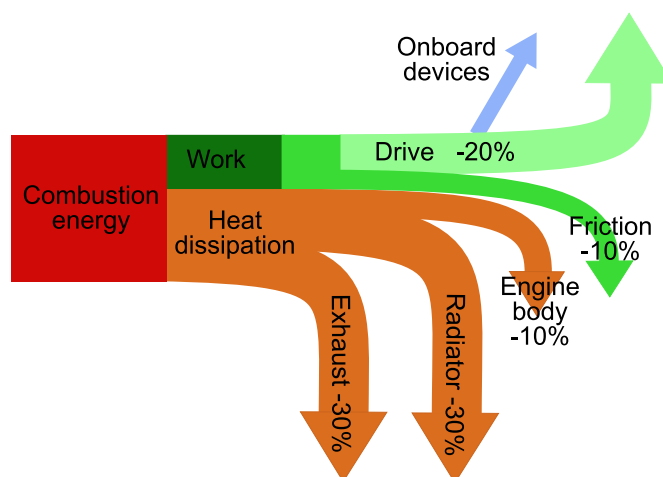


Figure 1.1: Fuel energy conversion for an internal combustion engine [12].

1.2.2 Definition and need of energy storage systems

A vehicle energy storage device is a subsystem of the vehicle that can, through an induced potential difference provide energy [13]. The main action a vehicle needs to perform, is moving. This means that whatever the nature of the potential difference, it must result ultimately in the provision of enough kinetic energy to move the vehicle. There can be several ways of achieving this goal.

1.2.2.1 Mechanical energy storage

The most obvious way of providing potential difference is through a mechanical mean. This could be operated either compressing a spring, or a gas or alternatively through a flywheel. Flywheel storage is perhaps one of the oldest energy storage systems available. The concept is simple: kinetic energy is stored in a rotating flywheel. The usable amount of energy is equivalent to the speed interval in which the flywheel operates formulated as follows [14]:

$$E_{\text{flywheel}} = \frac{1}{2} J \Delta \omega^2 = \frac{\omega_{\text{max}}^2 - \omega_{\text{min}}^2}{2} \int r^2 dm \quad (1.2)$$

where J is the moment of inertia with respect to the rotational axis and dm is a mass element at a distance r from the axis of rotation. Major issues in flywheel energy storage are the typology of bearings and the type of transmission used to retrieve the energy, most prominently whether the retrieved energy is to be transferred to the vehicle's wheels through a transmission or whether it needs to be used for generation in an electric machine [14]. Pneumatic energy storage is also a form of mechanical storage investigated in literature for the case of heavy vehicles, more specifically buses, despite showing a decrease of efficiency proportional to the cycling time [15]. Another option is hydraulic energy storage, a more consolidated and energy-dense methodology. In both cases, the energy is used to power a compressor (in the case of air) or a pump (in the case of hydraulic

systems) that moves the process fluid from one reservoir to another. In such way energy is stored in the form of pressure difference with respect to ambient pressure. Pneumatic and hydraulic storage can eventually be combined [16].

1.2.2.2 Fossil fuels and bio-fuels

Over the past two centuries of transportation, chemical storage has been the preferred method of energy storage. The principle is the following: the vehicle carries a tank filled with a chemical and a thermal machine in which such substance is processed, releasing heat and kinetic energy. The chemical compound provides heat energy, which is converted into kinetic energy either in an external combustor or boiler (for instance in steam engines) or inside the engine, as it happens in Internal Combustion Engines (ICE), for instance piston, rotary and jet engines processing petrol, oil, jet fuel, natural compressed gas, liquefied petroleum gas or bio-fuels, generally according to Otto, Diesel or Atkinson thermodynamic cycles [17].

The main advantages of such systems are their high power density and low initial cost. The main disadvantages are the generally low efficiency of the machines processing fuels, and the limited availability of fuels, especially the naturally sourced ones. Concerns have been raised on the toxicity of combustion residuals and exhaust gases and their detrimental effects on the atmosphere, since ICEs are the main source of urban pollution. ICE release exhaust gases composed by a mixture of Carbon monoxide, unburned hydrocarbons, particulate matter, Nitrogen oxides, Sulphur oxides and Carbon dioxide [17, 18].

1.2.2.3 Hydrogen and fuel cells

Fuel cells restore energy spent to produce hydrogen through electrolysis. There are different types of fuel cells, classified on the base of the electrolyte [19, 20]. Durability and cost are major issues preventing the widespread of fuel cells, since the cost is estimated to be approximately between 125 and 175 $USD \cdot kW^{-1}$ for mass-produced cells. Such value is approximately five times the correspondent value for an ICE-powered vehicle. In addition, performance of fuel cells start dropping after approximately 30,000 miles [21].

1.2.2.4 Electrical energy storage

Supercapacitors can store high power rates and have a very high volume specific power, however, their limit is the amount of charge storable, which is three to 30 times lower than electrolytic batteries. These devices can be charged and discharged in very short time intervals, making them an interesting option for energy recovery systems. There are three main types of supercapacitors: electric double layers capacitors, hybrid supercapacitors and pseudocapacitors [22].

Supercapacitors can also be used in hybridised energy storage systems, in combination with batteries, however such systems have more complicated layouts and put additional thermal stress on both batteries and supercapacitors [23].

1.2.2.5 Electro-chemical energy storage: batteries

Three types of batteries can be identified: i) galvanic cells (Figure 1.2), ii) concentration cells (Figure 1.3), iii) electrolytic cells (Figure 1.4) [24, 25]. Ion cells are re-chargeable batteries based on the reversible insertion and extraction of a guest species from a host matrix. This process witnesses a flow of ions through the electrolyte, together with a

redox (i.e. reduction and oxidation) reaction of the host matrix effectively resulting in an electron flow through an external circuit connecting the battery electrodes [26]. Preferred cells in the automotive are Lithium-ion electrolytic cells.

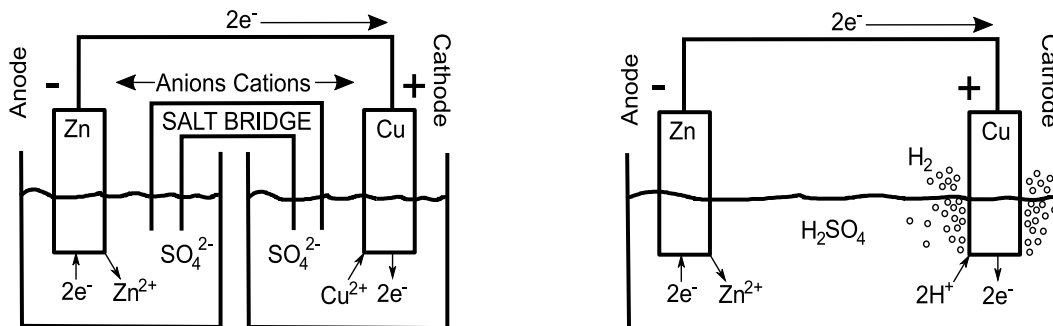


Figure 1.2: Galvanic cells, left Daniell's cell, right Volta's cell.

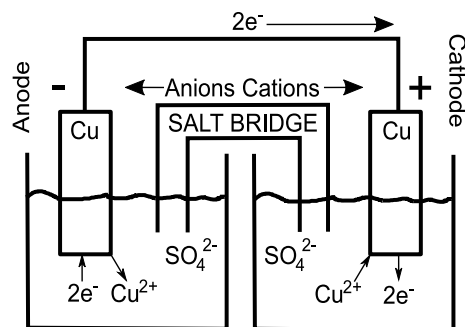


Figure 1.3: Concentration cell.

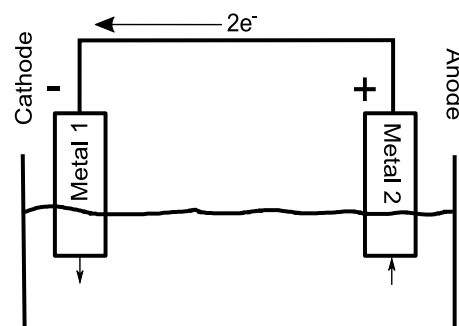


Figure 1.4: Electrolytic cell.

1.3 Motivations

Lithium-ion electrolytic cells work in a limited temperature range. Mahle-Behr, for instance, set 40°C as upper temperature limit and 5°C as maximum internal temperature gradient in each cell and as maximum temperature gradient between each two cells [27]. Other authors suggested that batteries achieve the best balance between performance and life between 25°C and 40°C also suggesting that temperature gradients within the cell should not exceed 5°C [28]. At temperatures higher than 60°C, loss of Lithium inventory followed by loss of active material takes place resulting in capacity drop [29]. Furthermore, batteries stored or cycled at above 45°C or below 0°C may be subject to accelerated ageing, due to accelerated reaction rates at high temperatures and reduced transport of ions and reaction rates at low temperatures, both leading to capacity and power fade [30, 31]. Moreover, side reactions start on the lithiated carbon at temperatures above 80°C. The decomposition of electrolyte forms protective layers on the electrode, the so-called solid electrolyte interphase layers, whose growth leads to loss of Lithium and decrease of active surface, leading to impedance rise and therefore capacity and power fade [32]. At temperatures between 90°C and 120°C the solid electrolyte interphase layer on the carbon anode decomposes exothermically, generating more heat and gas evolution as a result of the reaction between lithiated carbon and the electrolyte. At temperatures above 130°C, polymer separators melt, leading to local short circuits and further heat rejection [31]. Local short circuits may ignite the gases, resulting in a self-fed fire [33, 34]. These phenomena lead to catastrophic failures of battery cells such as fires or explosions [35, 36]. Furthermore, at low temperatures, metallic lithium plating takes place, leading to electrolyte decomposition and therefore capacity fade [32]. An average of 20% capacity fade for Lithium-ion battery cells is expected after 5000 full discharge and recharge cycles, such depletion must be taken into account when designing a battery pack, oversizing the

Cell type	Operating temperature range	Maximum $\Delta T_{internal}$	Reference
Li-ion, cylindrical cell 40140 ($\varnothing 40 \times 140mm$)	10 to 40°C (25°C optimal)	5°C	[27]
Li-ion pouch cells 150 × 150 × 8.5mm	10 to 40°C (25°C optimal)	3°C	
26650 LiFePO ₄ cylindrical 150 × 150 × 8.5mm	−30 to 60°C	6°C	[31, 41]
18650 NMC cylindrical cells $\varnothing 18 \times 650mm$	−20 to 70°C (25°C optimal)	9°C	[42]
GS Yuasa LEV50 NMC prismatic cells 113.5 × 171 × 43.8mm	−20 to 70°C (25°C optimal)	10°C	[43]

Table 1.1: Cell formats and types thermal constraints comparison, with maximum internal temperature gradient discovered by researchers cycling the battery at rates up to 4C (discussion on current rate in the next chapters) and ambient temperatures ranging from −10°C to 60°C .

battery in order to achieve the design requirements for minimum residual capacity at the end of life [37]. A description of the different battery degradation mechanisms is summarised in Figure 1.5. In addition, according to the European Automobile Manufacturers' Association, the average age of vehicles in Europe is currently over 11 years [38]. On the other hand, the average battery life for an automotive Lithium-ion battery pack has been estimated to be above 8 years and below 14 years, depending on severity of cycling, size and chemistry of batteries [39]. Furthermore, thermal modelling is required for battery management systems in which maximum allowed computational cost is a constraint, reducing computational expense of battery thermal models is a priority in the selection of models [40, 31]. A summary of cell formats and degradation mechanisms is presented in table (for further discussion on cell formats, please see Chapter 2). In summary operating temperature and internal temperature range affect battery life and performance as

discussed above. This leads to questioning how their effect can be taken into account from early stages of battery design.

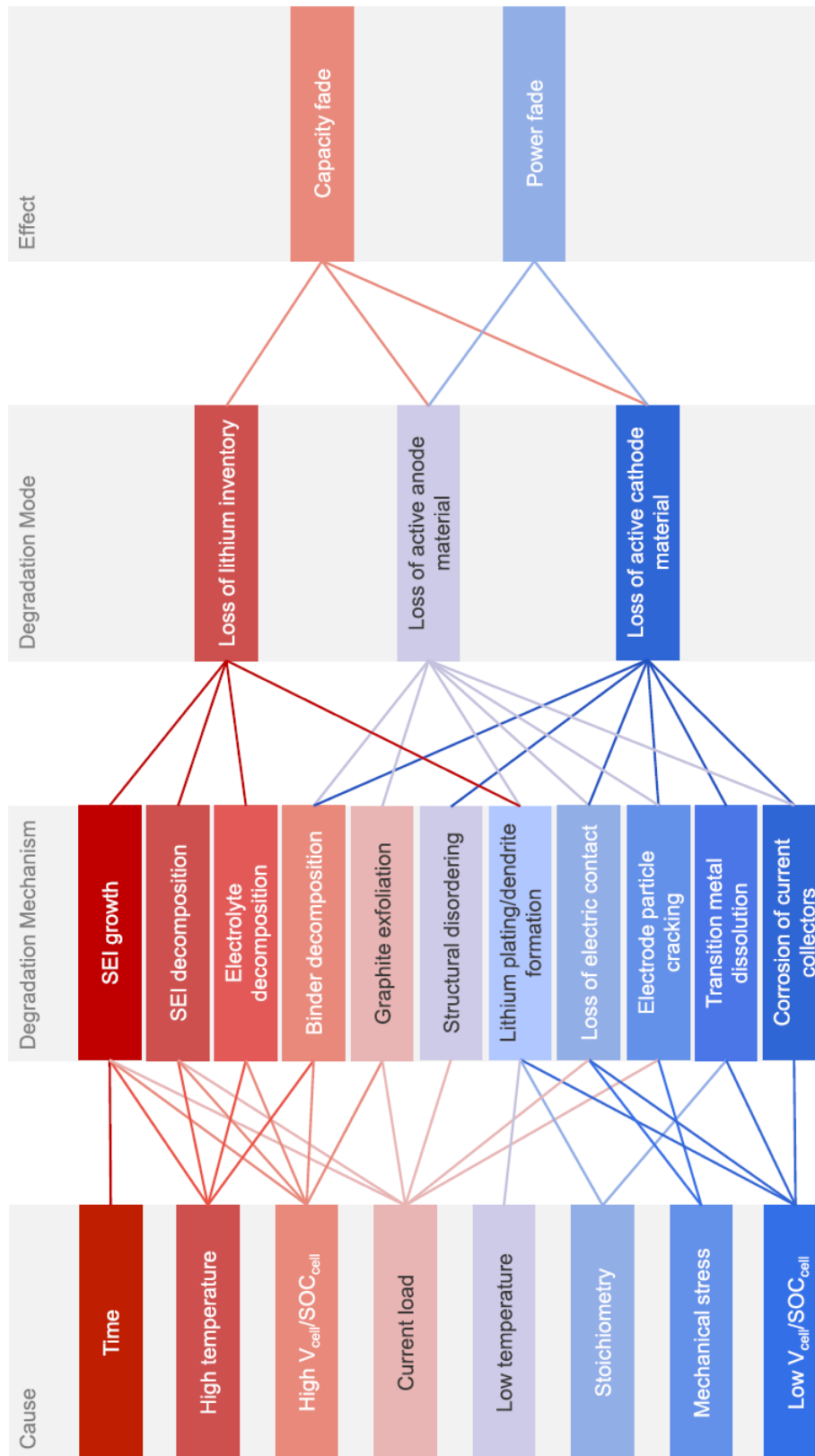


Figure 1.5: Summary of causes, modes and effects of battery degradation [33].

1.4 Goals and contribution

1.4.1 Research question and hypothesis

The main research question of this project was the following:

How can the design procedure of battery modules be made more systematic, more standardised and less expensive, while taking the thermal issues into account from the very beginning?

And the research hypothesis taken to answer such question is:

A re-scalable multi-domain modelling strategy can reduce computational time and provide more insight on the battery thermal behaviour. A flexible test-rig integrating cooling systems and battery cycling can reduce the cost of experiments and add more robustness to model validation.

Thermal behaviour of batteries is highly dependent on their duty cycle, average temperature and internal temperature gradient. On the other hand, heat rejection and operating temperature are highly dependent on the duty cycle of the battery. For such reasons more domains of physics need to be examined simultaneously with a methodology that is therefore called multi-domain simulation [44]. The computational cost, however, needs to be contained. A current gap in literature, as it will be outlined in the next chapter, lies in the development of low-computational cost multi-domain models. A way to reduce computational effort is developing a re-scalable model, by this term, we mean a model that is expandable from a small unit into a larger model [45]. In developing such models, an obstacle is describing the relationship between each two components or each two physical domains in a larger model. This issue is overcome by using modelling languages that do

not rely on procedural algorithms (i.e., inputting the commands to be executed as a list of actions to be performed at a given instant in time), but rather on the description between components that contain the procedures and the numerical methodologies to solve time derivatives [46]. Such languages go under the name of acausal languages. This strategy has proven to be effective in integrating models of different vehicle subsystems in previous research on internal combustion-engine powered vehicles [47].

1.4.2 Aims and objectives

The aims of this project are to establish a flexible, re-scalable, computationally lean procedure to model battery cells, and a flexible and re-configurable test-rig that can examine different battery thermal management layouts at a range of different charge/discharge duty cycles. The following objectives were set:

1. Delivery of the aforementioned battery cell model
2. Expanding the single cell model into a full-pack model
3. Designing and developing a flexible cooling systems test rig
4. Investigating removable cooling applications for fast-charging in vehicles without in-built battery cooling

1.4.3 Outcomes and deliverables

The main outcome of this work is a multi-domain simulation library that allows the implementation of battery models. A model of boundaries is also included and a single-cell model can be scaled up to implement battery-module models. The model fits a gap in research between the low computational expense of lumped-element models and the accuracy of finite-element models. In addition, the model can be used to generate different

module layouts from a single cell. A second major outcome is a re-configurable test rig that can host different battery modules and their thermal management systems. The test rig can be used for either model or layout validation.

1.5 Summary of introduction and thesis outline

In this chapter, we introduced the current scenario of energy storage in the automotive industry and outlined the challenges with batteries and their thermal behaviour. After that, we defined the research question and our hypothesis to tackle it. Finally we set aims and objectives and expected outcomes.

The thesis is organised in several chapters. The first one carries out a literature review on batteries, battery models, battery thermal models and battery thermal management systems. The following chapter describes the modelling technique developed in this work. A further chapter describes the test rig design, its purpose and the analysis of the uncertainty in measurements. Another chapter focuses, in its first part, on single-cell models and provides experimental validation of the proposed models. In the second part of the chapter, the attention shifts towards the scaling-up from the single-cell model to the module model. Experimental validation of simulated data is provided thanks to the test-rig. In the last chapters conclusions are drawn and an outlook to further research developments is outlined.

Chapter 2

Lithium-ion batteries and thermal management

In this chapter, the components of Lithium-ion batteries are then examined one by one and techniques to thermally model them are reviewed. After that, vehicle thermal management systems and, more specifically battery thermal management systems are examined. Finally, experimental techniques are discussed and evaluated. A benchmark of industrially adopted systems is also provided. Trends and gaps of the current research are remarked and analysed, explaining where this work fits, in the literary landscape.

2.1 Lithium-based electrolytic cells

Lithium-ion cells are electrolytic cells in which the guest species are Lithium ions and the host matrix undergoes the name of Lithium-insertion compound. In discharging phase, Lithium ions are inserted into the van der Waals gaps in the host matrix, while charge balance is maintained by the reduction of ions occurring in the host matrix. During a charging process, the opposite phenomenon occurs and the ions in the host matrix are

subject to oxidation instead. Such process can result in an Open Circuit Voltage (OCV, i.e. the battery voltage, without any load being connected to it) formulated as follows [26]:

$$OCV = \frac{\mu_{Li(cathode)} - \mu_{Li(anode)}}{F} \quad (2.1)$$

where μ_{Li} are the chemical potentials of anode and cathode respectively and F is Faraday's constant [26]. In any concentrated-solution-based device, mass transfer is driven by the gradient in electrochemical potential, defined as follows [48]:

$$c_i \nabla \mu_i = \sum_{j \neq i} K_{ij} (v_j - v_i) \quad (2.2)$$

where K_{ij} ($K_{ij} \neq K_{ji}$) are the frictional coefficients for the interactions between the two species, indicated by the coefficients i and j . Using the Lithium-insertion compound as reference and setting its velocity to zero, it is possible to describe the concentration ($c = c_i/v_i$) as follows:

$$\begin{cases} N_+ = -v_+ D \nabla c + \frac{it_+^0}{z_+ F} \\ N_- = -v_- D \nabla c + \frac{it_-^0}{z_- F} \end{cases} \quad (2.3)$$

where t^0 are the conductivities, v are the number of ions into which a mole dissociates, F is Faraday's constant, D is the diffusion coefficient, z is the charge number, c is the concentration of the electrolyte and i is the current density [48].

2.1.1 Battery components

Lithium-ion cells can use different materials for electrodes and electrolytes. The choice of the chemistry has a major effect on electrical and thermal properties.

2.1.1.1 Electrolytes

Electrolytes can be either liquid, solid or semi-solid. Interfacial resistance and chemical stability have led most manufacturer to prefer liquid electrolyte [49]. On the other hand, liquid electrolyte may cause formation of dendrites. In addition, the concentration of solute in the electrolyte solution is generally low. Conductivity and electrochemical stability drive the selection of liquid electrolytes [50].

Liquid electrolytes Electrolytes are generally selected according to some guidelines based on their properties. First of all, electro-chemical properties must be adequate: the electrolyte must be highly electrochemically stable, in order to tolerate differences of voltage around 4 V between the electrodes without being reduced or oxidised. Cathode materials, if doped can reach a potential of even 5 V. Anodic stability is therefore essential to ensure a relevant battery life. In addition, ionic conductivity must be high, so that cell resistance and therefore resistive heat rejection are minimised. Furthermore, the electrolyte must be chemically stable, since materials of the anode are highly reducing and materials of the cathode are highly oxidising. An essential requirement is that reduction of electrolyte species occurs at a potential higher than that of Li-insertion on the Carbon surface of an electrode. Beside such properties, the electrolyte must have a low melting point, in order to preserve conductivity and prevent solidification and phase separation. In addition, boiling point must be high, in order to minimise pressure build-up at high temperatures for reasons of safety. Lastly toxicity and cost of electrolyte are fundamental in determining electrolyte selection [50, 51]. Solutions of $LiPF_6$ in organic carbonates seem to best fit such requirements. Concentrations between 0.4 and 1.0M are a good trade-off between maximising the electrolyte conductivity and reducing salt precipitation. Alkyl carbonate solvents have higher anodic stability than esters and ethers. The latter two do

not promote good passivation of Lithium-Carbon electrodes. Typical examples of solvents are Di-Methyl Carbonate (DMC) 1:1 mixes of Ethyl Carbonate (EC) and Di-Ethyl Carbonate (DEC) [52, 53, 51, 54]. $LiPF_6$ is the generally accepted salt, due to its good conductivity when dissolved in Alkyl carbonate solvents. In addition thermal stability is good and a good passivation of Aluminium cathode current collectors is achieved. In addition, alternative Lithium salts presents serious safety issues: $LiClO_4$ is explosive at ambient temperatures and $LiAsF_6$ is highly toxic. Finally $LiPF_6$ is much cheaper than other Lithium salts [51]. Conductivity of liquid electrolytes increases with temperature. However, it is necessary to observe that, for instance, the boiling point of DMC is 90°C and that of DEC is 126.8°C . Although boiling points can be modified by the presence of a dissolved Lithium salt, it is recommendable to prevent the battery from reaching them, since local phenomena of boiling may occur, leading to the emission of gases [52, 51].

Gel and hybrid polymer electrolytes There are four different types of polymer electrolytes: i) solvent containing systems, ii) solvent-free ion-coupled systems, iii) single-ion systems and iv) decoupled systems. In the case of i) either the electrolyte is a gel, i.e. a liquid electrolyte is fully miscible with a single-phase swollen polymer matrix or the electrolyte is a two-phase hybrid, which means that a liquid electrolyte fills pores of a polymer membrane; in the case of ii) mobile anions and cations are hosted in a rubbery phase; in iii) anions are fixed to the polymer backbone and in iv) ionic mobility happens via channelled structures and is therefore reduced [55]. Issues generally affecting polymer electrolytes are low ionic conductivity, low oxidation voltage and formation of Lithium-dendrites [49]. Polymer molecular structure has a major effect on battery performance, especially reducing crystallinity helps in increasing conductivity at low temperatures. In addition, the polymer structure has a major effect on the melting point of the polymer. Furthermore, changes to the molecular structure of the polymer due to temperature can

have major effects on conductivity. Furthermore, interface surfaces have relevant effects on internal resistance [56]. Due to their cost, specific energy and performance, Lithium-polymer cells are not as wide-spread in the automotive as they are in other sectors .

Solid electrolyte Beside liquid and polymer electrolytes, solid electrolytes are also an option. Their main advantage is being single-ion conductors, allowing the conduction of Li^+ ions only. In such a scenario, higher voltages can be achieved. Notable examples are glass and crystalline ceramic electrolytes. This kind of electrolytes, however, find limited applications, due to their mechanical properties and to high manufacturing costs [57]. Beside ion-conductivity, the interface resistance between solid-electrolyte and electrodes is a fundamental issue in selecting a solid electrolyte material [58]. Moreover, solid electrolytes, in order to be effective need to be fabricated in a thin film in order to have values of impedance that make the battery a viable option [59].

Semi-solid electrolyte Aqueous semi-solid electrolytes are based on a suspension of energy-dense active materials in a liquid electrolyte. This technology may effectively simplify the cell manufacturing process, by means of a drastic simplification of the cell structure. When applied to aqueous chemistries, in flow cells, such electrolytes can deliver an energy density greater by five to 20 times than liquid electrolytes [60, 61, 62].

2.1.1.2 Electrodes material

High-voltage Li-Carbon intercalation compounds replace Li-metal anodes in Li-ion cells. Notable examples are $LiNiO_2$, $LiCoO_2$ and $LiMn_2O_2$, the latter being often doped with other materials to increase redox activity up to 5 V [51]. Graphitic carbons are the most used base for Li-ion cells anodes. Such material is extremely fragile and requires therefore to be used together with chemically and mechanically stable materials.

2.1.1.3 Anode materials

Early Lithium-ion cells were using Lithium foils as anodes, later such expensive and unsafe materials were replaced with Lithium-metal anodes TiS_2 and MoS_2 . Frequent and documented failures of such batteries led to the development of “rocking chair” batteries, based on the principle of simultaneous insertion and de-insertion of Lithium in both electrodes. Current anode technology space from carbonaceous materials, to Sn -, Sb - and Al -based composites and from metal oxides to Nitride phosphides [63]. Carbonaceous anodes appear the best trade-off between cost and performance in current battery industry. Carbonaceous anodes are used as host materials in which Lithium cations are electrochemically intercalated. Intercalation is a special case of insertion, in which a layered host receives the guests in the interlayer vacancies. Both graphitic and non-graphitic anodes are commonly used [64]. Non-graphitic carbons have recently been subject of research, especially in cooperation with other materials such as in the case of Carbon-Silicon composites [65]. It was shown that the factor that mostly influences thermal properties such as specific heat and cross-plane thermal conductivity is temperature. The influence of the State of Charge has proven to be negligible, while, the interaction of liquid and solid phase in liquid-electrolyte cells is remarkable [66]. For carbonaceous anodes, commonly observed values of specific heat are around $1400 J \cdot kg^{-1} K^{-1}$, while thermal conductivity can be represented as function of temperature and varies from a minimum of 7 to a maximum of $17.6 W \cdot m^{-1} K^{-1}$ being directly proportional to temperature [67, 54].

2.1.1.4 Cathode materials

Cathode materials must allow Li^+ intercalation, while granting a reasonable energy density, reasonable mechanical properties, the required voltage level and reasonable manufacturing costs and times. Material selection depends on the required voltage as presented

in Table 2.1 [68].

Cathode material	Cell voltage
FeS_2	1.5 V
S, Polysulphides	2 V
Mn Spinels, Li_xMnO_2 , $Li_xV_yO_z$	3 V
$LiFePO_4$	3.5 V
$LiMnO_2$, $Li_xMn_{1-y}M_yO_2$, $Li [Li_xM_yMn_{1-x-y}] O_2$	3 to 4 V
$LiNiO_2$, $LiCoO_2$, $LiMn_2O_4$, $LiCo_{1-x-y}Ni_xM_yO_2$, $Li_{1+y}Mn_{2-x}M_xO_4$ (x and y low)	4 V
$LiMn_{2-x}M_xO_4$ ($x \geq 0.5$)	5 V

Table 2.1: Summary of cell voltages achievable with different cathode chemistries [68].

A peculiarly promising methodology is coating cathodes with $Li[Ni_{0.5}Mn_{0.3}Co_{0.2}]O_2$, better known as NMC532. Artificial graphite electrodes were coated with NMC532, with an adhesion of 12.2 mg/cm^2 , with NMC532 accounting for 95.4% in weight of the electrode. Such cathode design has proved to provide cells capable of withstanding a 3700 full charge/discharge cycles, between 3.0 and 4.3V at a rate of C/3 and ambient temperatures ranging between 20 and 55°C; moreover, even in case of cells continuously cycled above 40°C in the aforementioned range of voltages and the aforementioned average charge/discharge rate, with peak rates up to 3C, 70% of capacity would be left after 10 years, it is estimated that a distance of 1,200,000 km could be covered on a Tesla battery pack should the duty cycle remain within the aforementioned boundaries [69]. As for the anodes, the interaction of liquid and solid phase has a considerable influence on the thermal properties [66]. Cathode coatings, in the case of NMC cells, are produced from a $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ active powder mixed with carbon black a polymeric binder and a solvent [70, 54]. Thermal conductivity and specific heat are temperature dependent and can be linearized in a temperature range within -40°C and 60°C [54, 71].

2.1.1.5 Materials and geometry of current collectors

Electrochemical reactions in battery cells happen in a wide potential window, exposing current collectors to passivation in anhydrous electrolyte. Such process depends on the upper cut-off voltage and leads to the selection of current collectors materials. Aluminium is chosen as anode current collector when dealing with lithiated transition metal oxides, due to its high resistance at voltage between 3.5 V and 5 V vs. Li/Li^+ . On the other hand, Copper is diffused in Cathode current collectors. In addition, some researchers point out Copper current collectors can elad to short circuits when the battery is over-discharged [72]. Current collectors can be either continuous or discrete, depending on packaging needs. Discrete anodes are an option where the cell is packed in a small container and weight and cost reduction are fundamental project specifications.

2.1.1.6 Separators

Separators prevent physical contact between positive and negative electrodes, isolating electronic flow and allowing free ionic transport. Separators are generally microporous layers consisting of polymeric membrane or non-woven fabric mat. They are chemically and electrochemically stable towards both electrodes and electrolyte and their mechanical properties allow them to withstand high stress during assembly [73]. Physical properties of separators affect their performance. An increased thickness, for instance, would reduce the power density, however, low thickness separators cannot withstand high mechanical stress and can therefore lead to local short-circuits causing safety issues. An industrial standard for separator thickness is 25.4 μm . Porosity is also influencing cell performances. Ionic conductivity is directly proportional to porosity. High porosity, however, limits the shutdown capability of cells and lowers the melting point of the separators. Manufacturers generally consider a 40% porosity. In addition, pore size must be smaller

than the particle size of electrode active materials and the conducting additives, while being tortuous enough to prevent particle penetration. Sub-micron order of magnitudes are generally accepted by manufacturers [73]. Porosity influences wettability and permeability. The former is the capability of the separator to get wet easily and retain the electrolyte permanently, increasing therefore battery life. The latter is a measure of the capability of the separator to allow the electrolyte to move through it. Permeability is usually quantified with the ratio of resistivity of wet separator divided by the resistivity of the electrolyte. Such ratio is called MacMullin number [73]:

$$N_M = \frac{\rho_{\text{wet separator}}}{\rho_{\text{electrolyte}}} . \quad (2.4)$$

In Lithium-ion batteries, MacMullin number is typically equal to 8. Such value enables an even distribution of current throughout the cell. In addition, separators must have adequate mechanical properties and dimensional stability. Separators are required to have a Young's modulus of at least $1000 \text{ kg} \cdot \text{cm}^{-2}$ and resist punctures up to 300 g for a thickness of $25.4 \mu\text{m}$. Separators are also required not to shrink more than 5% at 90°C . Finally separators are required to be capable of battery shutdown before thermal runaway occurs.

In Lithium-ion cells, this means they need to be capable of shutting down the cell at 130°C while having a melting point of approximately 165°C [73]. All the above property requirements led to the widespread use of Polyethylene-Polypropylene bilayer separators in Lithium-ion cells, which leads them to represent over 20% of the battery cell cost [73].

2.1.2 Battery cell format

Battery cells are built in different formats: cylindrical or prismatic, where prismatic cells can either have a hard-case, often featuring a gas-release valve, or a laminated pouch con-

tainer [74]. Cylindrical cells, if their height is extremely reduced, compared to their diameter, undergo the name of coin cells. Two layout cathodes are possible: in the case of hard-case cells, spirally wounded positive and negative electrodes, separated by a polyethylene and/or polypropylene separator, while in the case of pouch cells, more layers of electrodes are stacked on top of each other [75]. Cylindrical hard-case cells are manufactured by round winding, in prismatic cells, the jelly roll is rather flat-wound, in both cases, the jelly roll winding is placed inside a hard-case container which is then filled up with the electrolyte and sealed [74]. Energy density of cells is dependent on the volume of the cell, cylindrical cells are the format with the highest volume occupancy, prismatic cells have the highest volume-specific energy density [76]. Other authors outlined that cylindrical cells are the most resilient to mechanical shocks, while pouch cells provide the largest interface for heat exchange and therefore make the implementation of thermal management systems easier [77]. The DIN SPEC 91252 defines different types of cells, depending on the geometry of the connection as follows [75]:

- Type A: both connections on the top
- Type B: connections at the two ends
- Type C: positive connection at the top, negative connection on both bottom and side walls

Figure 2.1 summarises the different hard-case cell formats.

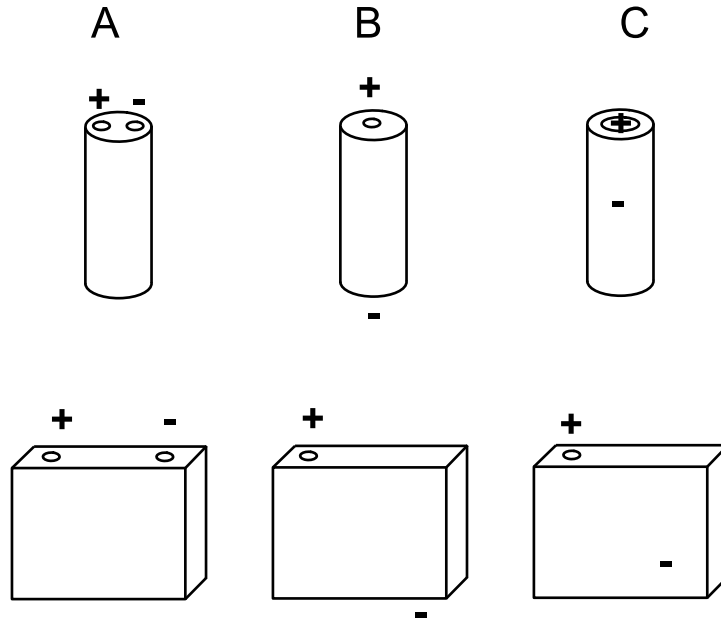


Figure 2.1: Hard-case cell formats according to the DIN SPEC 91252, first line shows cylindrical cells, second line shows prismatic cells [75].

2.1.3 Anisotropic thermal properties and temperature gradients

Thermal conductivities are strongly temperature-dependent, varying of a factor of 50% over a temperature difference of 60°C [54]. Previous research states that Lithium ion battery cells dissipate heat mostly as a consequence of overpotential under current load and also as result of changes in entropy; current density is unevenly distributed throughout the cell and regions subject to the highest current density reach the highest temperatures; such phenomenon accelerates degradation mechanisms in such areas further increasing the anisotropy of materials and therefore the internal temperature gradients [78]. Due to the anisotropy of cell thermal properties, the radial temperature gradient is expected to be greater than the axial temperature gradient [79]. The interface between the cell case and the active material and the fact that the active material thermal conductivity is by one order of magnitude axially and by two radially lower than that of the case material are a

cause of the non-uniform temperature distribution [80, 81]. In addition, the heat capacity of Lithium-ion battery cells decreases with increasing temperature, decreasing heating but also impeding heat dissipation [71]. Researchers have also determined that the heat flux throughout the battery cell is not uniform, since edge effect increases the heat flux on the perimeter of the active material [66]. In addition, temperature gradients throughout a battery cell have been found to result in a lower cell impedance than the theoretical value at uniform temperature [82]. The cell internal temperature gradient originates an uneven current distribution, since hotter part of the cell has a lower resistance, allowing a larger current to flow and generating more heat originating therefore a positive feedback mechanism [82, 83].

2.1.3.1 Challenges for parametrisation

As, previously discussed, battery cell active materials are anisotropic, researchers have investigated volume averaged models. Such models, however, would need to take into account intrinsic properties of physical phases, volume fractions of materials and electrode structure, the latter being subject to simplifications such as perfectly spherical particles, ultimately not fully capturing the anisotropy of materials [84]. Other authors have demonstrated how the microstructure and the active material layer arrangement need to be included in thermal properties modelling, together with the temperature-dependence of heat capacities and thermal conductivities [54]. Researchers also pointed out how experiments are required to validate theoretical modelling of thermal properties, presenting challenges such as maintaining a single-direction heat flow through materials when determining thermal conductivities, since such property, as previously showed, can vary by an order of magnitude in different directions [66]. In addition, other authors pointed out that the challenge in determining the thermal properties of electrolytes is found in the

pressure and temperature operating ranges and in the reactions of thermal decomposition occurring within the specific range, further stressing the attention on the previously mentioned safety temperature ranges [85].

2.1.4 Cell degradation: possible causes and consequences on performance and safety

Battery cell performance can degrade in terms of capacity and power through different degradation modes: i) loss of Lithium inventory, ii) loss of active anode material and iii) loss of active cathode material [33]. Mode i) is caused by different phenomena: solid-electrolyte interface growth and decomposition, electrolyte decomposition and Lithium plating and dendrite formation, while mode ii) is caused by a combination of binder decomposition, graphite exfoliation, Lithium plating and dendrite formation, loss of electric contact, electrode particle cracking and corrosion of current collectors and mode iii) [33]. The growth of the solid-electrolyte interface on the negative electrode is caused by Lithium plating which occurs during charging, at either low temperatures or at high rates or both and originates from charge transfer and solid Lithium diffusion, consequences of this process are a decrease in porosity and a decrease in active surface [86]. Dendrites are metallic Lithium deposits whose formation and growth poses additional mechanical stress on the internal layers of the battery cell while also damaging the structure of the cell, causing local short circuits, reducing the active surface and depleting the electrolyte [33]. Researchers have demonstrated that dendrite growth is dependent both on electrochemical process and on calendar time [87]. Aluminium cathodes experience serious corrosion at potentials higher than 3.5V as a result of reaction with Lithium salts combined with organic solvents, eventually resulting in loss of electric contact [88, 89]. Co-intercalation of solvent into the electrodes can lead to gas evolution and subsequent particle cracking,

resulting into graphite exfoliation, especially when the battery cell is overcharged, ultimately ending in a decrease in active material and a Lithium loss [32]. The reaction of fluorine-containing binders with the charged electrodes leads to a loss of contact the electrode and the current collector[32].

Extended battery cell cycling eventually results in electrolyte decomposition and the formation of solid-phase products, depleting Lithium ions and reducing Lithium transport at the interface between electrodes and electrolyte [90]. Lithium plating, dendrite formation, particle cracking and corrosion of electrodes can result in local short circuits and, as temperature increases above 150°C, Oxygen evolution [91, 33]. The above mentioned mechanisms lead to an increase of internal resistance and therefore heat generation. When a cell generates more heat than what it can dissipate the decomposition of the solid-electrolyte interface layer accelerates, solvent diffuses through the anode leading to exothermic reactions that further increase heat rejection and, when the temperature increase reaches $10^{\circ} C \cdot min^{-1}$, the process is irreversible. Such an event goes under the name of thermal runaway and is caused by over-charging, over-discharging and cycling at high ambient temperature and/or with very low heat dissipation [92]. Such an issue can result into catastrophic events ranging from rupture of cell enclosure and leakage of toxic substances to venting of flammable and toxic gases to explosions [93].

2.2 Battery cell models

A wide range of battery cell models are available in the literature. From single-dimension cell models to three-dimension models. Characterisation of cell properties can be delivered at different levels of detail [94].

Different models can be evaluated according to four fundamental parameters: i) accuracy, ii) computational complexity, iii) configuration effort, iv) analytical insight. Where i) refers to how close simulated and experimental values are, how broad is the range of loads and environmental condition that the model can handle. While ii) refers to the time needed to run a simulation, iii) refers to the number of parameters that can be estimated by the model and the amount of information needed for initial set-up. Finally for analytical insight iv) we mean the capability of the model to provide qualitative understanding of phenomena that are relevant and cannot be examined with other models [95, 96].

Different families of battery cell models can be identified: i) electrochemical models, ii) reduced-order models, iii) Equivalent Circuit Models (ECM), iv) empirical and black-box models [96].

- Electrochemical models are based on nonlinear equations explicitly representing the electrochemical processes happening within the battery cell [97]. Electrochemical models can include energy balance and capacity fading, providing therefore an insight on the reactions occurring within the cell. However, they require more than 50 input parameters and can require hours or even days to compute, finding, therefore, their weakness in configurational effort and computational complexity [95]. Accuracy is dependent on the level of discretisation, assuming uniform distribution of chemical properties can reduce the computational time to milliseconds at the expense of a much lower accuracy, since the information on temperature distribution and current distribution throughout the cell volume would be lost [97].
- Reduced-order models are developed by making assumptions on the physical phenomena occurring within the battery and assuming they happen uniformly across the battery, reducing therefore the number of dimensions represented, researchers

have proved that percentage error on estimated voltage ranges between 5% and 15% and computational time, for a single cell ranges between 2 and 3 *min* [98].

- ECMs are models that replicate the behaviour of a battery cell, through a network of electrical elements. Researchers demonstrated that total execution time of models is directly proportional to data precision, defined in number of bits used to represent the data and the number of elements composing the equivalent circuit model; root mean square percentage error of simulated versus modelled terminal voltage of such models lies between 0.02% and 0.18%, depending on the number of elements composing the layout [99]. In terms of configuration effort, ECMs need between 15 and 30 input parameters, which means more than reduced order models and less than electrochemical models [95].
- Empirical models use a set of equations to describe specific battery behaviours, black box model, starting from the same methodology, reproduce the behaviour of batteries from experimental data, without investigating the electrochemical processes occurring within the battery cell [96]. Empirical models have an average error on the estimated voltage ranging between 8% and 14% and they are applicable only in specific scenarios [95].

2.2.1 Electrochemical models

Electrochemical models can achieve a highly detailed chemical modelling of the cell. The basic underlying concept is obtaining the electrical and thermal behaviour of the battery cells from the description of mass transport and chemical reactions. From the definition of electrochemical potential and concentration as outlined earlier in Equations (2.2) and

(2.3), it is possible to express the variation in Lithium concentration as follows [48, 100]:

$$\varepsilon \frac{\partial c}{\partial t} = \nabla \cdot (\varepsilon \cdot D \cdot \nabla c) - \frac{i_2 \cdot \nabla t_+^0}{z_+ v_+ F} + \frac{a j_n (1 - t_+^0)}{v_+} \quad . \quad (2.5)$$

The current density conservation is expressed as follows [100]:

$$I = i_1 + i_2 \quad (2.6)$$

where the subscript 1 refers to current density through the solid material phase and 2 refers to the electrolyte phase and they are therefore defined as follows:

$$\begin{cases} i_1 = -\sigma \cdot \nabla \Phi_1 \\ i_2 = -\kappa \cdot \nabla \Phi_2 + \frac{\kappa R T}{F} \left(1 + \frac{\partial \ln f_A}{\partial \ln c} \right) \cdot (1 - t_+^0) \cdot \nabla \ln c \end{cases} \quad (2.7)$$

where σ is the conductivity of the solid matrix, κ is the conductivity of the electrolyte, Φ are the electrical potentials, R is the universal constant of gases and f_A is the activity coefficient of the dissolved Lithium salt. An alternative formulation of the current densities was proposed for low temperature charging

$$\begin{cases} i_1 = i_{0,1} \left[\exp \left(\frac{\alpha_{a,1} F}{RT} \eta_1 \right) - \exp \left(-\frac{\alpha_{c,1} F}{RT} \eta_1 \right) \right] \\ i_2 = \min \left\{ 0, i_{0,2} \left[\exp \left(\frac{\alpha_{a,2} F}{RT} \eta_2 \right) - \exp \left(-\frac{\alpha_{c,2} F}{RT} \eta_2 \right) \right] \right\} \end{cases} \quad (2.8)$$

The whole system is subject to the following boundary conditions:

$$\nabla c = 0 \quad \text{at} \quad \begin{cases} x = 0 \\ x = L \end{cases} \quad (2.9)$$

where L is the cell thickness [100, 101]. Different authors developed a wide range of models, starting from Newman's theories. They can vary from mono-dimensional electrochemical models to three-dimensional models. Such models prove excellent when characterising solid-electrolyte interface or phenomena as Lithium-plating at low temperatures [67, 101]. Such models provide accurate results when used to evaluate the behaviour of a specific battery chemistry, but prove difficult to set and computationally expensive. However, their contribution proves fundamental in the evaluation of certain heat generation terms

2.2.2 Reduced-order models

Reduced-order models are models that search for a solution in a governing equations subset [102]. Chebyshev and polynomial methods are preferred options in the development of such models, although orthogonal decomposition has been investigated as well. Such models can provide major benefits in computational costs, however, they need either data from higher order simulations or from experiments [103].

2.2.3 Equivalent circuit models

Equivalent Circuit Models (ECMs) are a network of voltage sources resistances and capacitors simulating the electrical interaction of electrolytes and solid phase. The simplest ECMs are resistor model, however such models are not particularly accurate, in order to take into account polarisation and increase accuracy, it is possible to add a resistance-capacity sub-network. Such model is called Thévenin equivalent circuit [36, 104]. A further variation on the theme of equivalent circuits is Randles circuit. This model integrates a Warburg impedance term, in series with the capacitance, to account for the diffusion of Lithium ions [104]. The Warburg impedance represents the effect of the combination of

the diffusional effects of Lithium ions on the interface between electrolyte and active material particles [105]. In on-board electric-vehicle applications, however, sampling rate of measurements is limited to 1 *Hz*, making it difficult to tell the solid-electrolyte contribute to resistance from the cell bulk resistance, in addition, in such scenario Warburg impedance is approximated as a number of parallels of resistance-capacitance pairs in series, adding further uncertainty to the estimation [106]. The extensive use of bi-directional ECMs has proved effective by automakers such as Renault-Nissan [107].

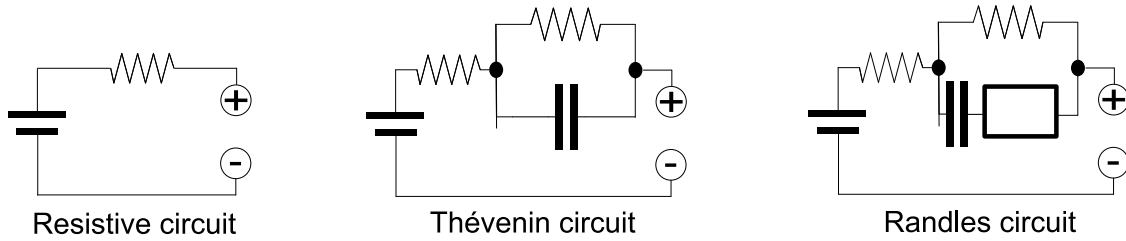


Figure 2.2: Different options of equivalent circuits.

2.2.4 Empirical models

In the case of tailored models for specific cells, it is possible to re-construct the behaviour of the battery cell from experiments. Data measured from cells are interpolated and used to feed equivalent circuit models [108, 109]. Alternatively, it is also possible to only model the voltage and current curves in order to feed other models. Such approach is what can be defined as a black-box model [110].

2.2.5 Battery thermal models

Thermal models of batteries can be developed as single-domain models or integrated in multi-domain models, in both contexts different levels of discretisation can be applied, from a lumped parameter element to a finite element model. Some authors have con-

centrated on providing a detailed electrochemical model that could correlate the ionic current with the electrolyte salt concentration in each layer, correlating it with the terminal voltage of the battery cell. However, such a model does not provide information on the thermal behaviour of the battery cell, and represents the battery layers as lumped elements [111]. Much work has been done on single-domain lumped models, focusing on one aspect of battery cell physics only, most of this work has found application in control theory. Some authors modelled the heat generation of the battery cell in correlation with modelling the cell volume as a lumped element and estimating its average thermal properties; the model proved to have a maximum error of 5% on the state of charge estimation, providing a good simulation of the general behaviour of the cell despite not investigating the local temperatures throughout the cell volume [112]. Others have pursued the implementation of battery thermal models that can be interfaced with lumped-element models of other vehicle components. In such a way it was possible to have a full system-level vehicle thermal management system simulation. However, information on battery internal temperature gradients was lost and only a generic average temperature of the battery pack was observed [113]. Other authors have developed electrochemical models that reproduce in less detail the concentration of ions, relying on describing the behaviour of single-particles at the surface of the active material. Such an option allows the integration of electrical, thermal and degradation models [114, 115]. A further step in the implementation of electrochemical models is their integration with lumped thermal models, providing a modelling of the different terms of heat generation: from contact resistances, from reaction and overpotentials and ionic ohmic heat. Such models, although still focusing on the battery cell as a lumped mass, have proven to be scalable up to a battery module model, composed of more cells [116]. Authors stressed the attention on multi-domain models that can reconstruct electrode reactions, ion transport through electrolyte, solid-state diffusion and charge transfer while accounting for

the conservation of thermal energy [117]. In addition, other researchers have proven the applicability of such techniques to cell characterisation experiments, in order to estimate state of charge and depleted capacity at different ambient temperatures [118]. On the other hand, others have proved that internal heat transfer models can be successfully coupled with equivalent circuit models and ageing models. However, such works rely on simplified heat generation models that only take into account the effect of voltage drop, beside only relying on a lumped-volume fed with averaged thermal properties of the battery cell in order to model internal heat transfer within the cell [119]. Others pursued chemistry-based equivalent-circuit models, proving that the chemical reactions occurring within a cell can be modelled by a network of electrical elements [120]. Such approach has also been used in the implementation of capacity fading models [121]. It was shown, however, how such models would need extensive experiments to characterise the battery cell parameters [122]. Researchers showed that, when coupling different domains of physics in simulation it is necessary to rely on different scales and dimensions in each domain, coupling a single-dimension chemical model, with a two-dimension electrical model and a three-dimensional thermal model [123]. Others showed how in coupled electrochemical-thermal models it is beneficial to take a two-dimensional approach, simulating the axial temperature gradient on a cylindrical cell, such approach, however, would not take into account radial gradients [124]. Others, however, preferred the implementation of single-dimension lumped-mass thermal battery cell models for battery pack model implementation, in order to reduce the complexity of the model. Such an option, however, does not investigate internal temperature gradient of cells within a pack [125]. Such models, however, often fail in portraying the interaction between each two material layers within a single battery cell. Different approaches can be taken when modelling the thermal properties of Lithium-ion cells presents challenges mostly due to the interaction of different materials and phases. Coupling different homogenous materials in series or in parallel

results in the following formulations of conductivity [54]:

$$\frac{k_{\perp}}{l_c} = \left(\sum_i^I \left(\frac{k_i}{s_i} \right)^{-1} \right)^{-1} \quad (2.10)$$

$$\frac{k_{\parallel}}{l_c} = \sum_i^I \frac{k_i}{s_i} \quad (2.11)$$

where $i=1, \dots, I$ are the phases, k_i are the thermal conductivities of the different phases, while s_i is the thickness of each layer and l_c is the overall thickness of the combined materials. The materials involved in battery cells, however present relevant levels of porosity that range between 30% and 50% and it is composed by a solid and liquid phase. In such cases, the approach is using the Krischer model, which features porosity [54]:

$$k_{\text{series}} = \left(\frac{\psi}{k_{\text{fluid}}} + \frac{1-\psi}{k_{\text{solid}}} \right)^{-1} \quad (2.12)$$

$$k_{\text{parallel}} = \psi \cdot k_{\text{fluid}} + (1-\psi) \cdot k_{\text{solid}} \quad (2.13)$$

where ψ is the porosity. Such methodology, however, has most prominently been used in order to estimate average properties of the whole cell. Properties are also influenced by the state of charge of the battery, however, such property has a much higher influence on the heat dissipation rather than on the thermal properties [54, 71].

2.2.6 Benchmarking battery models

Newman's model, represented in Figure 2.3 and further developed by other researchers is an interesting approach to the integration of different domains.

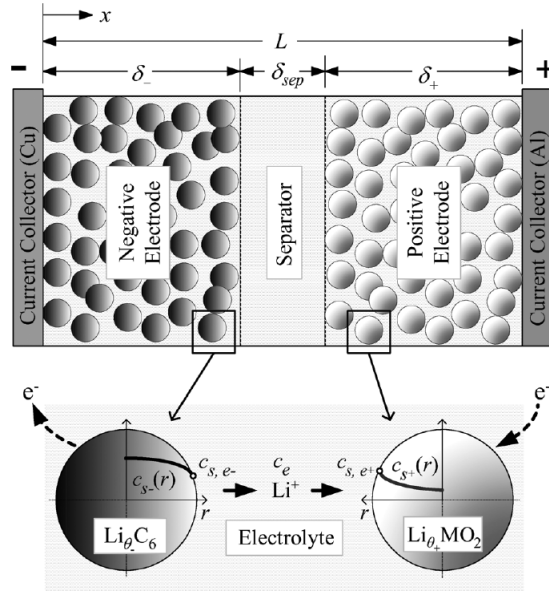


Figure 2.3: Lithium-ion insertion/extraction [115].

The core of the model is an electrochemical model that captures the solid-state and electrolyte diffusion dynamics and therefore predicting the physical limits of charge and discharge. The model is based on a network of infinite-dimensional Partial Differential Equations (PDEs), in two coordinates: the cell thickness and the radius of electrode particles in which the Lithium ions diffuse [100, 115]. The set of equations on which the model is based is composed by four PDEs coupled by a Butler-Volmer equation as follows, with the Lithium-ion conservation in the solid phase being described as [115]:

$$\begin{cases} \frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) \\ D_s \frac{\partial c_s}{\partial r} \Big|_{r=R_s} = \frac{-j^{Li}}{a_s F} \end{cases} \quad (2.14)$$

in which c_s is the solid-phase concentration, D_s is the solid-phase Lithium diffusion coefficient, a_s is the interface surface, r is the radial coordinate with respect to the particle, R_s is the particle radius, t is time, F is Faraday's constant and j^{Li} is the reaction rate. The

Lithium-ion conservation in the electrolyte being:

$$\begin{cases} \frac{\partial(\varepsilon c_e)}{\partial t} = \frac{\partial}{\partial x} \left(D_e \frac{\partial}{\partial x} c_e \right) + \frac{1-t_+^0}{F} j^{Li} \\ \frac{\partial c_e}{\partial x} \big|_{x=0} = \frac{\partial c_e}{\partial x} \big|_{x=L} = 0 \end{cases} \quad (2.15)$$

where c_e is the concentration of negative charge, x is the cell-thickness-wise coordinate, L is the cell's thickness, ε is the permittivity and t_+^0 is the Li^+ transference number. The e^- charge conservation in the solid phase is:

$$\begin{cases} \frac{\partial}{\partial x} \left(\sigma \frac{\partial}{\partial x} \phi_s \right) - j^{Li} = 0 \\ -\sigma \frac{\partial \phi_s}{\partial x} \big|_{x=0} = -\sigma \frac{\partial \phi_s}{\partial x} \big|_{x=L} = \frac{I(t)}{A} \end{cases} \quad (2.16)$$

in which σ is the solid phase conductivity, I is the current and A is the interface surface area. The e^- charge conservation in the electrolyte phase is:

$$\begin{cases} \frac{\partial}{\partial x} \left(\kappa^{eff} \frac{\partial}{\partial x} \phi_e \right) + \frac{\partial}{\partial x} \left(\kappa_D^{eff} \frac{\partial \ln c_e}{\partial x} \right) + j^{Li} = 0 \\ \frac{\partial \phi_e}{\partial x} \big|_{x=0} = \frac{\partial \phi_e}{\partial x} \big|_{x=L} = 0 \end{cases} . \quad (2.17)$$

where κ is the conductivity of the electrolyte and κ_D is the diffusional conductivity of the electrolyte. Butler-Volmer equation, describes the reaction current at the solid-electrolyte interface coupling the two equations as follows [115]:

$$\begin{cases} j^{Li} = a_s i_0 \left\{ \exp \left[\frac{\alpha_a F}{RT} \eta \right] - \exp \left[-\frac{\alpha_c F}{RT} \eta \right] \right\} \\ \eta = \phi_s - \phi_e - U \end{cases} \quad (2.18)$$

The diffusional conductivity of the electrolyte is calculated as follows [126]:

$$\kappa_D^{\text{eff}} = \frac{2RT}{F} \kappa^{\text{eff}} (t_+^0 - 1) \left(1 + \frac{d \ln f_{\pm}}{d \ln c_e} \right). \quad (2.19)$$

Such model has been subsequently integrated with a Thévenin ECM with a lumped thermal model, which was, on early models, fundamentally ohmic-generation only [108]. Other researchers have suggested that the interface between solid electrolyte and liquid can be modelled as a potential-dependent capacity. In such scenario, the equilibrium structure at the junction of a metal with a liquid electrolyte is represented as two elements, apart from the electronic charge layer: i) the inner “Helmholtz layer”, charge-free and of atomic width and ii) the outer “Gouy-Chapman” layer, semi-infinite, containing both unequally distributed anions and cations. The specific capacitance of the double layer is defined as the ratio of charge on the metal to the difference in electric potential in the liquid electrolyte between the metal surface and infinity [127]:

$$C_{\text{dl}} = \frac{q}{\phi(0) - \phi(\infty)} \quad (2.20)$$

where q is the charge and $\phi(x)$ is the potential at a distance x from the interface. In Equation (2.20), the concentration is subject to:

$$c_+ + c_- = 2c \quad . \quad (2.21)$$

Ions in this model are treated as spheres with a diameter equal to r . Equation (2.20) is

re-formulated as follows [127]:

$$\begin{aligned} \frac{1}{C_{dl}} &= \frac{\phi(0) - \phi(\infty)}{q} = \frac{\phi(0) - \phi(r)}{q} + \frac{\phi(r) - \phi(\infty)}{q} = \\ &= \frac{1}{C_{inner}} + \frac{1}{C_{outer}} \end{aligned} \quad (2.22)$$

in which the two terms account for the two layers and are calculated as follows [127]:

$$C_{outer} = \frac{\varepsilon}{\delta} \left[\frac{|q|}{\sqrt{2RT\varepsilon c} \cosh\{\exp(q^2/4RT\varepsilon c)\}} \right] \quad (2.23)$$

$$C_{inner} = \frac{\varepsilon}{r} \quad (2.24)$$

where R is the universal constant of gases, T is the temperature, ε is porosity, q is charge, c is concentration, r is the particle radius and δ is the Debye length. The Debye length is calculated as follows [127]:

$$\delta = \sqrt{\frac{RT\varepsilon}{2F^2c}} \quad (2.25)$$

The outer layer term in Equation (2.23), for small values of $q^2/RT\varepsilon c$ can be expanded in series in order to obtain an easier mathematical formulation. In the case of large values of the aforementioned quantity ($q^2 \gg RT\varepsilon c$), the outer layer capacitance can be simplified as follows [127]:

$$C_{outer} \approx \frac{\sqrt{2RT\varepsilon^3 c}}{\delta |q|} \quad (2.26)$$

Such model, despite providing terms of an equivalent circuit is more an analytical, reduced order model rather than an ECM. Alongside with reduced-order model and ECM, a further evolution are phenomenological models, which are a first attempt of reducing the computational time while performing a multi-domain analysis of battery cells. More specifically, phenomenological models available in literature couple chemical and electri-

cal domains, while accounting for three physical species: electrolyte, current collectors and electrodes, connecting them with a three-species-element ECM sub-network. In such a context, the interface between the electrolyte and the electrodes is rendered as a double species element. Researchers have also introduced terms to account for the heat dissipation of the battery cell, in relation to the electrical and chemical behaviour. The model is therefore organised in sub-circuits representing the transport of uncharged species and sub-circuits representing the transport of charged species, interfaced with each other. Such models manage to represent the amount of Lithium ions present in each layer and its consequences on the electrical behaviour. The conservation of thermal energy is therefore formulated in one dimension as follows [128]:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial t} \left(k_t \frac{\partial T}{\partial x} \right) + (q_{\text{reaction}} + q_{\text{Li-transport}} + q_{\text{ohmic}} + q_{\text{phase-change}}) - q_{\text{dissipated}} \quad (2.27)$$

where c_p is the heat capacity, x is the space coordinated, t is the time and the heat generation terms are expressed as follows:

$$\begin{cases} q_{\text{reaction}} = A_r \int_x^{x+dx} i_t (\phi^s - \phi^l - E^{\text{eq}}) dx \\ q_{\text{Li-transport}} = A_r \int_x^{x+dx} \left[\sigma_{\text{Li-interc}}^{\text{eff}} \left(\frac{\partial \phi^s}{\partial x} \right) + \kappa_{\text{Li-interc}}^{\text{eff}} \left(\frac{\partial \ln c_{\text{Li}^+}}{\partial x} \right) \left(\frac{\partial \phi^l}{\partial x} \right) \right] dx \\ q_{\text{ohmic}} = (I_{\text{battery}})^2 \frac{R_{\text{cathode}}}{L_x L_z} \\ q_{\text{phase-change}} = a_s i_t T \frac{\partial E^{\text{eq}}}{\partial T} \end{cases} \quad (2.28)$$

where i_t is the local intercalation current density, σ is the conductivity, κ is the solvent reduction kinetic constant, L terms are the length in the x and z directions and a_s is the particle active intercalation surface [128]. Such a model has proved effective in the implementation of health-aware charging/discharging strategies[129]. The path of the current inside the battery cell has been object of deep investigation by researchers, in order to

achieve accurate ECMs [130]. Damay et al. proposed models that, under the assumption of homogeneous properties throughout the battery cell, represent different sections in space, as equivalent circuits with different values of resistance and the same faradic capacitances, connected in parallel; such models are called multi-bunch models [131]. In this case the ECM was coupled with a thermal circuit representing the internal heat transfer and the heat dissipation towards the external environment. Different bunches have values of voltage and resistances that are determined by a Weibull distribution [132, 131]. Multi-bunch models has proven to perform better than other battery models. On the side of thermal models, much effort has been put on the delivery of either detailed finite-element models or alternatively reduced-order models. Some researchers have coupled reduced-order thermal models with a simplified heat generation, in order to analyse the radial heat distribution of cylindrical cells. The energy balance equation is obtained as follows [133]:

$$\begin{cases} \rho c_p \frac{\partial T(r,t)}{\partial t} = k_t \frac{\partial^2 T(r,t)}{\partial r^2} + \frac{k_t}{r} \frac{\partial T(r,t)}{\partial r} + \frac{Q(t)}{V} \\ \frac{\partial T(r,t)}{\partial r} \big|_{r=0} = 0 \\ \frac{\partial T(r,t)}{\partial r} \big|_{r=R} = -\frac{h}{k_t} (T(R, t) - T_\infty) \end{cases} \quad (2.29)$$

where h is the convective heat transfer coefficient, V is the volume of the cell and k_t is the averaged conductivity of the cell. The heat generation is assumed equal to the following term:

$$Q = i(U - V) - i \left(T \frac{\partial U}{\partial T} \right) \quad (2.30)$$

which neglects enthalpy of mixing, phase change and variations of heat capacity. The Equation (2.29) is then reduced with a polynomial approximation [133]. Although being computationally light and working well in a range of temperature in which physical propeties of the materials are not subject to major variations, such model only delivers an estimate of the radial profile of temperature of a cylindrical cell under the hypothesis of

a homogeneous material. For such reasons, it is only applicable to a reduced number of cases. Others have implemented empirical-data based ECMs, based on a structure as the one represented in Figure 2.4.

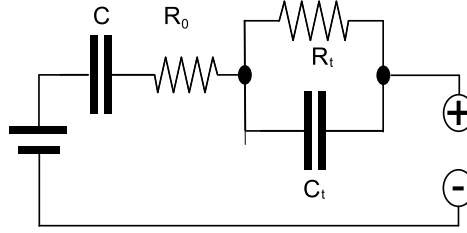


Figure 2.4: Experimental-data-based ECM as proposed by certain authors [134].

The first element of the network in Figure 2.4 is a capacitance that accounts for the ratio of charge variation on voltage variation as follows [134, 135]

$$\frac{1}{C} = \frac{\Delta U}{\Delta Q} \quad (2.31)$$

where ΔU is the voltage variation and ΔQ is the variation of charge. The resistance R_0 is obtained from experimental data for both charge and discharge. The network composed by R_t and C_t reproduces the influence of the electrochemical processes on the performance of the cell[134]. Such models prove fit as a base for the implementation of battery management strategies and are easily interfaceable with Hardware in the Loop (HIL) platforms [136]. A further implementation of empiric-based ECMs are acausal ECMs. In such models the interaction between each component is determined by their connections rather than declaring any variable a priori as input or output. Acausal modelling allows the coupling of different domains and enables the exploitment of computationally lean platforms such as Modelica modelling language and Dymola. A further advantage of such approach is the possibility of re-scaling models and generating a module of more cells from a single-cell model [46, 137]. Such models, however, are specific to a cell

chemistry and geometry and need extensive re-tuning each time a new type of cell needs to be simulated. It would therefore be much beneficial to have models that integrate experimental data specific to a certain cell with a stronger theoretical structure. There can be different ways of estimating the State of Charge (SOC). The simplest way would be estimating it from the OCV, i.e. the voltage of the battery without being connected to any load, however, such approach requires extensive characterising experiments. The most diffused method is Coulomb counting, defined as follows [138]:

$$SOC = SOC_i - \int_{t_0}^t \frac{\eta i(\tau)}{C_t} d\tau \quad (2.32)$$

where $i(t)$ is the current, η is the coulombic efficiency and C_t is the cell total capacity, t_0 is the initial instant of time, and t is the final instant in time and $d\tau$ is the infinitesimal instant of time. An improvement to such methodology could be the correction of the Coulomb count through a Kalman filter. Other methods such as support vector machine algorithm have been examined by some researcher [139, 138].

Some models also feature an estimation of the State of Health (SOH), i.e. the estimation of the residual battery capacity as percentage of the initial battery capacity. Most models of SOH are based on exponential laws obtained from experimental data [140]. Two main contributes to battery capacity decay were outlined: i) operational time and ii) cycling decay. It is therefore possible to formulate the remaining capacity as follows [141]:

$$Q_R = 1 - \left(A_P \cdot e^{-\frac{E_P}{RT}} \cdot \sqrt{N_P} + A_{cyc} \cdot e^{-\frac{E_{cyc}}{RT}} \cdot \sqrt{N_{cyc}} \right) \quad (2.33)$$

where A_P , A_{cyc} , E_P and E_{cyc} are constants depending on the battery chemistry, N_P is the operating time, N_{cyc} is the number of cycles, while T is the temperature and R is the

universal constant of gases [141]. Such Arrhenius-based methodology is employed by battery manufacturers and proves an accurate way of estimating remaining capacity.

2.2.7 Object-oriented, acausal modelling

Let us better investigate the peculiarities and benefits of acausal object-oriented modelling. Modelling is generally organised into more stages: describing a physical process, handling input data, implementing a solver and managing output data. The traditional way of dealing with this process is providing physical equations as input and defining variables that need to be obtained as output in a causal, sorted order, organising the code in several interacting subsystems. Sub-systems may be re-simulated more times while running the code. This approach may compromise the correct representation of physical parameters and result in a model that is difficult to adapt to different scenarios [142]. An object-oriented modelling strategy can allow a more modular approach, enabling the re-scalability of models and allowing the coupling of different physical domains [143]. In such modelling environments, no causal order of defined equations is applied, only a procedure is defined. In such a way it is possible to cover every single causality without re-configuring the model each time. One of the most consolidated acausal, object-oriented, multi-domain, equation-based environment is Modelica modelling language, which, for its multi-domain nature, eliminates the need for co-simulation. By doing so, any solver-synchronisation issue is removed [144]. Such strategies have been effectively applied to battery models by researchers, showing the possibility of coupling ECMs and heat transfer models [46, 137]. A bottleneck in object-oriented modelling is the choice of a solver. In Object-Oriented Modelling (OOM), physical systems are described with a set of differential-algebraic equations with an index (i.e. the number of differentiation steps required to obtain a system of ordinary differential equations) greater than 1. As

a consequence, models developed in OOM software platforms require stiff solvers, with step-size and order adaptations with error control. In addition, dealing with physical systems in which the derivative of a given property of a given discrete element depends on the values of few neighbouring elements. As it would happen in the thermal model of a battery cell, forces the solver to deal with a highly sparse Jacobian matrix, increasing computational time and allocated memory. Furthermore, in the selection of the time-step for the solver it is necessary to also take into account physical phenomena occurring locally in some regions of the modelled object and requiring a tighter time step [145]. In addition, researchers also pointed out that the size of the model should be defined by integer parameters allowing the model itself to set all physical parameters accordingly, i.e. a large physical system should be built from smaller units that can be combined together, being therefore re-scalable, in order to reduce computational effort and memory allocation [145]. Newton's solver is a widely diffused option, but an improved version of it, Petzold's Differential Algebraic System Solver (DASSL), has generally become the standard over the past decades. The algorithm replaces the derivatives with a k^{th} order backward differentiation, with k ranging from 1 to 5, and then solving with Newton's method. Such algorithm is a well-known, robust, multi-step solver with a controlled step-size and it is generally the default, in-built solver for Modelica solvers due to its high stability [146].

2.3 Research trends and research gaps

When designing a vehicle, priorities are typically maximising battery life, reducing weight, ensuring adequate safety standards and keeping manufacturing costs low. The current literary landscape outlines the need for re-scalable multi-domain battery models at a low computational cost. More specifically, what currently lacks is a modelling framework

that provides a convenient trade-off between the need for accuracy and the reduction of computational costs. Many of the available models concentrate on single cells and on a lumped element strategy, some focusing on a single domain of physics and being purely thermal models [147, 66]. Other lumped models, on the other hand, interface more domains of physics, but are still biased towards the thermal domain [140, 92]. Among finite element models, more examples of coupling of different physics domains can be found [148, 149]. The models with the most detailed discretisation, however, focus on the thermal domain only, concentrating on cell internal heat transfer [150], or on specific cooling applications [151]. A gap can be found at a lower level of discretisation, among coupled-physics domain models. Furthermore, much research has been carried out on single-cell models, especially on purely theoretical models [148, 150]. Some notable exception can be found on specific applications such as laptop batteries, in such case, single cell models were scaled up to generate a module model [110]. Most of the work featuring both simulation and experimental validation has been carried out at a single-cell level even for industrial applications [107]. A gap can therefore be found on re-scalable models that are interfaced with an experimental validation. The different aspects of the research literary landscape mentioned above are summarised in Figures 2.5 and 2.6, where the aforementioned gaps in the research are also outlined.

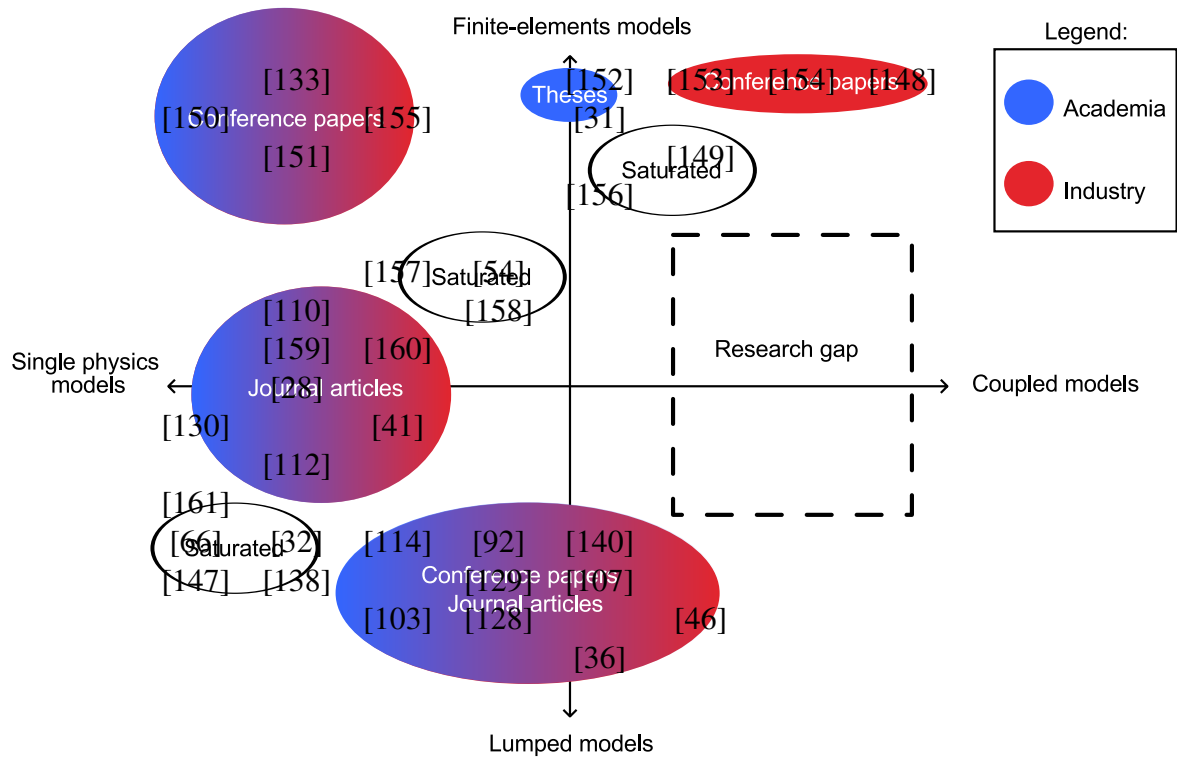


Figure 2.5: Literary landscape and research gap outline, from a modelling technique point of view.

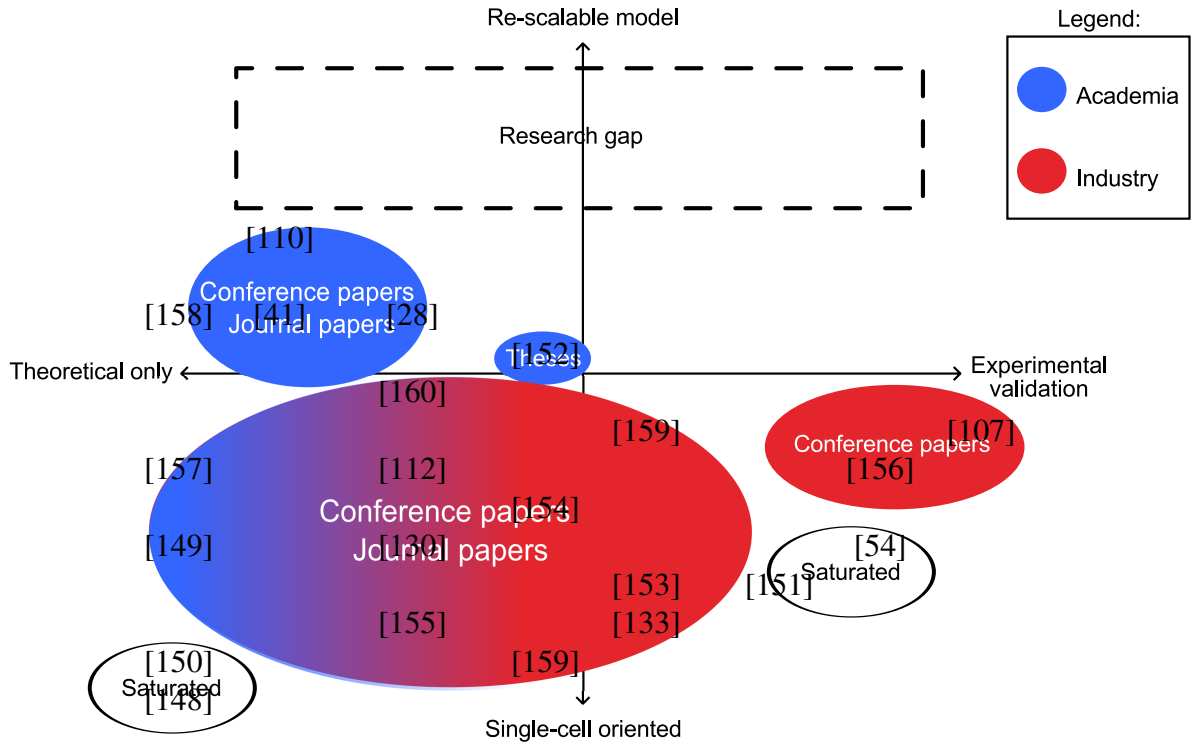


Figure 2.6: Literary landscape and research gap outline, from a modelling purpose point of view.

Major benefits would be granted by a rescalable model; the modelling procedure would be more streamlined and adaptable to different cells. In addition, it would be possible to generate module models from single cell models. It is also important to notice that a trend for the future is definitely that of multi-domain models. The outlined gap lays therefore in reducing computational cost of multi-domain models.

2.4 Battery thermal management systems

Battery thermal management systems are the devices in charge of managing the dissipated heat of batteries, while keeping them in their correct operating temperature range. In heat exchange, two elements need to be defined: a heat exchange mean, a difference of thermal

potential (i.e. temperature) is needed. In order to achieve such potential difference, it is necessary to rely on heat sources or heat sinks, depending whether the battery needs to be heated or cooled. They can be classified according to i) heat source/sink, ii) typology of contact between batteries and heat transfer mean, iii) physical state of heat transfer mean and iv) thermodynamic cycle of heat transfer mean [162].

2.4.1 Classification on the base of heat source/sink

Early battery vehicles only relied on ambient air for battery cooling, mostly for the sake of cost and weight reduction [163]. Battery Thermal Management Systems (BTMS) can either rely on the external environment as heat source/sink or they can feature an internal heat source/sink.

The former are defined as passive thermal management systems, the latter are defined as active thermal management systems. Some thermal management systems rely on a mixed strategy, integrating active and passive heat sources/sinks [162].

2.4.2 Classification as direct/indirect heat transfer

The heat transfer fluid can either be directly exchanging with the battery or their interaction can be mediated by a heat exchanger [163]. Each methodology has benefits and drawbacks. Above all, it is necessary to point out that heat transfer means in direct contact with battery cells need to be essentially electrical insulators. In indirect contact, the cells are cooled by the coolant flowing through the coolant passages in the heat sink plate. Flaws of such system can be found in the necessity of optimising the flow of the heat exchange mean on the battery surfaces.

In addition electrically conductive heat exchange means must be avoided and the system needs to be sealed from the external environment, to prevent any interference [164]. Air or dielectric oils can be used for direct contact. The latter undergoes the name of immersion cooling. Immersion cooling allows the battery to reach steady state much more quickly, but has much higher costs of maintenance and repair [163].

2.4.3 Physical phase of heat transfer mean

Heat transfer means are the materials which mediate thermal energy movement from the battery to a heat sink or from a heat source. They can be solid, liquid, aeriform or transition through different phases during the thermal managing process.

The latter refers either to a liquid to aeriform transition or to a solid to liquid transition. The former includes refrigeration cycles, the latter refers to paraffin-matrix-based thermal management systems, properly called Phase Change Material (PCM) thermal management systems.

2.4.4 Liquid cooling

In the case of liquid thermal management, both conduction and forced convection intervene in the process. Liquid coolant flows into channels which can be either in direct contact with the cells or positioned within heat sinks or plates, placed in contact with the cells.

The former is called direct liquid thermal management, the latter indirect liquid thermal management. Heat is first exchanged through conduction from the cells to the walls of the coolant channels and subsequently to the coolant through forced convection. Forced

convection can be modelled according to the following [165]:

$$\nabla \cdot (k \nabla T) + \frac{\dot{Q}}{V} = \rho c \frac{\partial T}{\partial t} \quad (2.34)$$

in which ∇ can vary depending on the coordinates selected. In the case of direct cooling, the shape of the pipes would determine the choice.

Squared section pipes would drive to the selection of a set of Cartesian coordinates, while round section pipes would drive to the selection of a set of cylindrical coordinates.

Under the hypothesis of pipes being made of metals such as Aluminium, it is possible to assume the material is isotropic and therefore the conductivity k is constant throughout the whole component.

When a base or side cooling plate is used, it look convenient to rely on a set of Cartesian coordinates to describe heat exchange from cells to plate and temperature distribution within the plate. From the pipe walls to the process fluid, heat exchange is mostly based on forced convection.

It is possible to define the heat flux across the heat sink and the coolant as follows [166]:

$$k_{hs} \nabla T_{wall} = h_c \nabla T_c \quad (2.35)$$

and energy conservation equation as follows:

$$\rho_c C_{pc} \frac{\partial T_c}{\partial t} = \nabla \cdot (h_c \nabla T_c) \quad (2.36)$$

where the subscript c refers to “coolant”. The equilibrium of momenta is expressed as follows:

$$\begin{aligned}\frac{\partial u}{\partial t} + \nabla u \cdot v_i &= f_{x_1} - \frac{1}{\rho} \frac{\partial P}{\partial x_1} + \nu \cdot \nabla^2 u \quad \text{in } \Omega, t > 0 \\ \frac{\partial v}{\partial t} + \nabla v \cdot v_i &= f_{x_2} - \frac{1}{\rho} \frac{\partial P}{\partial x_2} + \nu \cdot \nabla^2 v \quad \text{in } \Omega, t > 0 \\ \frac{\partial w}{\partial t} + \nabla w \cdot v_i &= f_{x_3} - \frac{1}{\rho} \frac{\partial P}{\partial x_3} + \nu \cdot \nabla^2 w \quad \text{in } \Omega, t > 0\end{aligned}\tag{2.37}$$

in which f is the body force, ρ is the density, P is the pressure and ν is the kinematic viscosity of the fluid (air in this case), $v_i = (u, v, w)$ is the vector of velocities and x_1, x_2 and x_3 are generic coordinates. Indirect liquid cooling is widely diffused.

LG Chem is currently supplier of many automotive manufacturers, including Volkswagen, BMW, Daimler, PSA, FCA, JLR, Hyundai-Kia and Renault-Nissan.

LG provides a system in which reconfigurable “bricks”, containing in most cases 12 NMC 60Ah (some manufacturers use SK 58Ah cells on the same layout instead) pouch cells connected in a 3s 4p configuration are assembled in modules, which then compose a pack [167].

Such pack is cooled with a bottom cold-plate heat exchanger as shown in Figure 2.7 for the case of the Audi E-Tron [168].

Audi e-tron 50 quattro

Flüssigkeitsgekühlte Lithium-Ionen-Batterie
Liquid cooled lithium-ion battery
07/19

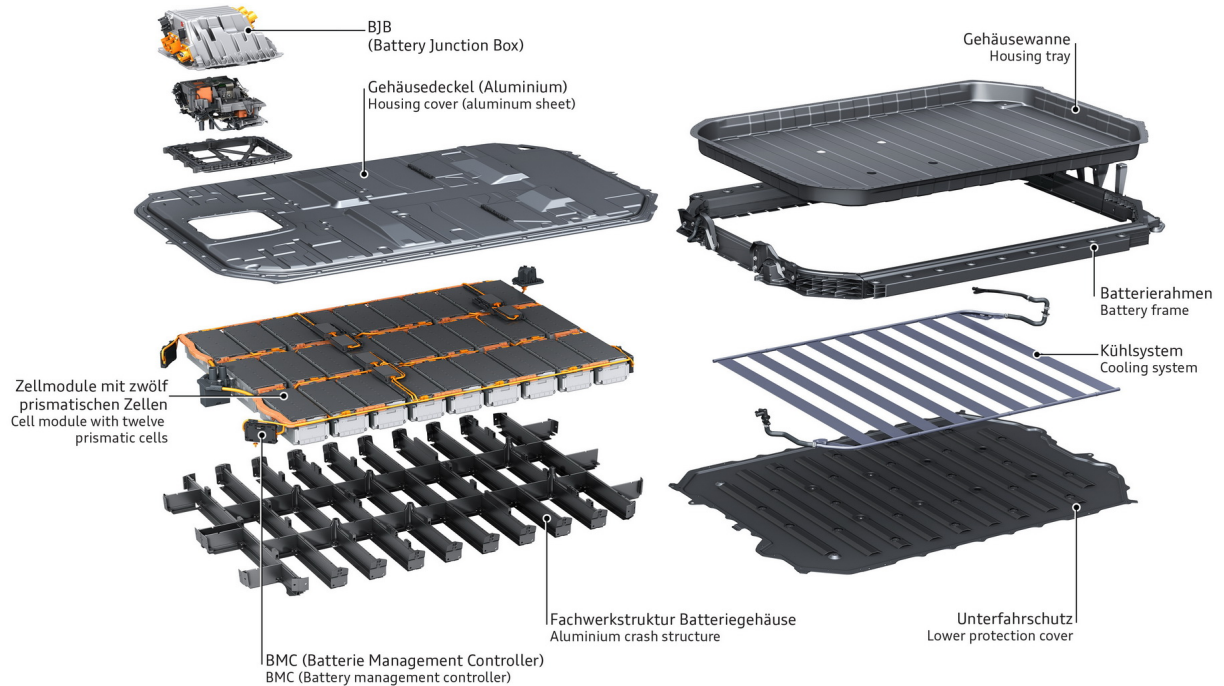


Figure 2.7: Audi E-Tron battery structure [167].

Alternatively, other options were side-cold plate heat exchangers, as in the system originally patented by Honda and later re-proposed by a Samsung-Bosch joint venture, illustrated in Figure 2.8 [169].

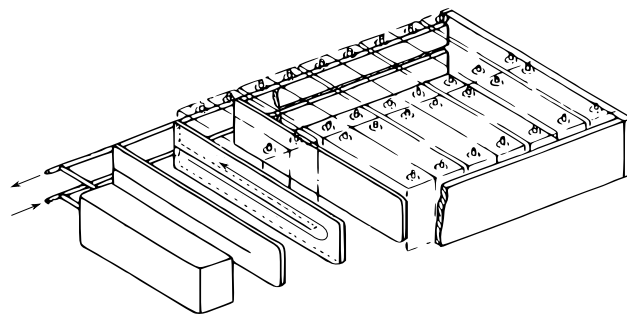


Figure 2.8: Side cold-plate indirect liquid cooling [169].

Another option of indirect liquid cooling is the layout chosen by Tesla, shown in Figure 2.9. In this case, finned pipes are arranged within the stacks of battery cells, in order to minimise the internal temperature gradient of each cell [170].

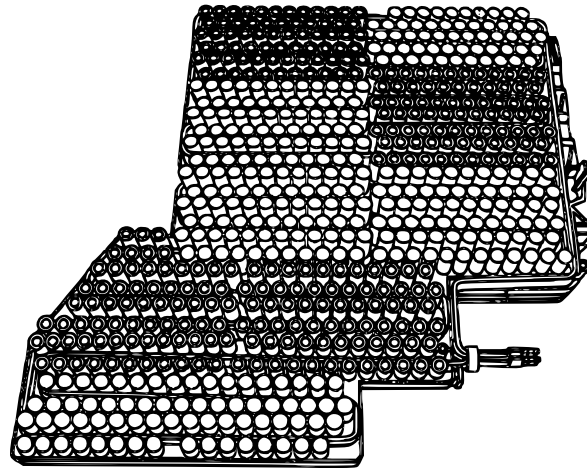


Figure 2.9: Tesla module layout, outlining the cooling strategy with pipes stretching through the cell stacks [171].

A further notable solution is the layout used on the Chevrolet Volt battery pack, featuring micro-channel cold plates, stacked between each two pouch cells as it can be seen in Figure 2.10 [172, 164].

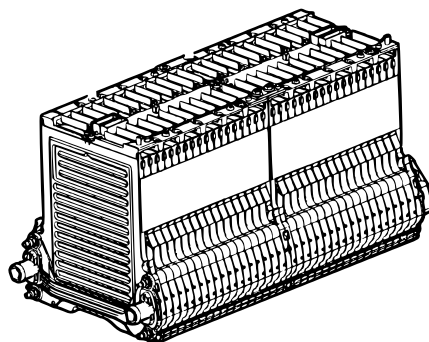


Figure 2.10: Battery module of a Chevrolet Volt, stack of prismatic pouch cells and liquid cold plates [173].

In liquid-based battery thermal management systems process fluids are usually either

water mixed with other fluids or mineral oils. The advantages of using water-based liquids are many. Such process fluids have a low friction, a high heat capacity and a high conductivity. The two latter properties result in a low temperature gradient between inlet and outlet. This would result in a good heat removal from the battery. On the other hand, dielectric mineral oils have a higher heat transfer coefficient at lower diameters and high mass flow. Such fluids can therefore be used to limit maximum peak temperature. Moreover they can reduce temperature oscillations in highly transient heat generating batteries [174].

It seems beneficial therefore, to use mineral oils for a battery thermal management system, especially in the case of direct battery thermal management systems. However, Tesla prefers to rely on a mix of 50% of either Ethylene or Propylene Glycol and 50% water. In addition, in the case of Tesla batteries, the main loop exchanges heat with a refrigeration loop, based on R134a refrigerant [175, 171].

2.4.5 Air cooling

In the case of an air-based strategy, the BTMS is essentially a cooling system. The main heat transfer mechanism is convection, since irradiation can be neglected within the operational range of battery cells. It is possible to describe the behaviour of the air surrounding the cells according to Navier-Stokes (NS) equations [176]. Continuity equation will be expressed as:

$$\nabla \cdot \bar{v} = 0 \quad \text{in } \Omega, t > 0 \quad (2.38)$$

where $\bar{v}$ is the vector of velocity and the gradient is expressed according to the selected coordinate set, depending on geometry and Ω is the computational domain. Equilibrium

of momenta can be formulated as:

$$\begin{aligned}\frac{\partial u}{\partial t} + \nabla u \cdot v_i &= f_{x_1} - \frac{1}{\rho} \frac{\partial P}{\partial x_1} + v \cdot \nabla^2 u \quad \text{in } \Omega, t > 0 \\ \frac{\partial v}{\partial t} + \nabla v \cdot v_i &= f_{x_2} - \frac{1}{\rho} \frac{\partial P}{\partial x_2} + v \cdot \nabla^2 v \quad \text{in } \Omega, t > 0 \\ \frac{\partial w}{\partial t} + \nabla w \cdot v_i &= f_{x_3} - \frac{1}{\rho} \frac{\partial P}{\partial x_3} + v \cdot \nabla^2 w \quad \text{in } \Omega, t > 0\end{aligned}\quad (2.39)$$

where f is the body force, ρ is the density, P is the pressure and v is the kinematic viscosity of the fluid (air in this case) and $v_i = (u, v, w)$ is the vector of velocities and the generic coordinates are expressed as x_1, x_2 and x_3 . The energy equation is then formulated as follows:

$$\rho C_p \frac{DT}{Dt} = h \nabla^2 (T) + \mu \Phi \quad \text{in } \Omega, t > 0 \quad (2.40)$$

where h is the convection coefficient. Concerning the latter, it is important to remark how boundary conditions depend on the model. It is therefore necessary to identify the geometry of the cell and allow the user of the model to set it depending on the vehicle, whose design will be optimised. In (2.40), C_p is the heat capacity, k is the thermal conductivity, μ is the viscosity and Φ is the viscous heating term.

Such a formulation, however, is not always practically applicable and therefore, it is essential to have a lumped parameter model which could provide a more viable solution, still retaining a satisfactory degree of accuracy. A basic lumped parameter model of heat transfer from the cells to the surrounding air, can be expressed as follows [177]:

$$\dot{Q} = N \cdot h \cdot A \cdot \Delta T_{av} \quad (2.41)$$

where N is the number of cells, h is the heat transfer coefficient, A is the surface area of

the cell and ΔT_{av} is the mean temperature difference between cell surface and surrounding air. From (2.39), (2.38) and (2.40) it is possible to see that the velocity of air plays a fundamental role in this kind of BTMS. This implies that an air-based BTMS is no longer much effective for large-sized batteries. It is difficult to maintain the required values of velocity throughout long channels. On the other hand, this solution is certainly cheap to manufacture and maintain and keeps the weight of the vehicle low.

Different applications of air cooling techniques are available on the market. The Renault-Nissan alliance preferred to rely on passive cooling on the first generation of Nissan Leaf and on a forced air strategy for vehicles like the Renault Zoe, as represented in Figure 2.11 [178]. This solution insures lightness and robustness to the system.

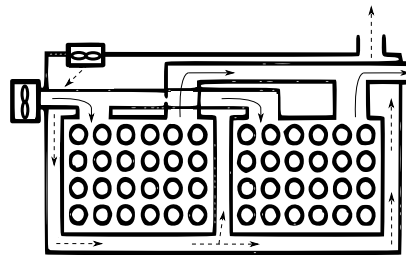


Figure 2.11: Renault-Nissan air cooling patent [178].

On the other hand, this layout makes the recovery of the heat dissipated by the battery pretty difficult and limited. Another relevant example is the battery pack developed by Williams for Formula E [179].

2.4.6 Current progresses in PCM

Phase change materials are generally speaking paraffin-based compounds, they can be used for both passive and active systems, the latter implying the PCM is combined with air or liquid cooling. They are particularly effective in reducing the internal temperature

gradient in each battery cell. When used as purely passive systems, they are unfit for automotive applications, since high-average heat output systems can provide them with a large amount of energy, which they store as latent heat. In such way, their peak-temperature-limiting power is less effective [180, 181]. In order to remove heat that otherwise would be stored as latent heat in the PCM, researchers suggested to further cool the PCM and battery cells assembly with forced convection air cooling at the external surfaces of the battery module, at a rate of $10W/(m^2K)$, showing how such option can increase the heat rejection rate by one order of magnitude in a 20-cell module of 7.5Ah 18650 cells organised in 4 5-cell stacks immersed in 0.250kg of AllCell PCM matrix, leaving the top and bottom plate of each cell exposed and welded to Nickel-plated Copper bus bars, under a duty cycle alternating recharge at a rate of 1.5C and discharge at a rate of 1.0C at an ambient temperature of $30^\circ C$ [182]. This material is generally considered safe up to $60^\circ C$ and it is not corrosive. Transition of phase occurs at $60^\circ C$ and the latent heat is $245 kJ/kg$, properties that make it a suitable material for this purpose [182, 180, 181]. Different methodologies can be used to improve PCM performance. The addition of graphite to the paraffin matrix of PCM can improve the thermal conductivity without increasing temperature dependence excessively, however the result would be a highly anisotropic material. Combining PCM with a Copper foam and/or Aluminium fins can help in achieving thermal conductivities up to above $2 W \cdot m^{-1} \cdot K^{-1}$, which result in a good improvement in cell temperature management, especially at high loads. Such composite heat exchanger can be combined with liquid cooling, resulting in effective heat dissipation and decreasing the internal temperature gradient of up to 30% in comparison with forced air cooling [183, 151, 184, 185]. It is possible to model the behaviour of the PCM material according to energy equations as well. It is possible to apply the same concept and write [181]:

$$\rho_{PCM} \frac{\partial H}{\partial t} = k_{PCM} \nabla^2 T \quad (2.42)$$

where H is the enthalpy of the PCM. In such scenario, it is important to define the initial conditions and the boundary conditions. The initial state is therefore defined as:

$$\begin{cases} t = 0 \\ T(x, y, z) = T_0 \end{cases} \quad (2.43)$$

while boundary conditions at the battery cell-PCM interface are, according to energy conservation, as follows:

$$-k_{\text{battery}} \nabla T = -k_{\text{PCM}} \nabla T \quad (2.44)$$

Furthermore, it is necessary to consider the boundary conditions between the PCM and its container:

$$-k_{\text{container material}} \nabla T = h(T - T_{\text{amb}}) \quad (2.45)$$

where h is the convective heat transfer coefficient. The above discussion shows it is possible to model such materials. PCM-based BTMSs, however, raise relevant questions in terms of control. Such systems cannot be fully independent from environmental conditions and therefore their use is, for the moment very limited.

2.4.6.1 Summary of notable vehicles

Different typologies of battery vehicles require different thermal management systems. Cooling battery modules through the immersion of the cells in an electrically insulating cooling liquid is an option proposed by Microvast Power Systems and currently being developed for industrial applications together with FPT and CNH Industrial, such option increases the contact surface of coolant with battery cells while reducing coolant pressure drops and containing battery pack size [186, 187]. On such vehicles space and packaging issues are less relevant than on small passenger cars. It is therefore possible to implement

systems that maximise the heat exchanging surface of the cells while having turbulent circulation of high specific heat fluids around them.

On the other hand, small passenger or goods vehicles such as compact or full-size cars, people carriers packaging plays a major role in battery design since the amount of space is limited. In addition, in order to maximise range, it is essential to keep power consumption of the thermal management system low. Air has lower thermal conductivity and lower density, compared to liquid coolants. However, it requires a lower number of thermal management components, reducing weight and cost. Beside air, indirect liquid cooling is also a preferred option since despite relying on heat exchangers to mediate the heat transfer between batteries and liquid, it allows the safe use of high-specific heat liquids and since it also ensures compliance with safety standards [163]. On small vehicle such as mopeds, forklifts or microcars, which, in some cases, are working in protected environments, minimising cost, weight, and energy consumption are the main targets. In these cases, therefore, passive cooling is often the most feasible option. Some notable BTMS from commercial and racing vehicles are outlined in Table 2.2.

	Heat source/sink	Contact	Phase
Audi E-Tron	Active	Indirect	Liquid
Jaguar I-Pace	Active	Indirect	Liquid
Porsche Taycan	Active	Indirect	Liquid
Tesla Model S	Active	Indirect	Liquid
Reanult Zoe	Passive	Direct	Air
Formula E	Active	Direct	Air

Table 2.2: Comparative table of different vehicle cooling systems.

2.4.6.2 Considerations on the most common layouts

A wide range of BTMS layouts is available on the market. The choice of a specific system depends mostly on the duty cycle expected for the vehicle. When the duty cycle is limited

to short urban drives, air passive cooling BTMS seem to be a preferred option. When reducing weight is the priority, active air cooling is chosen. When increasing mass of the vehicle is not an issue and the average duty is composed by sections of extra-urban roads and motorway, active liquid cooling is selected. Since opting for the wrong system would result in major performance drops and eventually safety issues, it is essential to correctly forecast the behaviour of the battery cells. This implies performing simulations on more domains. However, in early stages of vehicle design, the computational and time expense of such simulations may be inconvenient. There is therefore a need for computationally light, multi-domain models that can be used in early stages of vehicle design.

2.5 Summary of chapter

In this chapter we examined the literature on batteries, battery modelling and battery thermal management. First Lithium-ion cells were examined and their components, formats, and physics were described. After that, modelling strategies available in literature were examined and compared. Battery thermal management systems were then described. After having outlined the literary landscape and the current state of art in battery modelling and in battery thermal management systems, the proposed modelling technique will be introduced in the following chapter.

Chapter 3

A multi-domain battery modelling framework

The chapter introduces a computationally lean, re-scalable and multi-domain model that is used to generate a whole module model from a single cell model. Such a model is composed by more sub-models: a chemistry-based equivalent circuit model, which is an equivalent circuit model in which the circuit components are calculated from correlations depending on chemistry parameters of the cell, such as the concentration of the Lithium ions, and an internal heat transfer model. The equivalent circuit model exploits a mixed strategy, relying partly on interpolated data and partly on materials' properties. The internal heat transfer model reproduces the interaction between solid and liquid materials, through a network of elements used to build up the different layers. The two models are developed in an object-oriented acausal language, in order to avoid solver-synchronisation issues and grant a good coupling of different domains, while allowing the generation of matrices of single-cell models to populate a module model. The use of a single solver removes domain synchronisation issues.

3.1 The approach

The model in this work is developed relying on a network of interconnected lumped masses, solved in a multi-domain modelling network. Such technique has been previously applied by other authors to model air-ducts and its main advantage is relying on a single solver, not involving co-simulation and more simulations running in parallel on different solvers [143]. The model is composed by two main modules developed in Modelica: an equivalent circuit model, featuring heat generation and a single cell internal heat transfer model. The internal heat transfer model is defined as a network of lumped masses, each of which exchanging heat with the neighbouring masses, in a three-dimensional system of Cartesian coordinates (in the case of pouch cells) or cylindrical coordinates (in the case of cylindrical cells). Elements represent different layers, and those that represent the electrode and current collector layers are subject to heat generation, which is obtained from the ECM. The ECM is a network of resistive elements and capacitors, simulating the electrical behaviour of cell and the heat rejection, the latter being divided into more terms, each of which representing the contribution of one layer. Further details of the internal heat transfer model can be found in paragraph 3.1.2, while the equivalent circuit model is presented in paragraph 3.1.

This approach has a coarser discretisation than finite element methods, a finite element thermal model, however, takes approximately 3000s to simulate a steady-state constant heat generation case on 4 processors in parallel, and needs 16 processors running in parallel in order to run a single cell model in less than 1000s [158]. The proposed strategy requires simulation times in the order of magnitude of hundreds of seconds for a single cell, also providing a multi-domain strategy, as explained in the next paragraphs. The error and the accuracy of the model in different temperature ranges are discussed in

Chapter 5 which includes the outcome of simulations and experiments.

In summary, the choice of a modelling language can imply either representing physical objects as discretised in finite elements or as networks of lumped-mass elements, the chosen tool working in the latter way. The model provides local information on heat transfer and temperature profile, while keeping a low computational cost. Although being the discretisation coarse (in the order of magnitude of some tens of elements), the different domains of the model do not present issues due to solver synchronisation and can therefore easily be integrated in other larger vehicle models.

3.1.1 Equivalent circuit battery model

The ECM represents the electrical behaviour of the single cell and, scaled up, the electrical behaviour of the battery module. It is composed by a network of capacitor and resistor elements, represented in Figure 3.1, whose parameters are function of temperature and state of charge. The elements of the ECM are obtained from a simplified Newman's model, as in paragraph 2.2.6 with parameters estimated from electrode-averaged concentration, expressed as linear function of SOC as in 3.5 [188]. Capacitors account for the global charge/discharge process and also for layer-to-layer charge transfer, while resistors are function of materials' properties, geometry and chemistry. Parameters such as open circuit voltage are based on interpolated battery experimental data. The ECM is composed of the following elements: double layer capacitor, concentration-based capacitor, concentration-based resistors and tab resistors. There are three parallels of concentration-based resistors and capacitors, connected in series, each of them representing the electrolyte in cathode, separator and anode respectively.

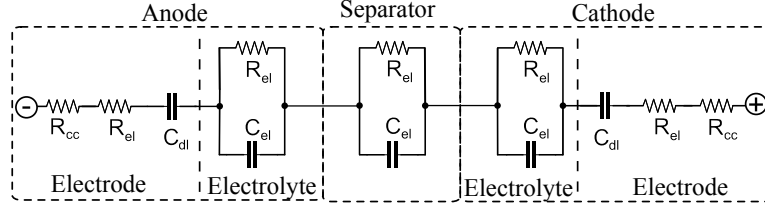


Figure 3.1: Equivalent circuit scheme proposed.

Two double layer capacitors at the beginning and temperature-dependent resistors at each end of the series represent the electrodes. Such elements represent the behaviour of porous electrodes, which are mechanically separated from each other by separators and electrically connected by the electrolyte. The capacitance of the double layer (C_{dl}) represents the interface between electrolyte and electrodes and can be represented as two capacitors in series as previously introduced in Chapter 2, Section 2.2.6. The electrolyte capacitance ($C_{Li^+}^{el}$) is expressed as a function of the concentration

$$C_{Li^+}^{el} = \frac{c_{Li^+}}{RT (x_j) (nF)^{-2}} \cdot A_S (x_j - x_{j-1}) \quad . \quad (3.1)$$

The electrolyte resistance (R_{el}) is represented by the following equation

$$R_{el} (x_j) = \frac{RT (x_j)}{c_{Li^+} (x_j) D_{Li^+} (nF)^2} \cdot (x_j - x_{j-1})^{-1} \quad . \quad (3.2)$$

The resistance is also subject to the effect of the time derivative of the temperature, through the use of a corrective coefficient, for the example, a generic resistance i of the ECM is corrected as follows:

$$R_{T\text{correction}} = R_{el_i} \left(1 + \alpha \frac{dT_i}{dt} \right) \quad (3.3)$$

where the coefficient α is a quadratic function of the time derivative of the temperature in

the local region of space as in

$$\alpha = A \left(\frac{dT_i}{dt} \right)^2 + B \left(\frac{dT_i}{dt} \right) + C \quad (3.4)$$

Variable	Symbol	Value	Unit	Reference
Equilibrium electrolyte concentration	$c_{Li^+, \max}$	$1.2 \cdot 10^3$	$mol \cdot m^{-3}$	[128]
Electrolyte diffusion coefficient	D_{Li^+}	$2.6 \cdot 10^{-10}$	$mol \cdot s^{-1}$	[128]
Faraday's Constant	F	96487	$C \cdot mol^{-1}$	[126]
Universal Constant of Gases	R	8.3143	$J \cdot mol^{-1} \cdot K^{-1}$	[126]
Particle Radius	r	$1.0 \cdot 10^{-6}$	m	[127, 128]
Dielectric Constant in Vacuum	ϵ_0	$8.854 \cdot 10^{-12}$	$F \cdot m^{-1}$	[127, 128]
Material Relative Permittivity	ϵ_r	20	$F \cdot m^{-1}$	[127, 128]
Molar Fraction at $SOC = 100\%$	θ_{Anode} $\theta_{Cathode}$	0.81 0.54	— —	[189]

Table 3.1: Summary of equation variables.

Ambient temperature	SOC	$R_{ccA} [\Omega]$	$R_{ccS} [\Omega]$	$R_{elA} [\Omega]$	$R_{elS} [\Omega]$	$R_{elC} [\Omega]$
$-10^\circ C$	100%	0.0012	0.0023	0.0182	0.0284	0.0254
	80%	0.0012	0.0023	0.0213	0.0284	0.0257
	60%	0.0012	0.0023	0.0256	0.0284	0.0261
	40%	0.0012	0.0023	0.0320	0.0284	0.0265
	20%	0.0012	0.0023	0.0428	0.0284	0.0269
	0%	0.0012	0.0023	0.0646	0.0284	0.0273
$25^\circ C$	100%	0.0010	0.0020	0.0043	0.0067	0.0060
	80%	0.0010	0.0020	0.0050	0.0067	0.0061
	60%	0.0010	0.0020	0.0061	0.0067	0.0062
	40%	0.0010	0.0020	0.0076	0.0067	0.0063
	20%	0.0010	0.0020	0.0102	0.0067	0.0064
	0%	0.0010	0.0020	0.0153	0.0067	0.0065
$40^\circ C$	100%	0.0011	0.0021	0.0033	0.0052	0.0047
	80%	0.0011	0.0021	0.0039	0.0052	0.0047
	60%	0.0011	0.0021	0.0047	0.0052	0.0048
	40%	0.0011	0.0021	0.0059	0.0052	0.0049
	20%	0.0011	0.0021	0.0079	0.0052	0.0049
	0%	0.0011	0.0021	0.0119	0.0052	0.0050

Table 3.2: Summary of circuit resistance terms for a 21700 cell, for ECM in Figure 3.1.

	SOC	$C_{dl_A} [F]$	$C_{dl_C} [F]$	$C_{el_A} [F]$	$C_{el_S} [F]$	$C_{el_C} [F]$
$-10^\circ C$	100%	734.88	224.86	84421.69	100502.01	44220.88
	80%	447.03	245.35	70753.41	100502.01	45024.90
	60%	343.66	273.18	57085.14	100502.01	45828.92
	40%	265.85	313.80	43416.87	100502.01	46632.93
	20%	195.42	385.68	29748.59	100502.01	47436.95
	0%	126.81	656.66	16763.73	100502.01	48200.76
$25^\circ C$	100%	737.36	230.27	74506.39	88698.08	39027.16
	80%	453.71	251.04	62443.45	88698.08	39736.74
	60%	350.24	279.21	50380.51	88698.08	40446.32
	40%	271.79	320.20	38317.57	88698.08	41155.91
	20%	200.36	392.41	26254.63	88698.08	41865.49
	0%	130.37	660.93	14794.84	88698.08	42539.60
$40^\circ C$	100%	738.14	232.03	70935.79	84447.37	37156.84
	80%	455.86	252.89	59450.95	84447.37	37832.42
	60%	352.37	281.17	47966.11	84447.37	38508.00
	40%	273.72	322.27	36481.27	84447.37	39183.58
	20%	201.97	394.58	24996.42	84447.37	39859.16
	0%	131.54	662.28	14085.82	84447.37	40500.96

Table 3.3: Summary of circuit capacitance terms for a 21700 cell, for ECM in Figure 3.1.

The average concentration ($c_{s,avg}$) is function of the State Of Charge (SOC) in the following equation:

$$c_{s,avg}(t) = [SOC(t)(\theta_{100\%} - \theta_{0\%}) + \theta_{0\%}] \cdot c_{Li^+,max} \quad (3.5)$$

where the dimensionless Li concentration is obtained as a ratio of actual concentration divided by maximum concentration $\theta = c_s/c_{s,max}$, in which $c_{s,max}$ is determined according to the cell chemistry. The state of charge (SOC) is obtained from

$$SOC = SOC_i - \frac{1}{3600 \cdot C_{cell}} \int_T i \cdot dt \quad (3.6)$$

where: SOC_i is the initial state of charge, C_{cell} is the cell capacity, T is the duration of the simulation and i is the current at a given instant in time. The Open Circuit Voltage (OCV)

is obtained from a polynomial interpolation from cell data as in:

$$\begin{aligned} OCV = & p_1 \cdot SOC^6 + p_2 \cdot SOC^5 + p_3 \cdot SOC^4 + \\ & + p_4 \cdot SOC^3 + p_5 \cdot SOC^2 + p_6 \cdot SOC + p_7 \quad . \end{aligned} \quad (3.7)$$

The OCV curve is also affected by the cycling history of the cell and more specifically by the average charge/discharge rate at which the cell has been previously cycled, where such rate is defined as follows:

$$C_{\text{rate}} = \frac{I}{I_{1h}} \quad (3.8)$$

where I_{1h} is the current necessary to discharge the battery in one hour. The effect, for state of charge between 90% and 10%, is equal to a fixed translation of the curve directly proportional to the rate at which the cell has been previously cycled. The translation term can be approximated with an additional linear term as in Equation (3.7):

$$\begin{aligned} OCV = & p_1 \cdot SOC^6 + p_2 \cdot SOC^5 + p_3 \cdot SOC^4 + \\ & + p_4 \cdot SOC^3 + p_5 \cdot SOC^2 + p_6 \cdot SOC + p_7 + \Delta V_{C-\text{rate}} \cdot (1 - C_{\text{rate}}) \quad . \end{aligned} \quad (3.9)$$

3.1.2 Internal heat transfer model

Assuming uniform initial temperature, internal heat transfer for a generic battery geometry would be defined by the following transient heat equation:

$$\nabla \cdot k \nabla T + \dot{q} = \rho c \frac{\partial T}{\partial t} \quad (3.10)$$

In the case of cylindrical cell, neglecting variation of temperature in circumferential direction, for the cylindrical cells the energy equilibrium is obtained as follows:

$$\rho c_p \frac{\partial T(r, z, t)}{\partial t} = \left(r \frac{\partial T(r, z, t)}{\partial r} \right) + \quad (3.11)$$

$$+ \frac{k_z}{r^2} \frac{\partial^2 T(r, z, t)}{\partial z^2} - \nabla \cdot \bar{q}(r, z, t) \quad .$$

In (3.11), r , z and t are the radial, axial and time coordinates, ρ is the density of the material, c_p is the specific heat, k is the thermal conductivity in directions r or z as specified in the subscript, T is the temperature and $\bar{q}$ is the dissipated and absorbed heat power, averaged on the analysed volume. In a similar manner, for pouch cells, it is possible to define the energy equilibrium as follows:

$$\rho c_p \frac{\partial T(x, y, z, t)}{\partial t} = \frac{\partial^2 T(x, y, z, t)}{\partial x^2} + \frac{\partial^2 T(x, y, z, t)}{\partial y^2} + \quad (3.12)$$

$$+ \frac{\partial^2 T(x, y, z, t)}{\partial z^2} - \nabla \cdot \bar{q}(x, y, z, t) \quad .$$

The general term $\bar{q}$ is therefore obtained averaging on the whole volume local $\dot{q}$ terms. Each local $\dot{q}$ is composed by more terms: reaction heat ($\dot{q}_r$), entropic heat ($\dot{q}_e$), ohmic heat ($\dot{q}_j$), contact ohmic heat occurring in current collectors ($\dot{q}_{cc}$) and the dissipated heat ($\dot{q}_{diss}$) as follows:

$$\dot{q} = \dot{q}_r + \dot{q}_e + \dot{q}_j + \dot{q}_{cc} - \dot{q}_{diss} \quad . \quad (3.13)$$

The contribution of phase change heat has shown to be negligible within the operating temperature range of road vehicles. The thermal contact resistance rejected heat is modelled through the current-collector resistances (cc subscript in the diagram in Figure 3.1). With reference to the previous chapters, the terms of equation (3.13) are expressed for

each element:

$$\dot{q}_e = A_s \cdot \int_0^L j_{Li} \left(T \cdot \frac{\partial E_{OCV}}{\partial T} \right) \quad (3.14)$$

$$\dot{q}_{cc} = i_{cc}^2 \cdot R_{cc} \quad (3.15)$$

$$\dot{q}_r = A_s \cdot \int_0^L j_{Li} (\phi_{solid} - \phi_{electrolyte} - OCV) \cdot dx_i \quad (3.16)$$

$$\dot{q}_j = i_j^2 \cdot R_j \quad (3.17)$$

A_s is the active surface, i_j is the current in the considered element and ϕ are the potentials of electrodes and electrolyte. R_{cc} is the current collector resistance and R_j is the resistance of the considered circuit element. Dissipated heat ($\dot{q}_{diss}$) is subject to boundary conditions and can occur either through conduction or through convection. Battery cell supports and electrical are also represented, in order to ensure an accurate reproduction of the thermal behaviour of the cell. Physical properties are defined locally as introduced in the previous sections. Boundary conditions are defined for each discrete element. Radiation heat transfer is neglected, as temperature gradient with external environment, surface and material properties make its contribution smaller, by several orders of magnitude, when compared to conduction and convection.

Each direction is represented separately. Computational effort is reduced as we can see by comparing the proposed model with strategies presented in literature which require longer computational time. For instance, a 5-cell stack CFD model inclusive of a thermal management system requires 14 hours of computation for a 3500 s long simulation at constant current discharge, on a 5-core Intel i7 CPU [190]. According to other authors, element models for battery cell heat conduction simulation of a single pouch cell, takes approximately 3000s to simulate a steady-state constant heat generation case on 8 processors in parallel [158]. The run time of the proposed model presented is less than 60s for a single cell. In addition, the different physics domains are better synchronized.

Each element of the ECM corresponds to a IHTM element. A simulation library that can represent different cell geometries and chemistries is generated. Simplifications are applied and the term of divergence of the heat in (3.11) is re-formulated as follows:

$$\rho c_p \frac{\partial T(r, z, t)}{\partial t} = \frac{k_r}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T(r, z, t)}{\partial r} \right) + k_z \frac{\partial^2 T(r, z, t)}{\partial z^2} + \frac{\dot{Q}}{V} \quad (3.18)$$

Equation (3.18) uses the total heat transfer $\dot{Q}$ divided by the volume V instead of using the term of volume-unit-specific heat. The energy balance of the thermal problem is defined according to a coordinate system that assigns positive sign to heat generated by each element ($\dot{Q}_{\text{gen}}$) and negative sign to heat dissipated by each element to the surrounding external environment ($\dot{Q}_{\text{diss}}$) as

$$m_{\text{tot}} \bar{c}_p \frac{\partial \bar{T}}{\partial t} = \sum_{i=1}^n (\dot{Q}_{\text{gen}_i} - \dot{Q}_{\text{diss}_i}) \quad (3.19)$$

where, m is the mass of the element and n is the number of discrete elements, $\dot{Q}_{\text{gen}}$ is the heat generated in that specific element, such information is obtained from the ECM.

Different composite materials are used in Li-ion battery cells. There are three main elements: solid electrodes, solid separators and liquid electrolytes. Cell electrodes include a base material, a coating and host a metal current collector inside them, as explained in the previous chapters. Current collectors are made of Copper for the anode and Aluminium for the cathode. The electrolyte is a solution of Lithium Hexafluorophosphate (LiPF_6) in the ratio of 1 mole per litre using a 50-50 mix of Ethyl Carbonate (EC) and Diethyl Carbonate (DEC) as a solvent. Within the operating temperature interval of automotive cells (between -15°C and 50°C) it is possible to linearise both conductivity (k) and specific

heat (c_p) in the following form

$$k = m_k \cdot T + b_k \quad \text{and} \quad c_p = m_c \cdot T + b_c \quad (3.20)$$

in which m is the angular coefficient, b is a translation coefficient and subscript k and c refer to conductivity and specific heat respectively. Constant thermal properties cause a divergence of simulation results from experimental data, as a cumulative error when modelling long drive cycles can be substantial. The liquid-phase electrolyte fills all internal regions of the cell. In the liquid phase, the ratio between heat exchanged through conduction and heat exchanged through convection is evaluated through the Nusselt number (Nu) as

$$Nu = \frac{hL}{k} \quad (3.21)$$

in which h is the convective heat transfer coefficient and L is the characteristic length of the electrolyte layer. Due to the reduced thickness, values of Nusselt number are in the 10^{-3} order of magnitude. Convective heat transfer phenomena are therefore neglected and internal heat exchange is modelled as conduction only. Each element of the internal heat transfer model is connected with a corresponding one of the ECM, receiving heat generation from it. Each single element of the cell is defined as follows:

$$m c_p \frac{\partial T_{be}}{\partial t} = \dot{q}_{cc} + \dot{q}_r + \dot{q}_j - \sum_j \left(k_j \cdot l_{el_j} \cdot (T_{el} - T_{el_{j+1}}) + k_j \cdot l_{el_j} \cdot (T_{el} - T_{el_{j-1}}) \right) \quad (3.22)$$

boundary conditions expressed according to cylindrical coordinates illustrated in Figure 3.4, which corresponds to the following formulation for different regions of the battery

cell:

$$\begin{cases} T(r, z, t) = T_0 & \text{at } t = 0, r = 0, z = 0 \\ \frac{\partial T(r, z, t)}{\partial r} = 0 & \text{at } t = 0, r = 0, z = 0 \\ T(r, z, t) = T_0 & \text{at } t = 0, r = 0, z = H \end{cases} \quad (3.23)$$

while, in cartesian coordinates for a pouch cell, boundary conditions are formulated as follows:

$$\begin{cases} T(x, y, z, t) = T_0 & \text{at } t = 0, x = 0, y = 0, z = 0 \\ \frac{\partial T(x, y, z, t)}{\partial x} = 0 & \text{at } t = 0, x = 0, y = 0, z = 0 \\ \frac{\partial T(x, y, z, t)}{\partial y} = 0 & \text{at } t = 0, x = 0, y = 0, z = 0 \\ T(x, y, z, t) = T_0 & \text{at } t = 0, x = 0, y = 0, z = H \end{cases} \quad (3.24)$$

In both cases temperature at the initial instant in time is assumed equal to a value of T_0 and internal gradient with respect to radius, in cylindrical cells and x and y directions in pouch cells is assumed equal to zero. Temperature gradient and initial temperatures can eventually be set to a specific initial value. Thermal properties per each element are obtained including the effect of porosity and mass percentages as follows:

$$k_{\text{parallel}} = \psi \cdot k_f + (1 - \psi) \cdot k_s \quad (3.25)$$

$$\frac{1}{k_{\text{series}}} = \left(\frac{\psi}{k_f} + \frac{1 - \psi}{k_s} \right) \quad (3.26)$$

where ψ is the porosity expressed in percentage and k is the thermal conductivity. The specific heat of the discrete element will be defined as follows:

$$c_p = \frac{c_{p,f} \cdot \rho_f \cdot \phi + c_{p,s} \cdot \rho_s \cdot (1 - \phi)}{\bar{\rho}} \quad (3.27)$$

where:

$$\bar{\rho} = \rho_f \cdot \phi + \rho_s \cdot (1 - \phi) \quad (3.28)$$

where c_p is the specific heat (f for the electrolyte phase and s for the solid phase), ρ ($\bar{\rho}$ when averaged) is the density and ϕ is the percentage of liquid phase. Specific heat in the electrolyte is defined as

$$c_{pel} = x_{sol} \cdot c_{psol} + x_{el} \cdot \left(m_{c_{pel}} \cdot T + a_{c_{pel}} \right) \quad (3.29)$$

x_{sol} and x_{elt} are the percentages of each material, m and a are the angular coefficient and the offset of the specific heat of electrolyte. The last two parameters are used since the temperature dependency of electrolyte specific heat is linearised. As it can be seen in (3.29), as a simplifying hypothesis, the specific heat of the solvent was assumed constant. Such approach allows a better representation of the internal heat exchange within the battery cell with higher precision than a simple weighted average of material properties. This approach effectively reproduces the interaction of the two phases in different directions in space, which would not be allowed by other methods. The introduced modelling technique reduces computational costs on two fronts: coupling of different physical phenomena and coupling of different discretisation scales. Working on coupled Cauchy problems interacting with each other prevents the user from relying on different solvers working in parallel. A different scale of discretisation can be allowed in the ECM and in the Internal Heat Transfer Model (IHTM), enabling, for instance, either a very detailed IHTM coupled with a single bunch ECM or a multi-bunch ECM coupled with a very rough IHTM or even a very fine IHTM coupled with a multi-bunch ECM. This model was implemented in a 1D system simulation platform, based on Modelica language. Each model was coded separately. A simple Graphic User Interface (GUI) was implemented to

interface ECM and IHTM, as shown in Figure 3.2.

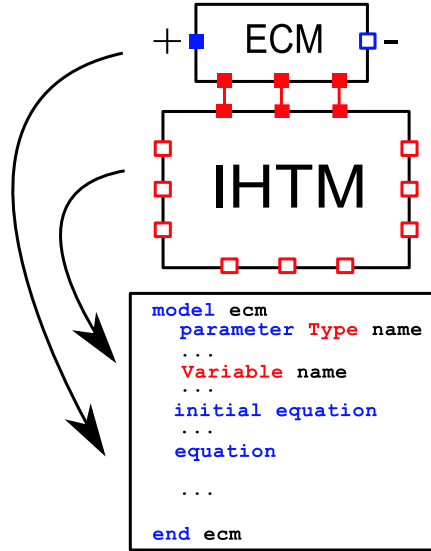


Figure 3.2: Block GUI of the Modelica model.

3.1.3 Coupling of different domains

The main challenge in multi-domain modelling is synchronisation of different solvers. Different fields of physics rely on different numerical methods of integration. Often time-step and computational time needed for integration differ from one solver to another, being an obstacle to information exchange among different domains in the model. Domain solver synchronisation issues are overcome by the selection of an appropriate simulating tool.

The solution proposed in this work is the analytical integration in space and matching of domains, using numerical methods for time derivatives only. Such method eliminates the need for the use of multiple solvers while allowing to take into account transients with much less computational effort. Modelica proves an effective modelling language for the implementation of such approach.

This methodology allows the coupling of different discretisation scales in different domains of physics. Since a single solver is used, there are no issues concerning the synchronisation of solvers in different domains. With respect to finite element models, the level of accuracy is lower since discrete elements are lumped masses rather than multi-node elements available in a set of different geometries. On the other hand, the model can handle transients, or, more specifically, process time derivatives, more effectively and cell temperature gradients are still effectively captured. The model is re-scalable at a lower computational cost and it can be integrated into a full-scale vehicle model, both on a Modelica-based platform and on a Matlab-Simulink platform.

Equations of different domains of physics are analytically integrated in space, by representing the materials as a network of lumped mass elements and by representing the electrical behaviour through an equivalent circuit whose elements are reproducing the electrical behaviour of each element of the cell. The result is a set of differential algebraic equations which are then processed by the same solver.

3.2 Battery model, algorithm and code implementation

Different Modelica scripts implemented in Dymola compose the model. Each script is organised in different sections. In the first section the units are defined, such section is replicated in every sub-model, in order to prevent incongruence in units. Such addition does not draw additional computational power, but actually reduces it since there is no need to link every constant and every variable to a pre-defined unit from Modelica libraries.

A second section of the code is the definition of the constants, followed by the definition of variables. Some variables are defined as “ports”, i.e. elements exchanging information with other sub-models. The last two parts are the initial equation section, where the model is initialised and the equation section, which is where the Cauchy problem of each sub-model is defined and where the sub-models are connected in space domain, in the main script.

The core of the model are an ECM, with chemically-based parameters and an Internal Heat Transfer Model (IHTM) interfaced with each other. The two models are both nested into a higher level model that solves the equations in both of them simultaneously, as previously mentioned.

Beside the two main models, simpler heat conduction models are also nested into the main script, in order to simulate the boundary surrounding the cells, which can either be a supporting sled for a single cell or the internal structure of a whole model.

3.2.1 Nickel-Manganese-Cobalt Oxide Cells

Two specific cases study are analysed, both featuring Nickel-Manganese-Cobalt-Oxide (NMC) cells, whose properties are summarised in Table 3.4. For some properties, a range of temperature-dependent values was available in literature, temperature dependence was linearised as explained in the previous paragraphs. Influence of variation of state of charge has shown to be affecting thermal properties by less than 5% and is therefore neglected [66].

Layer	Conductivity [$W \cdot m^{-1} \cdot K^{-1}$]	Specific heat [$J \cdot kg^{-1} \cdot K^{-1}$]	Reference
Separator	0.21 – 0.22	700	[54, 191, 192, 193, 194, 67]
Cathode	0.375 – 4.1	1437	[54, 67]
Cath. Coating	0.375 – 2.25	1050	[195, 54]
Cath. Current Collector	240	900	[196, 197]
Anode	7 – 17.6	1269	[54, 67]
And. Coating	2 – 5	1050	[195, 54]
And. Current Collector	380	385	[197]
Electrolyte	0.60	994.67 – 1301.43	[67, 85]

Table 3.4: Material properties in NMC cells.

3.2.2 Cylindrical cells

Cylindrical jelly roll cells are composed by a layered structure of electrodes and separators rolled around a central carbon (graphite) core as shown in Figure 3.3. The assembly of cell active materials and core is then placed inside a cylindrical can and filled with liquid electrolyte.

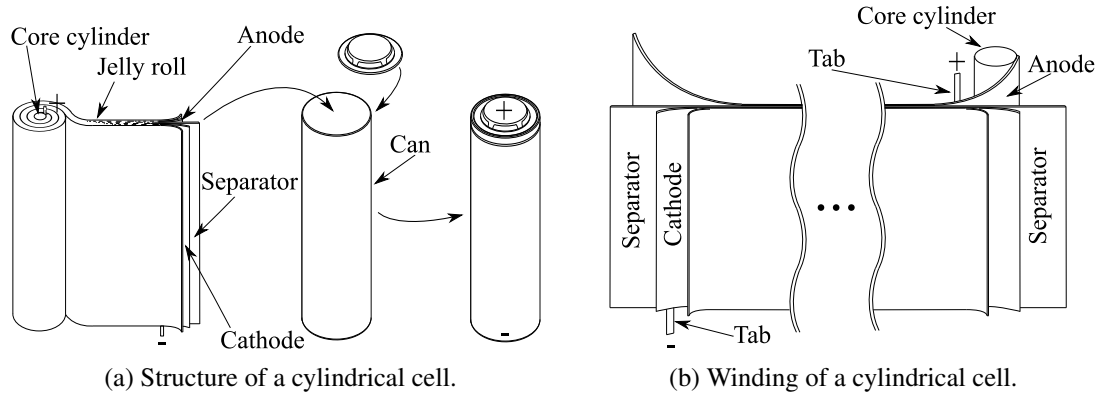


Figure 3.3: Cell structure.

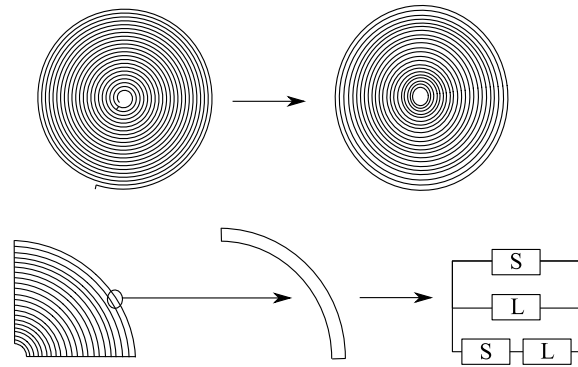
Several composite materials are used in Li-ion battery cells. There are three main elements: solid electrodes, solid separators, and liquid electrolytes. Cell electrodes include a base material, a coating, and host a metal current collector inside them. Current collectors

are made of Copper for the anode and Aluminum for the cathode. Cathode coatings are modelled according to the materials and the properties outlined earlier in the literature. The IHTM was implemented applying the principles introduced in the above paragraphs, developing a discretized model in a Modelica-based simulation platform operating in multiple physics domains. A matrix of elements is defined and temperature-dependent properties are assigned to each of them. Boundary conditions and interactions between each pair of elements are then set. Physical properties are defined locally for each element, effectively representing an anisotropic material as locally isotropic. Discrete elements of the cell represent: (i) anode, (ii) cathode, (iii) separators and (iv) electrolyte. The model also features heat exchange with the external environment. The interaction between liquid (iv) and solid phase in (i), (ii) and (iii) is modeled with purpose-built discrete elements.

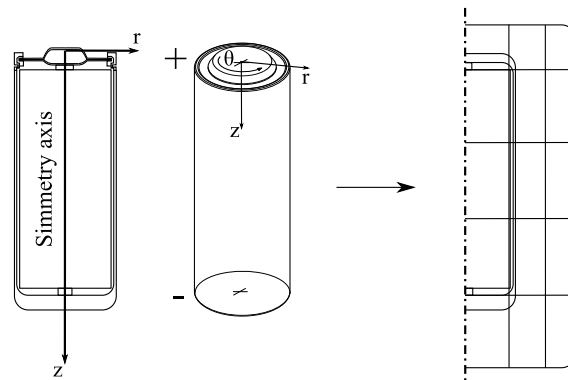
Figure 3.4 shows how discrete elements are joined to form a section of a battery cell on a plane perpendicular to the axis. Figure 3.4, shows how the original spiral in Subfigure 1 is simplified as a series of concentric cylinders. Subfigure 3 it is possible to see how just a quarter of such section is considered. Each winding is then composed by external separator, anode, internal separator and cathode. Subfigure 3.4a represents the discrete element composed by solid-phase components (S) and liquid-phase components (L) connected. Three discrete layers of axial discretization are considered, obtained by simplifying the original geometry as shown in Subfigure 3.4b. Boundaries are included in the model, so that any supporting structure can be represented. In doing so, thermal contact resistance between the cell and any adjacent structure is taken into account. In circumferential direction, as shown in Subfigure 3.4a, such discretization was allowed by the reduced thickness. Such technique is reliable in this scenario since the jelly roll has a high number of windings and a reduced thickness per winding. Concerning the top of the cell, the simplification of the geometry of the positive connector still takes into ac-

count the mass of the original component and, at the given level of discretization it does not result in substantial modifications to the level of accuracy. Symmetry does not affect geometry but allows a leaner computation.

The combination of simplification of geometry and symmetry can result in neglecting an irregularity accounting for approximately 2% of the diameter, with thickness being directly proportional to transferred heat. The error is therefore negligible.



(a) Radial and circumferential discretisation.



(b) Axial discretisation and symmetry exploitation.

Figure 3.4: Cell discretisation strategy, including the cylindrical coordinates [198].

3.2.3 Pouch cells

Pouch cells are composed by more layer of active materials on top of each other. Continuous current collectors are preferred in this type of cells, since not rolling the cell on itself puts less torsional shear stress on the material.

As a drawback, however, such cells lack of structural rigidity, requiring additional supports when a module is assembled. Each layer of the cell is represented by a network of lumped masses. Each mass exchanges heat with the neighbouring masses. At the boundaries, another network of lumped masses represents the materials used for the battery support.

A simplified two-layer layout was assumed and each layer was discretised into 9 elements, with the addition of current collectors tabs as represented in Figure 3.5.

The number of elements was chosen as the best trade-off between a single-lumped mass and a finely discretised finite element model. Other authors have chosen to represent the battery as stack of lumped elements, one per layer [129]. Others, have decided to use an adaptive mesh finite element model [158].

The proposed strategy is based on a network of lumped masses, therefore the chosen strategy was driven by the need of representing at least one element per tab, and one element representing the cell between the two tabs and at least three elements axially. Current collectors are modelled as single-phase lumped elements networks, while the same discrete element used for the cylindrical cells is applied to the other layers.

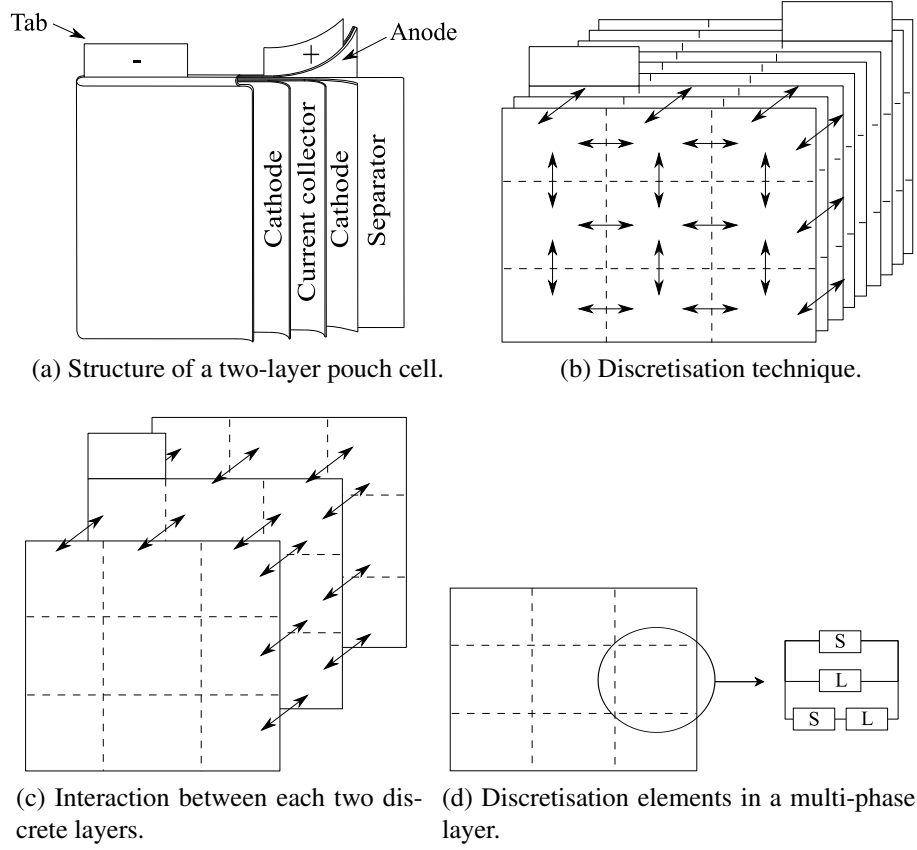


Figure 3.5: Pouch cells, structure and discretisation technique.

3.2.4 Boundary conditions

A critical step in developing a single-cell model in order to allow its scalability up to a module or pack model is the boundary modelling. Thermal contact resistance and natural or forced convection models, together with information on the potting materials surrounding a battery cell contribute in providing a realistic model. Conductive heat transfer resistance can be expressed as follows:

$$R_{\text{conduction}_i} = \frac{T_{s1} - T_{s2}}{Q_i} = \frac{r \cdot L_i}{A_i} \quad (3.30)$$

where the subscript i indicates a generic coordinate in which heat transfer is considered, subscripts s_1 and s_2 indicate the two surfaces in contact, r is the thermal resistivity, depending on contact surface, A is the contact surface and L_i represents the length through which conductive heat transfer is examined.

Beside conduction heat transfer with potting materials, cells within modules may be exposed to convection, if not completely immersed in the potting material. For instance, in the case of passive or liquid cooling, certain portions of surface are exposed to natural convection. On the other hand, in the case of air-cooled or liquid-immersed battery thermal management, heat transfer at the boundaries of cell, occurs through forced convection. The arrangement of the cells has a major effect on the convective heat transfer coefficient. It is possible to obtain such coefficient from the velocity of the fluid and the geometry of the stack of cells. In order to do that, it is necessary to start from dimensionless coefficients, such as stack-averaged Nusselt number ($\bar{Nu}$) and maximum Reynolds number (Re). Stack-averaged Nusselt number, can be used to obtain the convective coefficient, as it can be seen in (3.31), referring to the diameter of cells (D) as basic dimension, conductive coefficient (k) and averaged convective coefficient of fluid ($\bar{h}$):

$$\bar{Nu}_D = \frac{\bar{h}D}{k} \quad (3.31)$$

from which it is possible to obtain:

$$\bar{h} = \frac{\bar{Nu}_D k}{D} \quad (3.32)$$

With reference to the maximum velocity of the fluid at inlet (u_{max}), cell diameter (D) taken as hydraulic diameter and referring to fluid viscosity (ν), it is possible to determine

the maximum Reynolds number as in (3.33):

$$Re_D = \frac{u_{max} D}{\nu} . \quad (3.33)$$

In order to correlate (3.31) with the system geometry, it is necessary to rely on a further dimensionless coefficient, such as Prandtl number, evaluated at bulk fluid temperature (Pr) and at cell wall temperature (Pr_w) as shown in (3.34).

$$Pr_i = \frac{\mu c_p}{k} \quad (3.34)$$

where μ is the local dynamic viscosity, c_p is the specific heat and k is the conductivity of the fluid. Such properties are evaluated in the aforementioned point. Through (3.33), (3.34) can be expressed as in (3.35).

$$\bar{Nu}_D = A \cdot Pr^{0.36} f(Re_D) \quad (3.35)$$

Further details can be found in the appendices.

3.2.5 Module heat exchanger

In the case of the battery module, a bottom cold-plate heat exchanger provides cooling. A simplified Modelica model of the cold-plate was implemented, taking into account conduction through a solid plate of Aluminium and forced convection through the coolant, modelled according to the fluid velocity and fluid properties, with a discretisation grid matching the one applied to the battery, as shown in Figure 3.6.

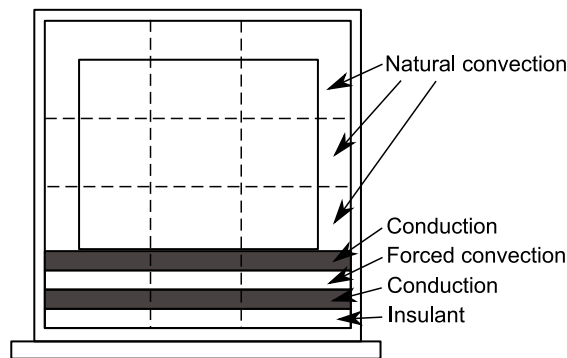


Figure 3.6: Front view of the battery module within the enclosure, with the cold-plate heat exchanger at the bottom.

3.2.6 Code implementation of models

The aforementioned model sections are organised as represented in Figure 3.7. The initial “model” declaration specifies the solver is used to integrate a differential algebraic equation system. The “initial equation” section defines the initial equations, while the “equation” section contains the Cauchy problem to be integrated in time.

```
Model Model
  initial equation
  equation
end Model;
```

Figure 3.7: Generic structure of a Modelica model section.

The initial section contains the definition of units, constants and variables. Variables could have been initialised to a specific value in this section. However such fashion is unfit for a full initial equation definition.

3.3 From cell to module model

The single cell model is scaled up in order to simulate a battery module. The nature of the modelling language allows the generation of matrices of identical components from a single one. It is then possible to modify the properties of each of such components and connect them in a suitable way.

A pouch cell model was considered, with the addition of potting material, bus bars sections and sections of enclosing box around it. Such model is effectively a slice of a battery module. Such slice was used to generate a matrix of identical components, with the addition of a front panel and a back panel.

The model was implemented in Modelica code and the number of cells in parallel and the number of cells in series were defined as input parameters. These parameters were used as sizes, i.e. number of rows and number of columns, to generate a matrix of cell models, as represented in Figure 3.8. Two matrices of ECMs and IHTMs are generated, the ECMs in each row are connected with each other in series.

Each row is connected with the same input and output at each end. Every single ECM model is connected with an IHTM model. Each IHTM model is connected to the neighbouring ones, exchanging heat with them. More details on the code implementation of the module model can be found in Appendix A.

```

model module
mEC ecm[parallel, series](
    USER-SET VARIABLES
    ...);
cy2 ihtm[parallel, series](
    USER-SET VARIABLES
    ...);
...

equation
for i in 1:parallel loop
    for j in 1:series-1 loop
        connect(ecm[i,j].pinN,ecm[i,j+1].pinP);
    end for;
    for k in 1:series loop
        connect(ecm[i,k].portAnd,ihtm[i,k].andGEN);
        connect(ecm[i,k].portAnd,ihtm[i,k].sepGEN);
        connect(ecm[i,k].portAnd,ihtm[i,k].catGEN);
    end for;
    connect(ecm[i,1].pinP,pinPmodule);
    connect(ecm[i,series].pinN,pinNmodule);
end for;
...
end module;

```

Figure 3.8: Code implementation of battery module model, from single cell ECM and IHTM models.

3.4 Simulation algorithm

The Modelica code is run externally from a Matlab script. This option allows the automatization of the simulation procedure. In addition, a much leaner data processing is enabled. The procedure is described in Figure 3.9. From the initial input data, taken from both the manufacturer's data sheet and the available literature on materials, a Matlab algorithm generates a Modelica script (*.mos format) that manipulates a Modelica model (*.mo format). Dymola, the chosen Modelica solver is called by the Matlab script and the Modelica script is executed. Results, stored into a *.mat format file are retrieved by Matlab and compared with experimental results.

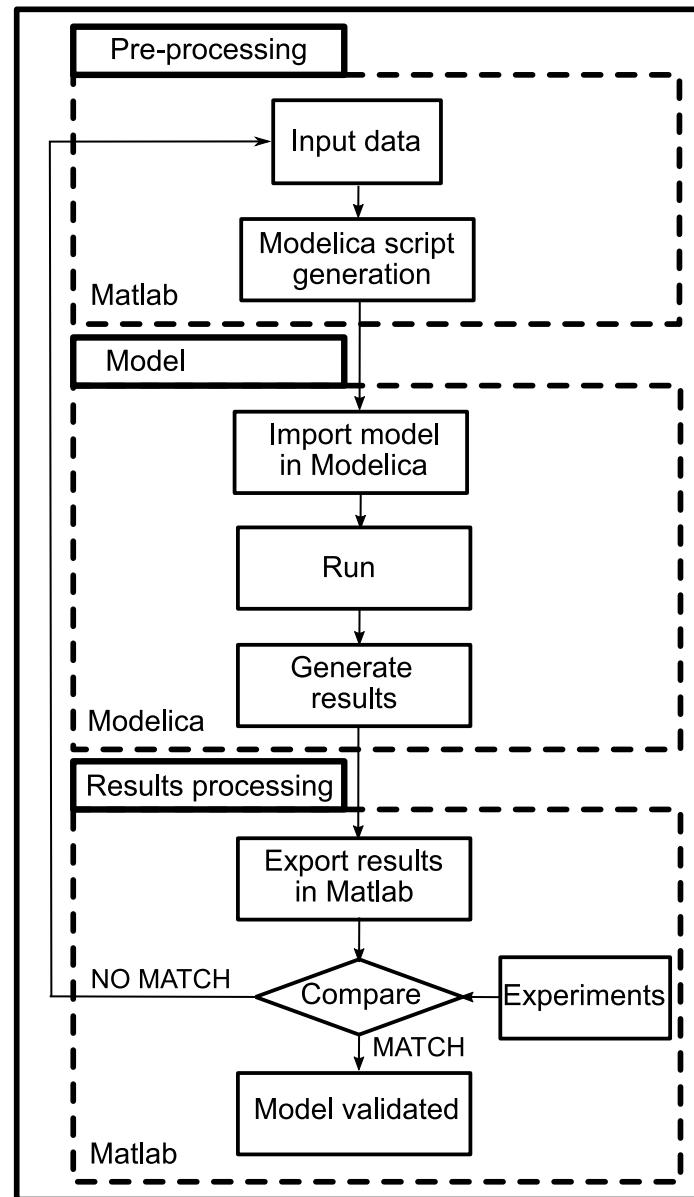


Figure 3.9: Scheme of the developed simulation algorithm.

3.5 Summary of chapter

In this chapter the modelling technique was explained. First the electrical modelling was discussed, explaining the equivalent circuit model and how its parameters were calcu-

lated. Subsequently, the internal heat transfer model was introduced and its parameters discussed. Finally, the scaling up of the model and the simulation algorithm were introduced. In the next chapter, the design of the validation test rig will be discussed.

Chapter 4

Test-rig design, assembly and uncertainty analysis

The chapter describes the development of the test-rig outlining its purpose and its benefits. The experimental layout is designed to test indirect liquid-cooling. It can host one battery module. Several different pressure and temperature sensors are mounted in the cooling loop and on the surface of the battery. Measurements provide model validation and the comparison of different scenarios. Attention was stressed on fast-charge procedures, jointly with urban drive cycles. In the first two chapters we outlined how high-rate cycling is the most stressful scenario for battery thermal management. High current rates are reached during fast charging, in order to minimise the time needed to restore battery capacity. The electric bike market is in rapid expansion in large and densely populated cities [199]. For medium and small-size batteries, urban drive cycles are therefore the most likely scenario.

4.1 Test-rig aims, objectives and layout design

In the research question in Chapter 1, we wondered how the design procedure of battery modules can be made more systematic, including thermal issues from the very beginning. In our objectives, beside the development of a battery cell model and its re-scaling up to a module model, we outlined the development of a flexible cooling test-rig layout and the investigation of removable cold-plate cooling as objectives of this work. More in detail, the test rig was implemented for three main aims: i) validating the scalability of the single-cell model up to a module mode, ii) evaluating different cooling strategies and iii) outlining the most stressful scenarios for battery modules. In order to do so, a controlled-temperature room was selected as location and a small scale liquid-cooling layout was implemented around a battery module. Module potting and enclosing materials were characterised and temperature was sampled on the external walls of the battery module and on the cooling loop, heat exchange conditions were fixed and well characterised. The final outcome is a device that helped in model validation and in critical cases definition, outlining under which scenarios the battery module is at risk of exceeding the safety temperature range and what counter-measures could be adopted to avoid it, at what energy consumption.

4.1.1 Test-rig Objectives

The specific objectives were the following:

- Cycling a battery module in a controlled-temperature environment, under a pre-defined duty cycle, without cooling system and with a specific cooling system applied. The battery module is placed inside an enclosure that can host modules of a size up to $600 \times 400 \times 300 \text{ mm}$. The selected case study is a battery module from Zero motorcycles, which has been chosen for its layout simplicity: a stack of 28 pouch

cells connected in series with copper bus bars on the top, covered with an epoxy potting material and enclosed in an Aluminium case. A module has been ripped apart and benchmarked in order to implement the model, as shown in the next paragraphs. The test-rig layout has been assembled in a temperature-controlled room.

The cooling loop has been sized in order to ensure a constant heat dissipation rate, by measuring the inlet temperature and pressure, the ambient temperature and the mass flow rate, as specified in the next paragraphs. The duty cycle has been chosen according to what was outlined in the literature (see Chapter 2) as the most stressful scenario for a battery thermal management, i.e. high-rate cycling. Details of the examined duty cycles are provided in Chapter 5. The battery enclosure is provided with an inlet manifold and an outlet manifold, the system can therefore host different indirect- or eventually direct-contact liquid cooling systems. The selected case study is an indirect-contact cold-plate-based liquid cooling system. Such option was selected as a case study, since, as shown in the literature (see Chapter 2) it is currently the preferred layout by many manufacturers. In addition, such layout allows the implementation of removable cooling devices that can be used in some scenarios such as battery charging, as explained in Chapter 5.

- Measuring the temperature profile in different location on the battery module in order to provide a validation of the proposed modelling technique and examine specific scenarios (presented and discussed in Chapter 5). A battery module was ripped apart and benchmarked in order to characterise materials and architecture of the battery (more details in the next paragraphs).
- Outlining the temperature profile under different duties and providing a guideline for the battery cooling.

4.2 Test-rig sizing

The aim was to investigate the effectiveness of heat exchange through an external and removable cold-plate heat exchanger. In order to do so, the module was placed into an enclosure, in a controlled-temperature room, in order to minimise the effect of convective heat transfer. The bottom of the enclosure, in contact with the test-rig supporting structure was covered by a double layer of thermally insulating material, in order to minimise the conductive heat exchange from the battery and the heat exchanger to the supporting structure. Details of the thermal management sizing are provided in the next section.

Properties of the fluid are presented in Paragraph 4.3.1, the cold plate, if coolant is circulated rates varying from 1 to 5l/min, the energy balance is calculated as follows:

$$\dot{Q} = \rho \dot{V} \cdot c_p \Delta T \quad (4.1)$$

where ρ is the equivalent density of the coolant, $\dot{V}$ is the volume flow rate, c_p is the fluid specific heat and ΔT is the temperature difference. Considering an ambient temperature of 25°C and a maximum cell temperature of 60°C and an ohmic heat rejection of 0.375kW per cell at a continuous discharge rate of 2C, the maximum ohmic heat rejection of the module will be of 10.5kW during a continuous discharge at a rate of 2C, as per battery specifications [200].

Assuming the system to have reached steady state and the cold plate to be therefore at the same temperature as the battery walls, the cold plate is capable of removing 11.1kW at a flow rate of 5l/min, which, considering an overhead of over 5%, makes the system capable of handling cooling at current rates up to 2C.

In terms of hydraulic sizing, considering a section 1, upstream the pump and a section 2, downstream the pump, the following energy balance equation needs to be satisfied:

$$p_1 + \rho \frac{v_1^2}{2} - \Delta p_{loss} + \gamma \cdot z = p_2 + \rho \frac{v_2^2}{2} - \Delta p_{loss} + \gamma \cdot z \quad (4.2)$$

where p is the pressure, ρ is the density of the fluid, v is the local velocity of the fluid, γ is the specific weight of the fluid (calculated as $\gamma = \rho \cdot g$, where g is the gravitational acceleration), Δp_{loss} is the sum of local and distributed pressure losses, calculated as explained in Paragraph 4.3.1 and showed in Figure 4.5 and z is the height. The height is constant throughout the test rig and can be removed and the fluid velocity, can be assumed identical in section 1 and 2. It is possible to observe that the selected pump (characteristic curve in Figure 4.3) manages to cope with the pressure drop, while ensuring the required flow rate.

4.3 Hardware implementation

The test rig is composed by a battery module assembled on top of a liquid heat exchanger and a coolant loop. A scheme of the layout is shown in Figure 4.1, while a picture can be seen in Figure 4.2. The coolant loop, beside the heat exchanger features a pump, a radiator with a double fan, a de-gassing tank, and temperature and pressure sensors. Temperature and pressure sensors are placed upstream and downstream the heat exchanger and the radiator.

The chosen temperature sensors are resistive transducers (RTD). Such sensors have a reduced operating range and a good accuracy. The selected pressure sensors are strain-gauge-based transducers, measuring absolute pressure. Absolute pressure measurement

is preferred to increase system robustness.

In addition to such devices, an ultrasonic flowmeter is also provided. The test rig was built in a controlled-temperature room. Such feature allows a good repeatability of the experiments and minimises the influence of the environment on the outcomes. The test-rig supporting frame is mounted on damping feet, in order to insulate the sensors from vibrations that may affect the measurements.

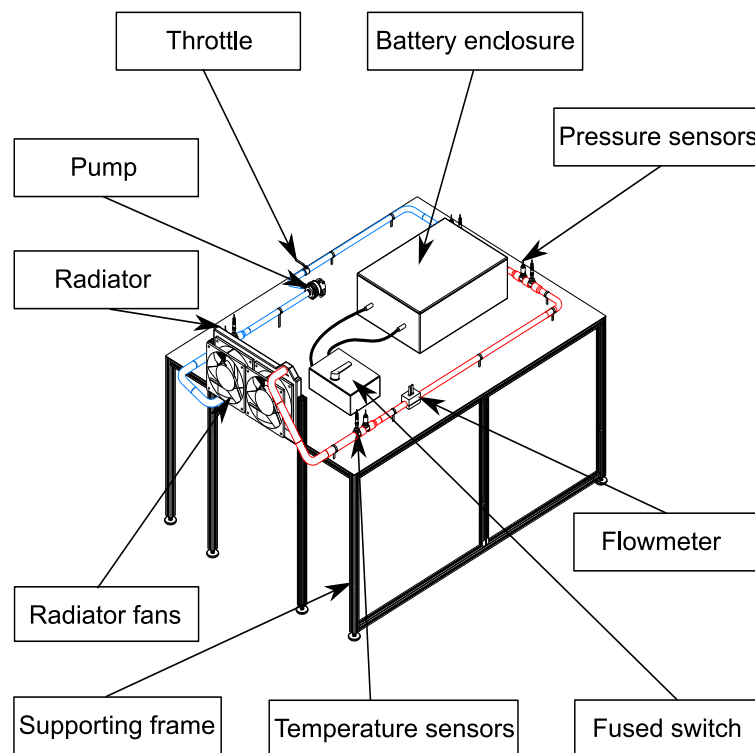


Figure 4.1: Isometric-view of the test rig.



Figure 4.2: A photograph of the test rig.

4.3.1 Hydraulic loop

The chosen coolant is a mixture of water and ethylene glycol. This cooling fluid is common in ICE cooling and often used in electric powertrains as well. Such choice was made due to the high specific heat and low cost of such material. These two features make the mixture highly interesting for cooling purposes, especially in indirect cooling, since the coolant is not in contact with the battery walls. The specifications of the radiator are summarised in Table 4.1, while the properties of the coolant can be found in Table 4.2. The radiator can ensure a convective heat transfer coefficient of $20 \text{ W} \cdot \text{m}^{-2}\text{K}$ when operated at maximum fan speed.

Radiator size (wetted area)	$65 \times 640 \times 320$ mm
Fan shroud size	$90 \times 640 \times 400$ mm
Maximum air flow	1.085 $m^3 \cdot s^{-1}$
Convective heat transfer coefficient	20 $W \cdot m^{-2} \cdot K^{-1}$

Table 4.1: Radiator properties at at 25°C, with the cooling fluid in Table 4.2.

Property (at 25°C)		Water	Ethylene Glycol
Density	ρ	998.2 $kg \cdot m^{-3}$	1111.4 $kg \cdot m^{-3}$
Dynamic Viscosity	ν	0.001003 $Pa \cdot s$	0.0157 $Pa \cdot s$
Specific heat	c_p	4181.6 $J \cdot kg^{-1} \cdot K^{-1}$	2300 $J \cdot kg^{-1} \cdot K^{-1}$
Thermal conductivity	k	0.6 $W \cdot m^{-1} \cdot K^{-1}$	0.258 $W \cdot m^{-1} \cdot K^{-1}$
Mass percentage	x	75 %	25 %

Table 4.2: Properties of coolant used in experiments.

The selected pump is a 24 V cooling booster pump, whose characteristic curve can be observed in Figure 4.3. Such a device is normally used when additional head is needed in cooling circuit. It is therefore designed to minimise energy consumption and the amount of space needed.

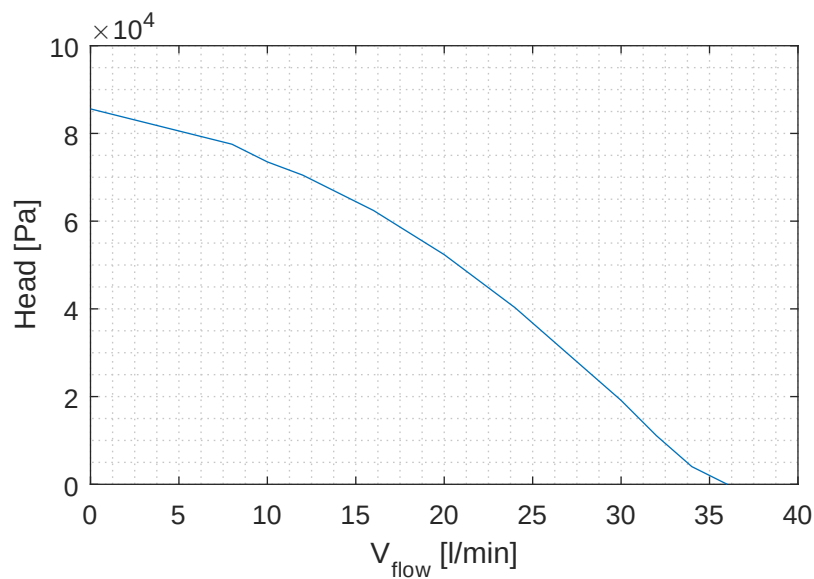


Figure 4.3: Characteristic curve of the test-rig pump.

The fluid circulation loop features sections of different diameters, elbows and section reductions. Figure 4.5 summarises the pressure drops, also including the cold-plate heat exchanger and the radiator.

Pressure drops in both elements are measured including the inlet and outlet sections as well [201]. Losses on straight sections are calculated according to

$$\Delta p = \gamma \cdot \lambda \cdot L \quad (4.3)$$

in which the coefficient λ is obtained from Moody's graphs from diameter and Reynolds number, calculated as follows

$$Re = \frac{\rho v D}{\mu} \quad (4.4)$$

While losses on elbows are obtained from the following

$$\Delta p = \zeta \cdot \rho \cdot \frac{v^2}{2} \quad (4.5)$$

where ζ is obtained from

$$\zeta = \zeta_{local} + \zeta_{friction} \quad (4.6)$$

in which the specific terms are calculated as

$$\begin{cases} \zeta_{friction} = 0.0175 \cdot \lambda \frac{R_0}{D_H} \delta^0 \\ \zeta_{length} = A_1 B_1 C_1 \end{cases} \quad (4.7)$$

with A_1 , B_1 and C_1 being geometry-dependent parameters. In addition, losses from section

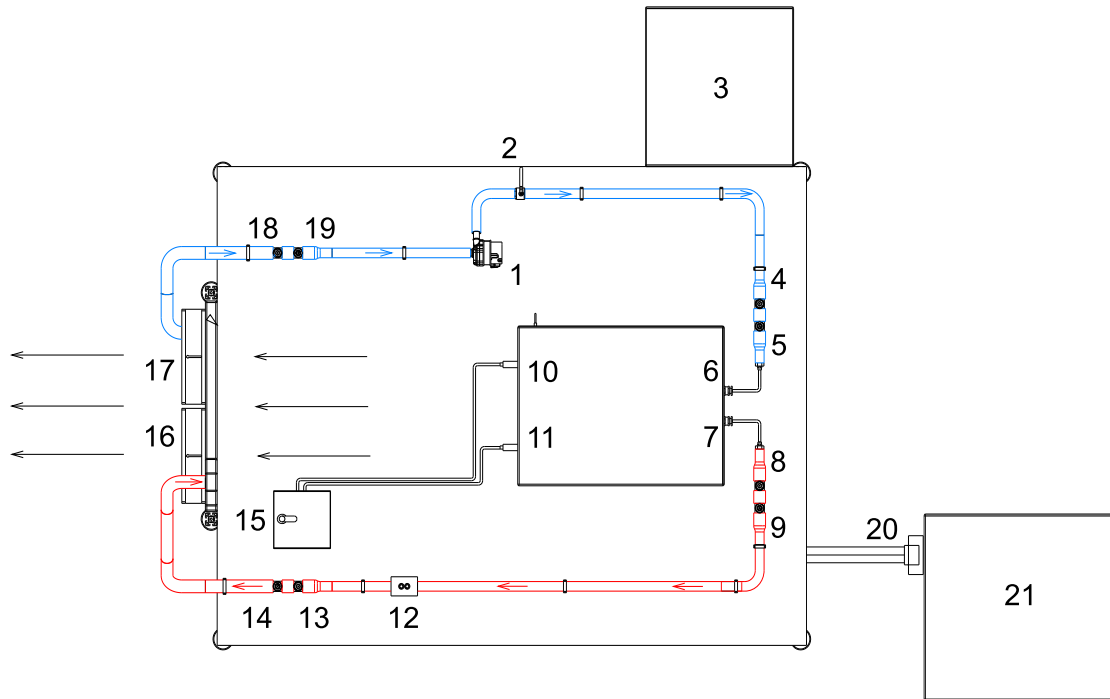
reducers are calculated as follows:

$$\Delta p = \alpha \cdot \rho \cdot \frac{v^2}{2} \quad (4.8)$$

where the coefficient α is obtained as sum of different components

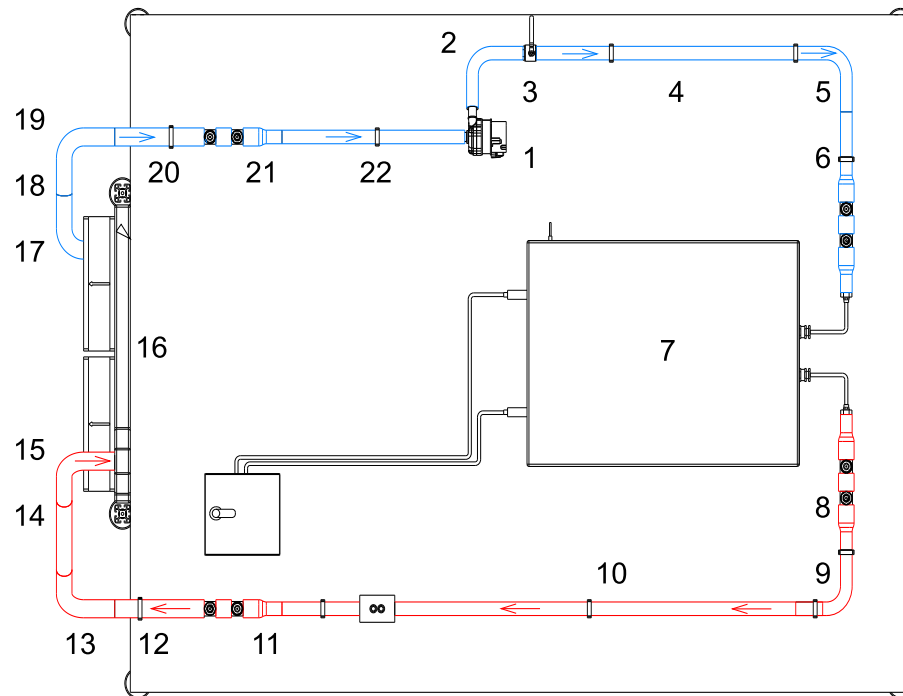
$$\alpha = k_1 \cdot \alpha_{expansion} + \zeta_{friction} \quad (4.9)$$

where the term $\zeta_{friction}$ is obtained from look-up tables and $\alpha_{expansion}$ is also taken from look-up tables, using the reduction angle β as an input parameter [201]. Having characterised the hydraulic and thermal performance of the test rig, it is possible to know its impact on the battery operating temperature. Test rig components are listed in Table 4.4, specifying the position of the Resistive Temperature Detectors (RTD), pressure transducers and flowmeter. On the other hand, Table 4.5 shows the pressure drops throughout the test rig. It is important to notice that adaptors for pressure transducers and RTDs cause pressure drops, although most of the losses are caused, as expected, by the cold plate and by the radiator. Minimising the test-rig pressure drops and maximising the pump head allows testing a broad range of heat exchangers.



No.	Description
1	Pump
2	DAQ cabinet
3	Manual throttle valve
4	Pressure transducer
5	RTD
6	Cold-plate inlet
7	Cold-plate outlet
8	Pressure transducer
9	RTD
10	Battery negative connection
11	Battery positive connection
12	Ultrasonic flowmeter
13	Cold-plate inlet
14	Cold-plate outlet
15	Main switch and fuses
16	Radiator fan 1
17	Radiator fan 2
18	Pressure transducer
19	RTD
20	Power supply to battery connection
21	DC power supply

Figure 4.4: Functional scheme of the test rig, arrows represent the direction of the coolant flow and air flow through the radiator.



No.	Section (at 25°C, 5 l/min)	Δp [Pa]
1	Pump	+80000.00
2	∅19 elbow	−35.91
3	Manual throttle	<i>negligible</i>
4	∅19 straight hose	−115.77
5	∅19 elbow	−35.91
6	∅19 to ∅32 expansion	−3.57
7	Cold plate (including inlet and outlet)	−68055.52
8	∅32 to ∅19 restriction	−1.78
9	∅19 elbow	−35.91
10	∅19 straight hose	−124.91
11	∅19 to ∅32 expansion	−3.57
12	∅32 straight hose	−9.09
13	∅32 elbow	−8.82
14	∅32 straight hose	−6.06
15	∅32 elbow	−8.82
16	Radiator (including collectors)	−407.54
17	∅32 elbow	−8.82
18	∅32 straight hose	−3.33
19	∅32 elbow	−8.82
20	∅32 straight hose	−7.57
21	∅32 to ∅19 restriction	−1.78
22	∅19 straight hose	−60.93

Figure 4.5: Scheme of the test-rig, outlining the variation in coolant pressure.

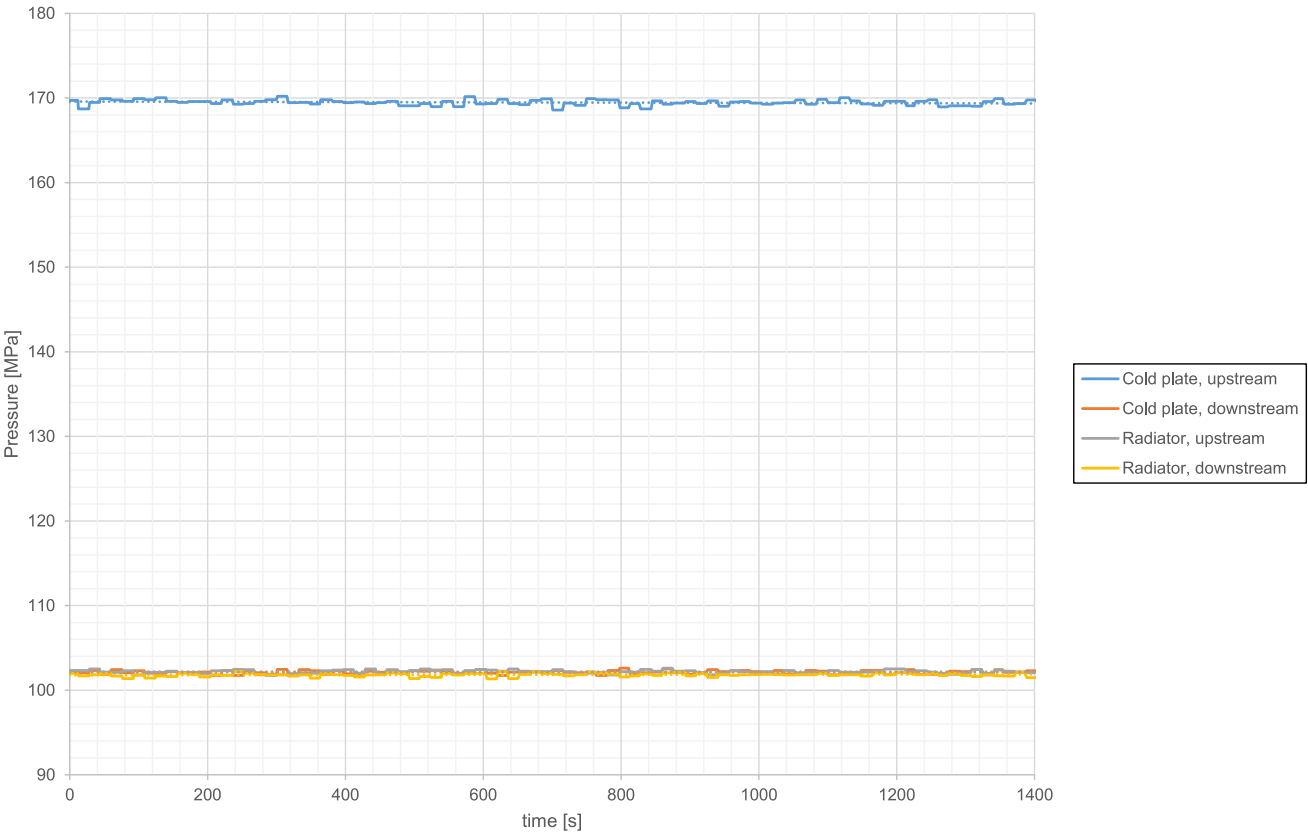


Figure 4.6: Sampled pressure downstream pump at 5l/min.

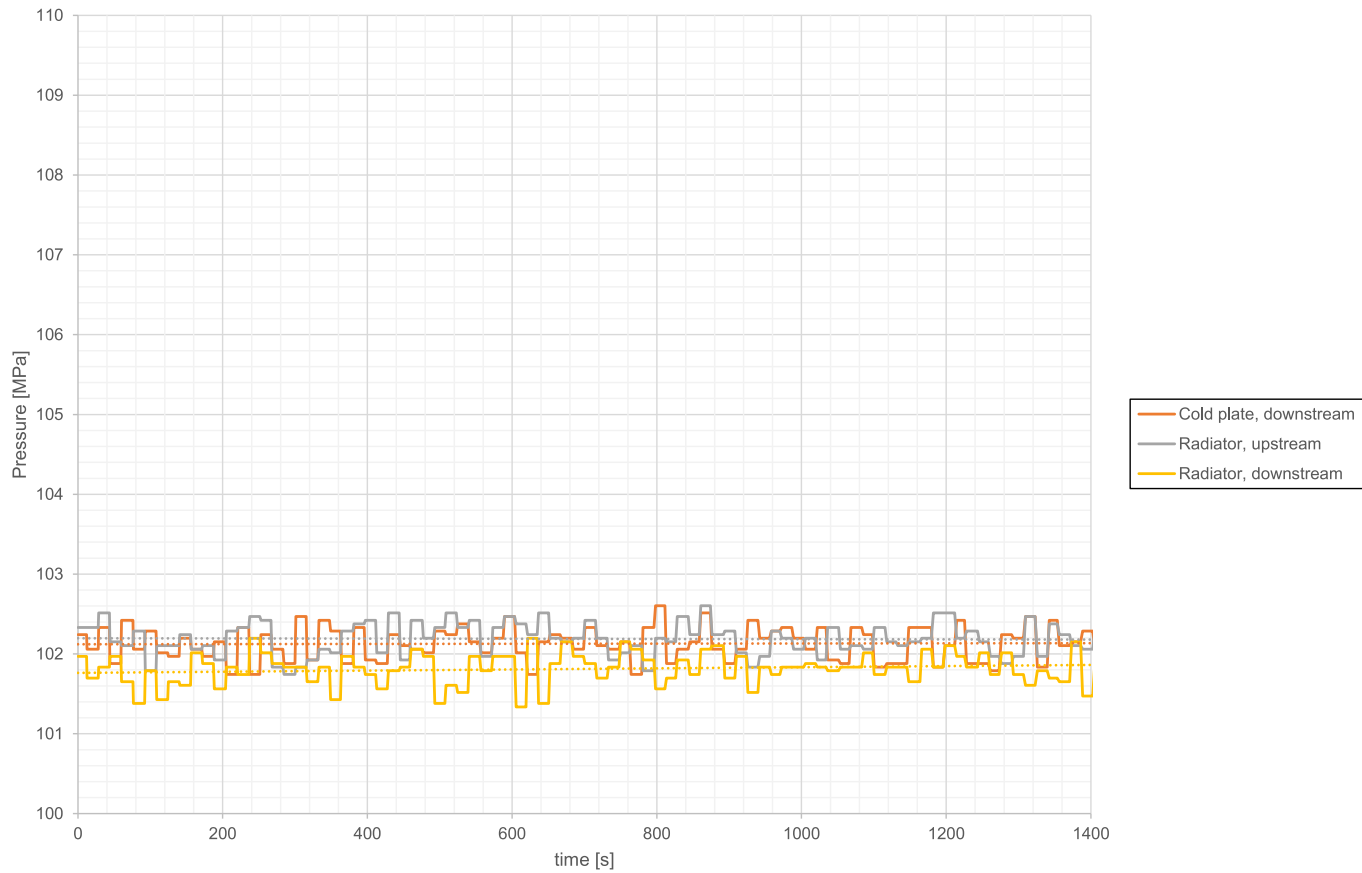


Figure 4.7: Sampled pressure drops of components at 5 l/min .

4.3.2 Electrical loop

The battery is connected through a fused switch to a 100 V power supply equipped with an extra emergency switch. The specifications of the power supply are summarised in Table 4.3 the power supply is connected to the grid through a 32 A plug. A scheme of the system is represented in Figure 4.8. Pump, fans, flowmeter and data acquisition system are powered by separated power supplies.

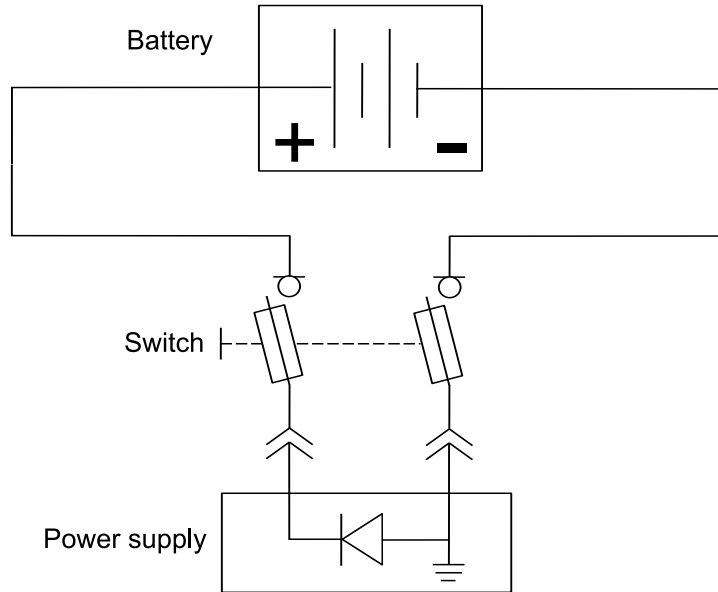


Figure 4.8: Test-rig circuit macro-scheme.

ETPS TC.GSS.32.400.S.HMI			
Input			
Voltage	V_{AC}	3×400	V_{AC}
Current	I_{AC}	3×32	A_{AC}
Frequency	f_{AC}	50	Hz
Output			
Voltage	V_{DC}	0 to 400	V_{DC}
Current	I_{DC}	-100 to 100	A_{DC}
Power (max)	P_{AC}	18	kW

Table 4.3: Specifications of the bi-directional power supply.

4.3.3 Battery temperature sampling

The current section focuses on temperature sensor positioning. More details about the battery will be introduced in Chapter 5, in Subsection 5.4.2. Sensors were placed on the external walls of the battery according to the scheme presented in 4.9. The rear view represents the surface in direct contact with the cold-plate heat exchanger. Eleven sensors were placed on the battery surface, a further one (sensor No. 10) was positioned inside

the enclosure to measure the ambient temperature as a reference.

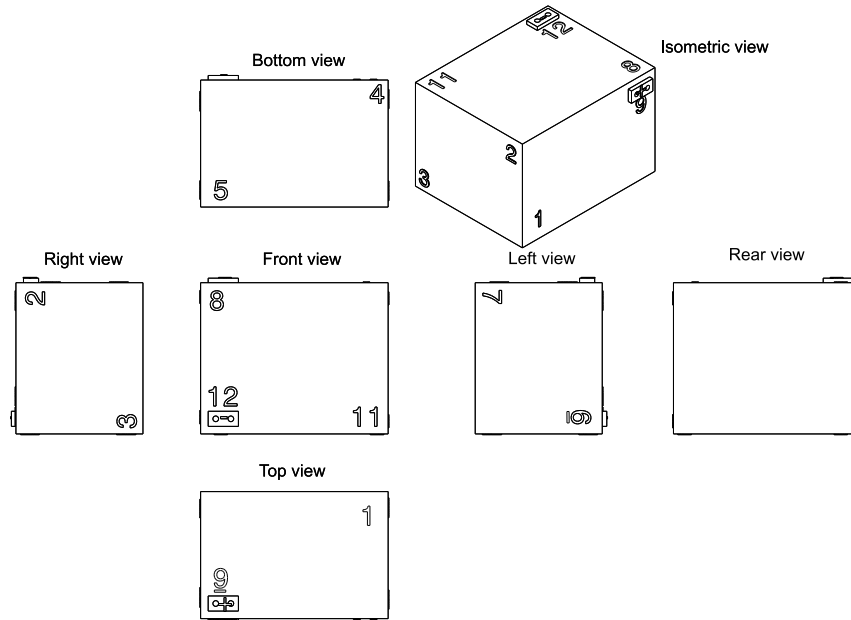


Figure 4.9: RTD sensor positioning on the external walls of the battery module.

Firstly, surface temperature of the module is relevant to the final output, in order to estimate the thermal stress on neighbouring components. In addition, since the materials within the battery module are known, together with its geometry, it is still possible to estimate the battery surface temperature. The module used in the tests is taken from a commercial motorcycle. The battery was positioned inside an enclosing box, in order to ensure conditions that would have been the closest to the final vehicle. The temperature of the room hosting the test-rig was controlled and kept constant. In Paragraphs 4.2 and 4.3.1 the performance of the cold-plate, the radiator and the hydraulic loop of the test-rig were characterised in order to run the experiment under known conditions. Two sensors were placed close to the positive connection, one close to the negative connection. A battery module identical to the tested one was ripped apart and its structure was observed for modelling purposes with more data further presented later, in Paragraph 5.4.2, Tables 5.15 and 5.14. The structure of the battery can be seen in Figure 4.10, from the size of

the bus bars and from the specifications of the cell, we expect the positive connection to be the warmest spot.

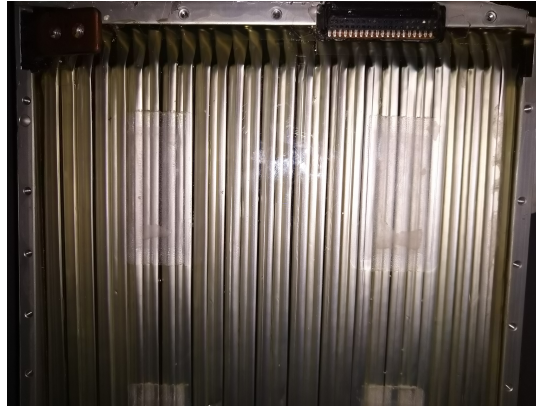


Figure 4.10: Structure of battery module, pouch cells, potting material (epoxy resin) and Aluminium enclosure, note that an insulating rubber mat is placed every two cells.

4.4 Experimental strategy

4.4.1 Sensors used in the test-rig

Different types of measurements are taken in the test rig. Temperature, pressure and volume flow rate are sampled with specific sensors. Temperature is sampled with Resistance Temperature Detectors (RTD) sensors, pressure with strain gauge-based pressure transducers and volume flow with an ultrasonic flowmeter. RTDs log the variation of resistance and interpolate it in order to obtain a temperature measurement. Temperature is directly proportional to resistance, according to a specific law for each class of sensors. A summary of the sensors and their interaction with data acquisition is presented in figure 4.11, and the arrangement of the devices in the auxiliary cabinet is displayed in Figure 4.12. Twelve class C TE RTDs were used for sampling on the battery module external walls while 4 Omega RTDs were measuring coolant temperature. Coolant pressure is measured in four different spots on the cooling loop. The temperature was sampled up-

stream and downstream the cold-plate heat exchanger and upstream and downstream the radiator. The cooling fluid inlet temperature was therefore kept under control in order to ensure known heat exchange conditions, so that modelling was possible. The ultrasonic flowmeter is an Omega FDT42, connected to an Omega logging unit. The flowmeter measures fluid speed, the volume flow is calculated from fluid properties in the logging unit.

Component	Manufacturer	Model	Reference
Class C Pt 100 RTD	TE	NB-PTCO-058	[202]
Class A Pt 100 RTD	Omega	RTDM12-1/8NPT-3MM-13MM-A	[203]
Pressure transducers	Omega	PX309-100A5V	[204]
Ultrasonic flowmeter	Omega	FDT-42	[205]
Flowmeter logging unit	Omega	FDT-40E-VDC-HT	[205]
RTD logging module	NI	9216	[206]
Pressure logging module	NI	9205	[207]
Data acquisition platform	NI	cDAQ 9133	[208]

Table 4.4: Summary of sensors and data acquisition.

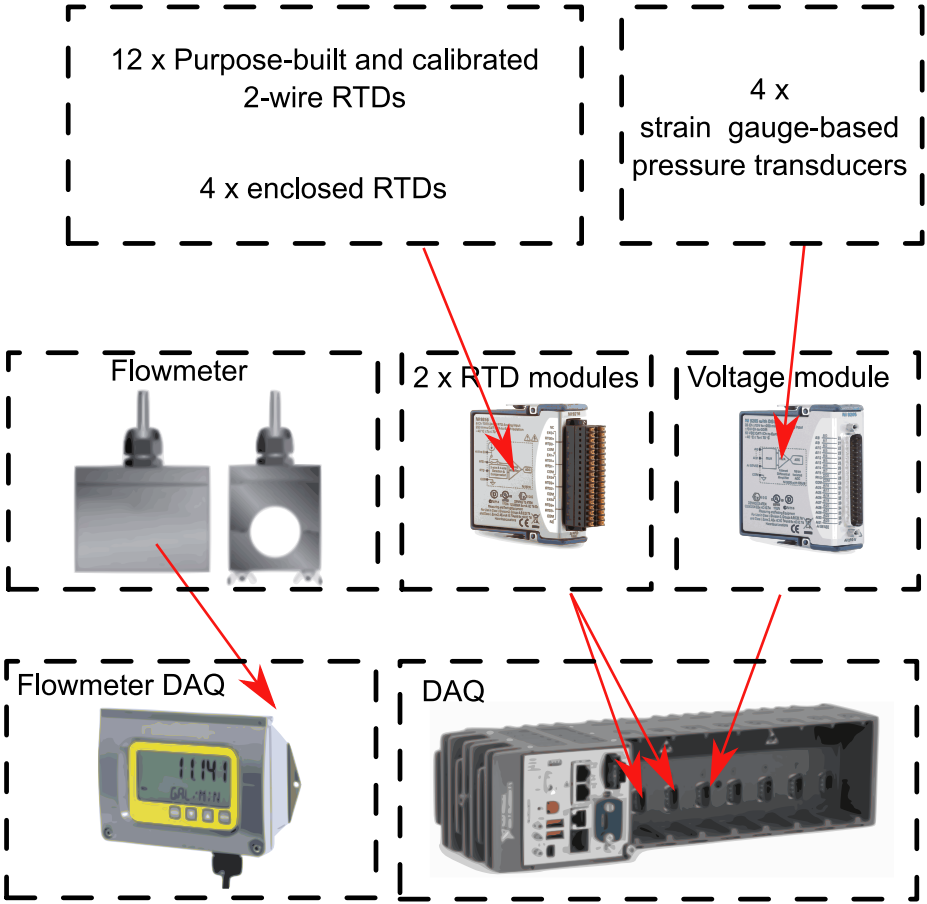


Figure 4.11: Data flow for sensors and data acquisition modules.

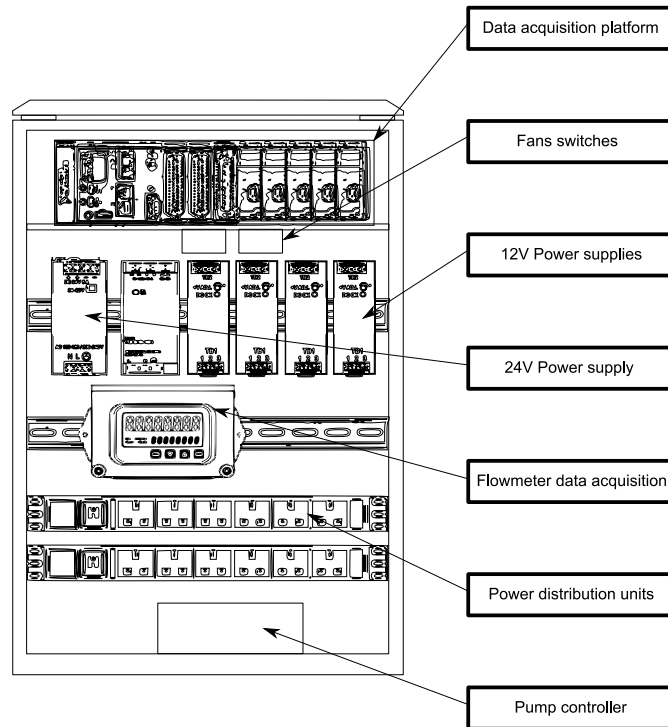


Figure 4.12: Data acquisition cabinet.

4.4.2 Uncertainty analysis

Given a generic measured quantity R , depending on parameters $(X_1, X_2, \dots, X_n)$ uncertainty is defined as follows [209]:

$$dR = \sum_{i=1}^n \frac{\partial R}{\partial X_i} dX_i \quad (4.10)$$

Defining the reliability of measurements prior to any experiment is essential. The first step is the definition of the accuracy of sensors. After that, the accuracy of the sensors is combined with the accuracy of the data acquisition platform. As a consequence, the final measurement will not be an exact value but a most likely value lying in an interval of confidence instead.

4.4.2.1 Confidence interval of RTD sensors

Uncertainty was estimated on both resistance and temperature. The temperature may vary by a term defined as follows:

$$dT = \pm (a_T + b_T \cdot |T|) \quad (4.11)$$

where a and b are two coefficients specific to each sensor. Table 4.5 summarises the coefficients values for the two sensor classes

Sensor	a_T	b_T
Class C Pt 100 RTD	0.6	0.007
Class A Pt 100 RTD	0.15	0.002

Table 4.5: Temperature uncertainty parameters.

Uncertainty on resistance is expressed for class C sensors as follows:

$$\begin{cases} \text{if } T \geq 0: & R = R_0 \pm R_0 (a_R \cdot T + b_R \cdot T^2) \\ \text{if } T < 0: & R = R_0 \pm R_0 (a_R \cdot T + b_R \cdot T^2 + c_R (T - 100) \cdot T^3) \end{cases} \quad (4.12)$$

where the temperature is expressed in °C. While, in the case of class A it is

$$\begin{cases} \text{if } T \neq 0^\circ\text{C}: & R_{1/3DIN} = R_0 \pm \frac{1}{3} \cdot (a_R + b_R \cdot T) \\ \text{if } T = 0^\circ\text{C}: & R = 100 \pm 0.10 \end{cases} \quad (4.13)$$

where 1/3 DIN is the standardised class of the sensor. Parameters are summarised in Table 4.6.

Sensor	a_R	b_R	c_R
Class C Pt 100 RTD	$3.9083 \cdot 10^{-3}$	$-5.775 \cdot 10^{-7}$	$-4.183 \cdot 10^{-12}$
Class A Pt 100 RTD	$3.0 \cdot 10^{-1}$	$5.0 \cdot 10^{-3}$	—

Table 4.6: Resistance uncertainty parameters.

Wiring resistance accounts by 0.375% of nominal resistance on the longest wiring of the system, which has a length of 3 m. Wiring resistance is therefore neglected. In addition, uncertainty of the data acquisition module must be considered. Data is retrieved from the RTDs with the help of two National Instruments 9216 modules. The additional errors on temperature and resistance must be considered:

$$dT_{NI} = T_{signal} \pm e_{TNI} \quad (4.14)$$

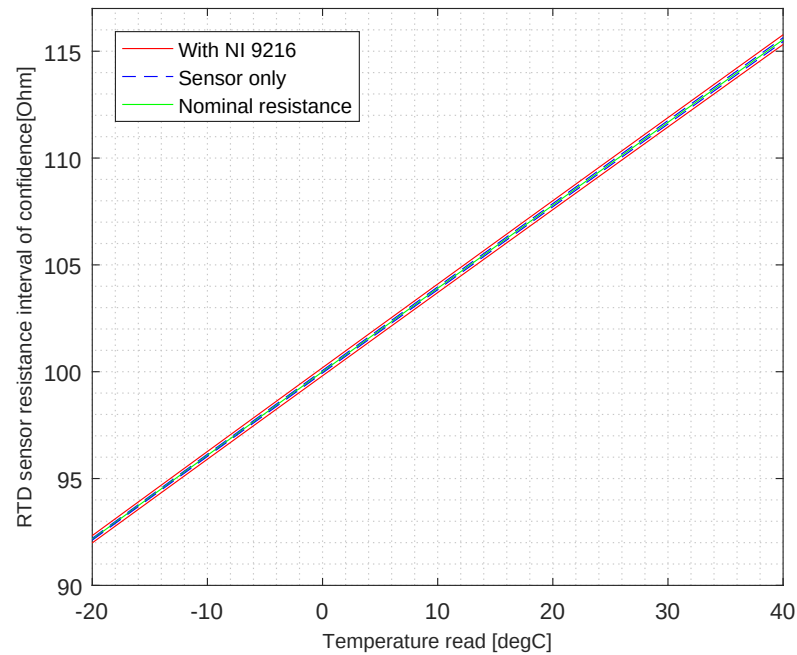
$$dR_{NI} = (1 \pm e_{gainNI}) \cdot (R_{signal} \pm e_{offsetNI}) \quad (4.15)$$

in which T_{signal} and R_{signal} are temperature and resistance signals inclusive of sensors' uncertainties. The parameters are summarised in Table 4.7.

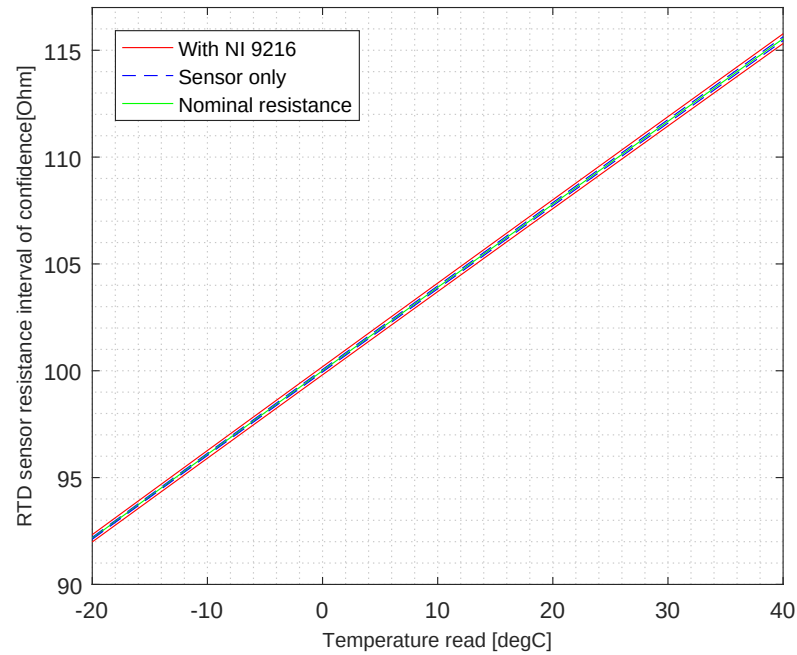
Parameter		Value	Reference
Temperature error	e_{TNI}	$\pm 0.4 \text{ } ^\circ\text{C}$	[206]
Resistance offset	e_{gainNI}	$\pm 0.006 \text{ } \Omega$	
Resistance gain	$e_{offsetNI}$	$\pm 0.007 \text{ } \%$	

Table 4.7: Error parameters of data acquisition platform.

Evaluation of uncertainty of resistance in the case of Omega RTDs is shown in Figure 4.13a, while Figure 4.14b shows the uncertainty of measurement of resistance for TE RTDs. The uncertainty in temperature of Omega RTDs is represented in Figure 4.14a, while Figure represents the temperature uncertainty of TE RTDs 4.14b.

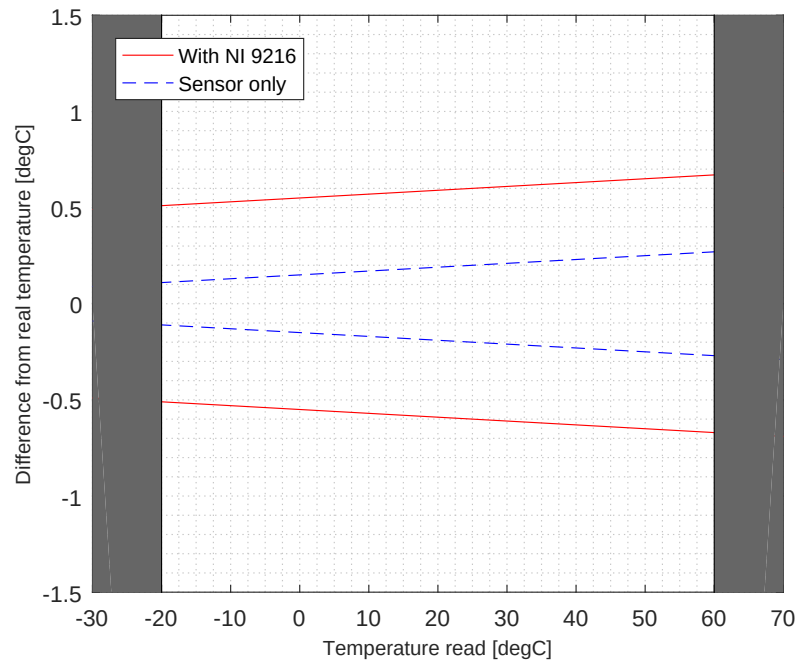


(a) Resistance accuracy for Omega RTDs.

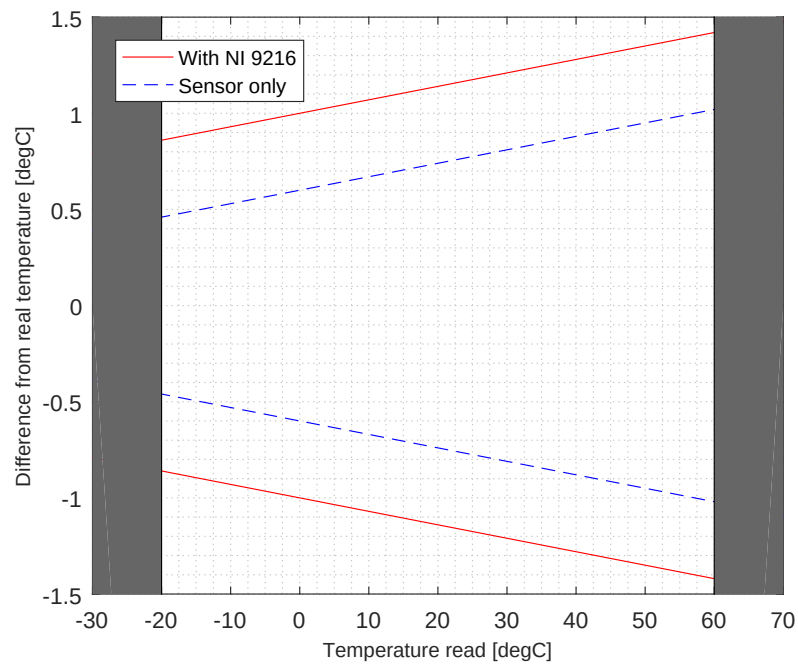


(b) Resistance accuracy for TE RTDs.

Figure 4.13: Accuracy of resistance.



(a) Temperature accuracy for Omega RTDs.



(b) Temperature accuracy for TE RTDs.

Figure 4.14: Accuracy of temperature measurements.

4.4.2.2 Confidence interval of pressure transducers

Uncertainty on pressure samplings was estimated according to the following formula:

$$dp = \pm (1 \pm n_{\text{years}} \cdot e_{\text{yearly}}) (p_0 \cdot e_p) \quad (4.16)$$

where p_0 is the actual pressure, e_p is the error of measurement, n_{years} is the number of years the sensor has been running without calibration and the other parameters are summarised in Table 4.8.

Parameter		Value	Reference
Percentage error	e_p	$\pm 0.25 \%$	[204]
Yearly error	e_{yearly}	$\pm 0.25 \%$	

Table 4.8: Error parameters of data acquisition platform.

In the case of the pressure transducers the uncertainty of the data acquisition platform was taken into account too. The error in pressure measurements needs therefore to be further adjusted as follows:

$$dp_{\text{tot}} = \left(1 \pm \frac{e_{pNI}}{V_{\text{full scale}}} \right) \cdot dp \pm e_{\text{noise NI}} \quad (4.17)$$

the parameters of the data acquisition platform are summarised in Table 4.9

Parameter		Value	Reference
Percentage error	e_{pNI}	3230 μV	[207]
Full scale voltage	$V_{\text{full scale}}$	5 V	
Yearly error	$e_{\text{noise NI}}^1$	116 μV	

Table 4.9: Error parameters of data acquisition platform.

The device has a sensitivity of 46.4 μV . The uncertainty in pressure measurements is shown in Figure 4.15.

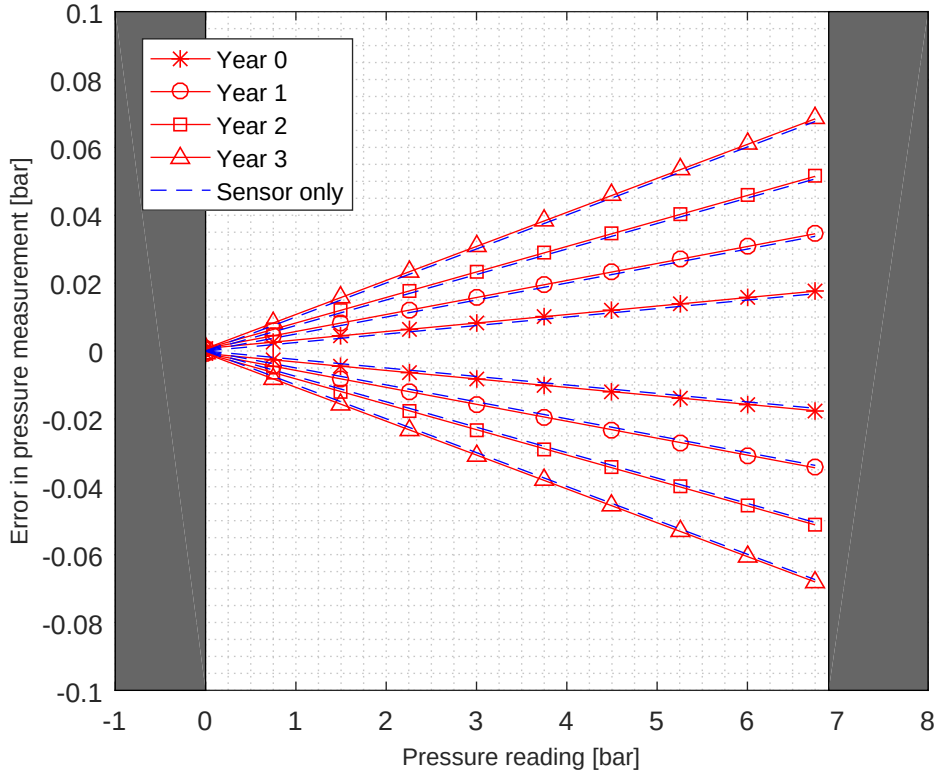


Figure 4.15: Error in pressure measurement.

4.4.2.3 Confidence interval of flowmeter

The ultrasonic flowmeter can measure flow rate in both directions. The absolute value of the error is directly proportional to the absolute value of the flow speed, being $\pm 1\%$ of the flow speed or 0.003 m/s , at a flow speed ranging from -12 m/s to 12 m/s as summarised by the following formula

$$\begin{cases} \text{if } v_{fluid} > 0.003 \text{ m/s} & dv = 0.003 \text{ m/s} \\ \text{if } v_{fluid} < 0.003 \text{ m/s} & dv = \pm 0.01 \cdot v_{fluid} \end{cases} \quad (4.18)$$

Uncertainty of the data acquisition module is, in this case, negligible. Figure 4.16 represents the error of the flowmeter at different speeds.

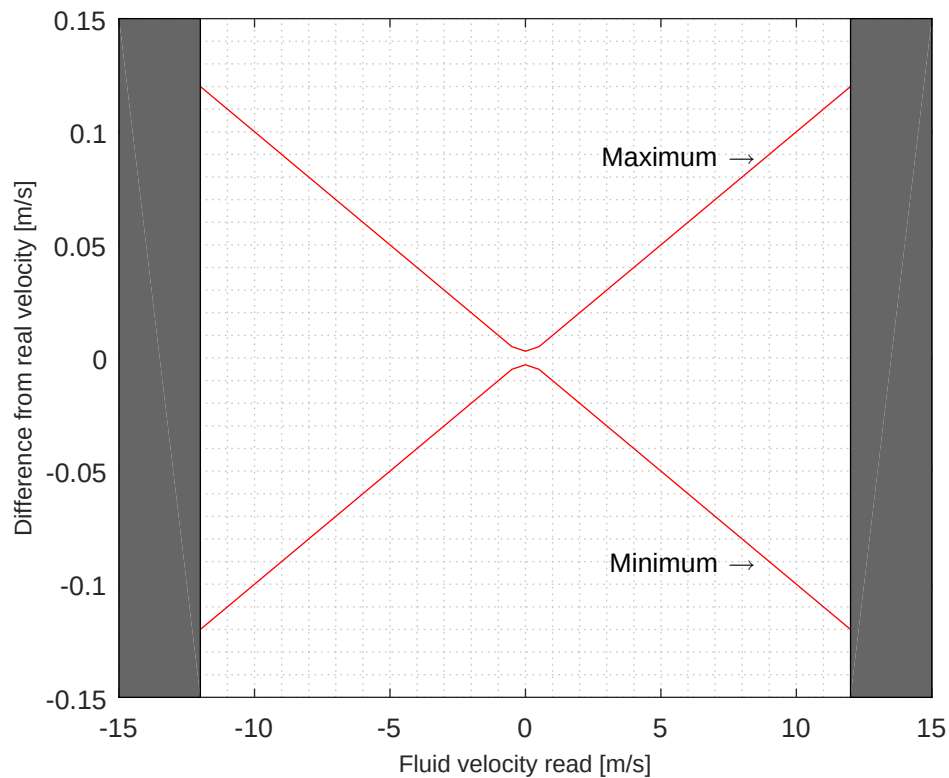


Figure 4.16: Flowmeter measurement error.

4.4.3 Testing procedure

The test-bench replicates in a smaller scale a vehicle battery cooling loop. It can accommodate different battery modules and it can be used to study solutions like removable external cold-plate indirect liquid cooling applications. The latter is an interesting future development in motorcycle fast charging. Motorcycles have weight and reliability requirements that often force designers to opt for passive cooled batteries. Oversizing the pack can allow normal road use, since the torque request is relatively low. However fast charging cycles may need to be terminated too early, due to battery overheating. Removable cold-plate heat exchangers can overcome such issue. The test-rig allows the testing of such devices as well as more traditional cooling systems. Temperature is sampled in different regions of the battery external walls and on the cooling loop. In order to have a full

understanding of the cooling loop, temperature and pressure are also sampled at different spots throughout the test-rig. In additions, a flowmeter is also added. The power supply logs voltage, absorbed and dissipated power and current profile. The measurements taken on the test-rig reproduce a real life scenario, allowing the measurements to be the least invasive possible but grating a satisfactory level of accuracy. As on a real vehicle, the battery is kept into an enclosure and the ambient temperature within the enclosure is monitored during the tests.

4.4.4 Strategic contribution

The battery was cycled over different current profiles and the temperature was logged as it will be presented in Chapter 5, and the pressure was logged at different locations to make sure the pressure drops were as per sizing, as in Paragraph 4.3.1. Major benefits derived from having laboratory observations on a real vehicle sub-system. With respect to measurements on a real vehicle, it is possible to avoid disturbances and perform tests in a controlled environment. Such details allow a more precise characterisation of the battery. Previous test rigs were either layout-specific or not flexible enough to allow the testing of different layouts, or alternatively they were too large and expensive to run. The new test rig is cheap to run and can examine a broad range of layouts. The layout presents a battery module within an enclosure, on top of a cold plate, with thermal insulation at the bottom, a layout which, although being limited to one module, is structured in the same way as that of the Audi e-tron and other similar vehicles [167].

The implemented test-rig provides a different approach to model validation, more flexible and cost-effective and fully integrated with the simulation library. On the other hand, the test rig is not designed to host a whole battery pack and a powertrain. How-

ever the combined use of simulation and test-rig validation overcomes such limitation, achieving a balance between a fully theoretical and a fully empirical approach. The test rig is therefore capable of shortening the design process effectively decreasing the cost of prototyping.

4.5 Interim conclusions

The test rig proves flexible and re-configurable. It is possible to test different layouts of battery module and cooling systems. Measurement uncertainty has been minimised, the ambient conditions controlled and the input fluid temperature and velocity is controlled as well. The test rig provides therefore cheap and reliable results and it can be re-used for several different applications.

4.6 Summary of chapter

This chapter presented the experimental test-rig layout. It started from some initial sizing considerations, presenting then the test-rig subsystems. The data acquisition system was then introduced together with the uncertainty analysis of the sensors. The contribution of the experimental set-up was outlined and conclusions were drawn. In the next chapter the simulations and their experimental validation will be presented, making use of the samplings taken from the test-rig layout.

Chapter 5

Experimental validation and results

The chapter introduces the modelling results and matches them with the outcome of experiments. First the single-cell case is examined, then the module. In the case of the single cell, after an aggressive validation duty, a full drive cycle and the combination of two urban drive cycles and a fast-charge duty are examined. In the case of the module first an aggressive duty and then a drive cycle followed by a fast-charge duty are observed. In both cases, temperature and electrical parameters are sampled, the discrepancy is examined and commented and observations are raised on the correlation between the current rate and the temperature increase, examining how accurate the model is. The criticality of fast charge is underlined and an option to contrast its effect is proposed. The model manages to accurately reproduce the temperature profile and the electrical performance of both the single cell and the module while keeping computational cost low.

5.1 Model implementation and validation

The model was combined with test-rig results, in order to prove the viability of the methodology. First, simulation and tests were extensively performed on a single cell,

then on battery module. Two typologies of battery cells were examined: cylindrical cells with a rigid Aluminium enclosure, in the case of single cell tests, while module testing was performed on a stack of 28 pouch cells connected in series and enclosed in a rigid prismatic Aluminium container filled with epoxy potting material. In an initial stage, aggressive cycles were performed on a single cell at different temperatures. Subsequently, some drive cycles were scaled down to the single cell level and the cell was tested at 25°C. After that step, the battery module was tested in a controlled-temperature room, with both charge-discharge cycles, drive-cycles and, “taxi cycles” alternating the urban section of a drive cycle with fast-charge. The aim of the whole procedure was to prove the effectiveness of the model under different duties and boundary conditions and its re-scalability from a single cell to a whole module model.

5.2 Definition of duty cycles

Duty cycle definition was organised in two major steps: definition of the single cell cycles and definition of the module cycles. The single cells were initially tested with a 10s pulsation of 1.5C current, at temperatures of -10 , 0, 12 and 25°C. After such test was carried out, a pack current profile was calculated from vehicle and powertrain data. From the pack profile a single-cell profile was obtained, using the information on the pack and modules layout. On this first step, extreme scenarios, featuring changing current direction at low temperatures, provided validation of the single cell model, testing whether the estimated internal temperature gradient was accurately reproduced, and whether the temperature increases and decreases were correctly simulated. The electrical performances were also subject to careful comparison. In the second case, the model was scaled up, from the same chemistry, but on a different geometry. In this case, the battery module was positioned into a test-rig which reproduces a small scale cold-plate indirect liquid

cooling system. In this case, the current profile was scaled down, in order to reproduce the behaviour of a module inside a full pack.

5.3 Single cell

The single cell was modelled as showed in the previous chapters, the work has been recently presented in the in aforementioned publication [198]. The model relies on geometrical simplifications, representing the spiral winding of the cell as a pack of concentric cylinders instead. Each cylinder is circumferentially discretised in four elements and axially discretised in three elements. The geometry of the top and bottom connections is also simplified. The connections, the insulating material and convective heat exchange around the battery are also modelled. The simulation was coupled with experiments on LG 21700M50 cells. The cell, held by a supporting sled and covered in thermally insulating material was fitted 3 K-type thermocouples on the external walls, near the top plate, at half height and near the bottom plate. The cell was then positioned inside a thermal chamber at a controlled temperature and connected to a bi-directional power supply. Voltage and current were monitored throughout the whole test. The objective was to develop a computationally lean multi-domain model that could provide an accurate representation of the battery temperature profiles in a wide-range of environmental conditions. We expected to obtain a robust, lean, efficient and effective methodology for battery testing that conveniently matches the experimental data. Our expectations were to obtain a larger amount of information on the thermal behaviour of the battery cell, with respect to currently available lumped-parameter, reduced-order models at a lower computational cost than currently available finite-element models. The model takes simplifying assumptions on the geometry and therefore it cannot be used for those applications that require detailed modelling of cells, e.g. for optimisation of a battery container, electrode

and electrode coatings thickness sizing et similia. On the other hand, the model proves extremely beneficial in combining cell internal temperature gradient estimation and module temperature gradient estimation. The proposed methodology represents a beneficial trade-off between accuracy and extensiveness of multi-domain capability.

5.3.1 Procedure

The insulating material wrapped around the cell is assumed to be isotropic and represented by a network of lumped masses each of which is connected to a discrete element of the cell enclosing can model. The contact resistance is assumed to be constant and the convective heat transfer coefficient is assumed to be constant all around the cell. The model specific cell model was not designed to capture sudden variation in the air flow around the cell. Although such practice would be possible, it is out of the scope of the experiments.

The main purpose of the experiments was to validate the internal heat transfer model of the battery cell. Tested cells are NMC, hard case jelly roll, model LG21700M50. The external boundary is reproduced in the model as well, taking into account heat transfer contact resistance between the insulating material and the cell wall. The electrical resistance of the connections is included in the model as well.

Thermally insulating layer	
Material	Calcium Magnesium Silicate
Density	128 $kg \cdot m^{-3}$
Thermal conductivity	0.04 $W \cdot m^{-1} K^{-1}$
Thickness	6 mm
Connections	
Electrical resistance of connection	< 1 $m\Omega$
Electrical resistance of cables	2 $m\Omega$

Table 5.1: Material properties for experimental layout.

The internal heat transfer model is developed by simplifying the spiral windings into concentric circles and breaking each circle into lumped mass elements. Each concentric circle is discretised axially in three elements and circumferentially in four elements. The initial circumferential temperature gradient is assumed to be zero. Such hypothesis is plausible, since the product of thermal conductivity and length in circumferential direction is high.

The same concept would apply in axial direction too, however, the different geometry of the connections affects the heat exchange surface. Most electrically conductive materials, also have a good thermal conductivity. In the experiments performed in this work, connectors were made of Aluminium. Due to the specific design of cylindrical cells, a lower contact surface and a lower contact pressure are allowed on the positive connection. It was therefore preferred to measure the initial axial temperature gradient on the external wall of the battery cell and start both experiments and simulations from the same initial conditions.

5.3.2 Vehicle data and description

Experiments are based on a single cell current profile calculated on the data of the Arrival Pod experimental vehicle summarised Table 5.2. Powertrain specifications are summarised in Table 5.3. Two different battery layout were examined. In the first case, the largest pack available was examined. In this layout, three series of 8 modules were put in parallel, as represented in Table 5.4. The second layout considered featured a smaller battery pack. In this case the pack is built out of two stacks of four modules connected in parallel, with properties showed in Table 5.5.

Vehicle specifications		
Mass	2000	<i>kg</i>
Weight on front wheels	50	%
Weight on rear wheels	50	%
Final drive ratio	2.71	
Front section area	1.8	<i>m</i> ²
Aerodynamic drag coefficient	0.31	
Rolling resistance coefficient	0.01	
Power regeneration ratio	30	%

Table 5.2: Summary of Arrival Pod specifications.

Motor specifications		
Peak torque	370	<i>Nm</i>
Continuous torque	200	<i>Nm</i>
Peak power (at 700 <i>V_{DC}</i>)	160	<i>kW</i>
Continuous power	20 to 100	<i>kW</i>
Speed	0 to 8000	<i>rpm</i>
Peak efficiency	96	%
Dry mass	24	<i>kg</i>

Table 5.3: Specifications of the Arrival Pod motor.

Battery specifications		
Cell nominal capacity	5000	<i>mAh</i>
Cell nominal voltage when fully charged	4.25	<i>V</i>
Number of cells in parallel in a module	20	
Number of cells in series in a module	12	
Module nominal capacity	40	<i>Ah</i>
Module specific energy	175.2	<i>Wh · kg</i> ⁻¹
Module nominal voltage when fully charged	51	<i>V</i>
Number of modules in series in a pack	3	
Number of modules in parallel in a pack	8	
Pack nominal capacity	120	<i>Ah</i>
Pack specific energy	168.2	<i>Wh · kg</i> ⁻¹
Pack nominal voltage when fully charged	408	<i>V</i>

Table 5.4: Specifications of battery pack layout 1.

Battery specifications		
Cell nominal capacity	5000	<i>mAh</i>
Cell nominal voltage when fully charged	4.25	<i>V</i>
Number of cells in parallel in a module	20	
Number of cells in series in a module	12	
Module nominal capacity	40	<i>Ah</i>
Module specific energy	175.2	<i>Wh · kg⁻¹</i>
Module nominal voltage when fully charged	51	<i>V</i>
Number of modules in series in a pack	4	
Number of modules in parallel in a pack	2	
Pack nominal capacity	80	<i>Ah</i>
Pack specific energy	156.7	<i>Wh · kg⁻¹</i>
Pack nominal voltage when fully charged	204	<i>V</i>

Table 5.5: Specifications of battery pack layout 2.

5.3.3 Simulation setup

The experimental results were compared to a cylindrical-cell model as a case study, in order to evaluate the effectiveness of the proposed modelling strategy. The cell model chosen for validation is composed by 21 concentric cylinders, each of them composed by anode, main separator, cathode and external separator, with temperature-dependent thermal properties, connected to an ECM model. A core cylinder and an Aluminium enclosure were also added. The interaction between each layer and the liquid electrolyte was modelled as shown in the previous chapters. The overall weight of the cell is 68 g, the diameter is 21 mm and the height is 70 mm. The central core is made of graphite and its diameter is 2 mm. The material data are modelled accordingly in the IHTM. The electrolyte is Lithium hexafluorophosphate.

The discretisation strategy is shown in Figure 5.1. As a first step, a single bunch ECM was considered. The anode heat generation term was connected to the discrete element closest to the anode current collector connection with the top plate, while the cathode heat

generation term was placed in the discrete element positioned the closest to the cathode tab connection. Both the simulations and the experiments were performed with an initial SOC of 90%.

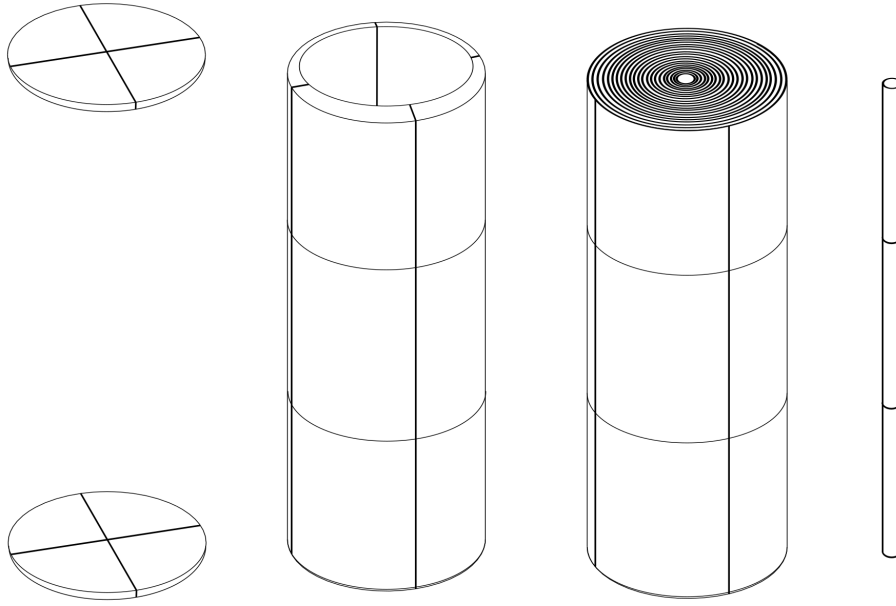


Figure 5.1: Discretisation of the cylindrical cell, left to right: end plates, Aluminium cylinder, jelly roll, central cylindrical element.

The Modelica script was executed through Dymola, with Petzold's DASSL solver, setting a tolerance of 0.0001 and 500 intervals. The Modelica script was generated automatically, from user-set parameters, i.e. simulation time, solver and time step, through a MATLAB script, the results, retrieved by the same Matlab script, were then compared to the experiment results to provide validation.

The procedure is semi-automated, it requires user to intervene after the Modelica script has run, at that stage, user checks no relevant errors have been issued on the result window. If no issues occurred, the user closes Dymola. At that stage the Matlab script automatically resumes and runs until its completion. The algorithm structure is

outlined in Figure 5.2. The setup runs smoothly and completes the simulation of 1000 s of cycle in less than 40 s.

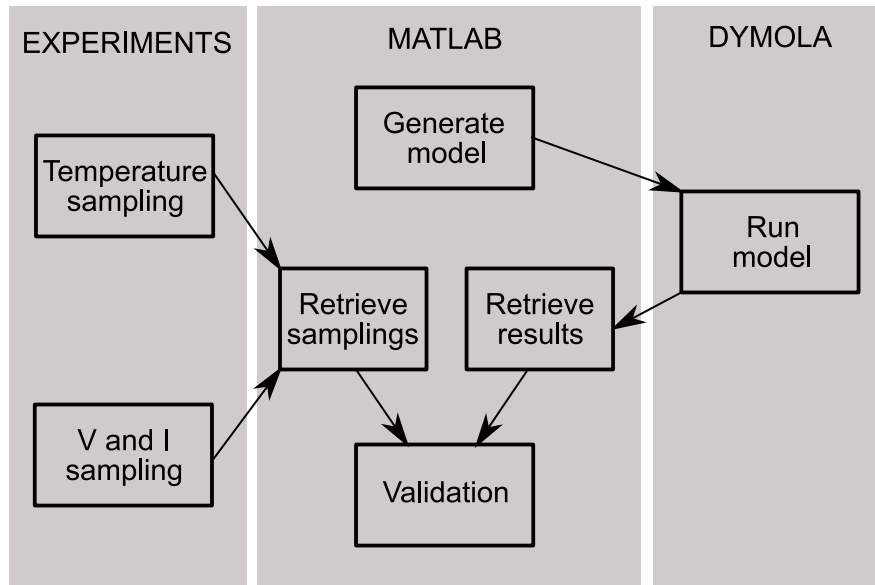


Figure 5.2: Algorithm layout.

5.3.4 Optimal simulation parameters

The selection of solver and number of discretising intervals per each instant of the time scale is a major issue when running simulations. Since the problem is represented by non-stiff differential algebraic equations and there is a limited number of events in the problem, most prominently only current and temperature variations, influencing other parameters, a DASSL solver is selected. The selection of the number of discrete intervals in which each point in the time scale should be divided is made by running different models and comparing the outcome. Most prominently three parameters were examined: i) the Central Processing Unit (CPU) time for integration, ii) the average time needed for each grid interval and iii) the Fourier number. These parameters were examined on the first duty cycle, at 25°C for 100, 500 and 1000 intervals. The decrease of Fourier

number is much steeper before reaching 500 intervals, as it can be seen in Figure 5.3. Fourier number is too high at 100 intervals and reaches an optimum of 0.5 at around 100 intervals, while the benefit of increasing the number of intervals above 500 is minor. However, above 500 intervals, the increase in CPU time for integration keeps increasing at a remarkable rate, as per Figure 5.4. It is to be observed that the time needed for each grid interval decreases as the number of intervals increase. Such decrease, however, is by two orders of magnitude smaller than the increase in CPU time for integration. The final selection is therefore a DASSL solver with a 500 intervals of discretisation. Tolerance is set to be one order of magnitude smaller than the smallest interval of time.

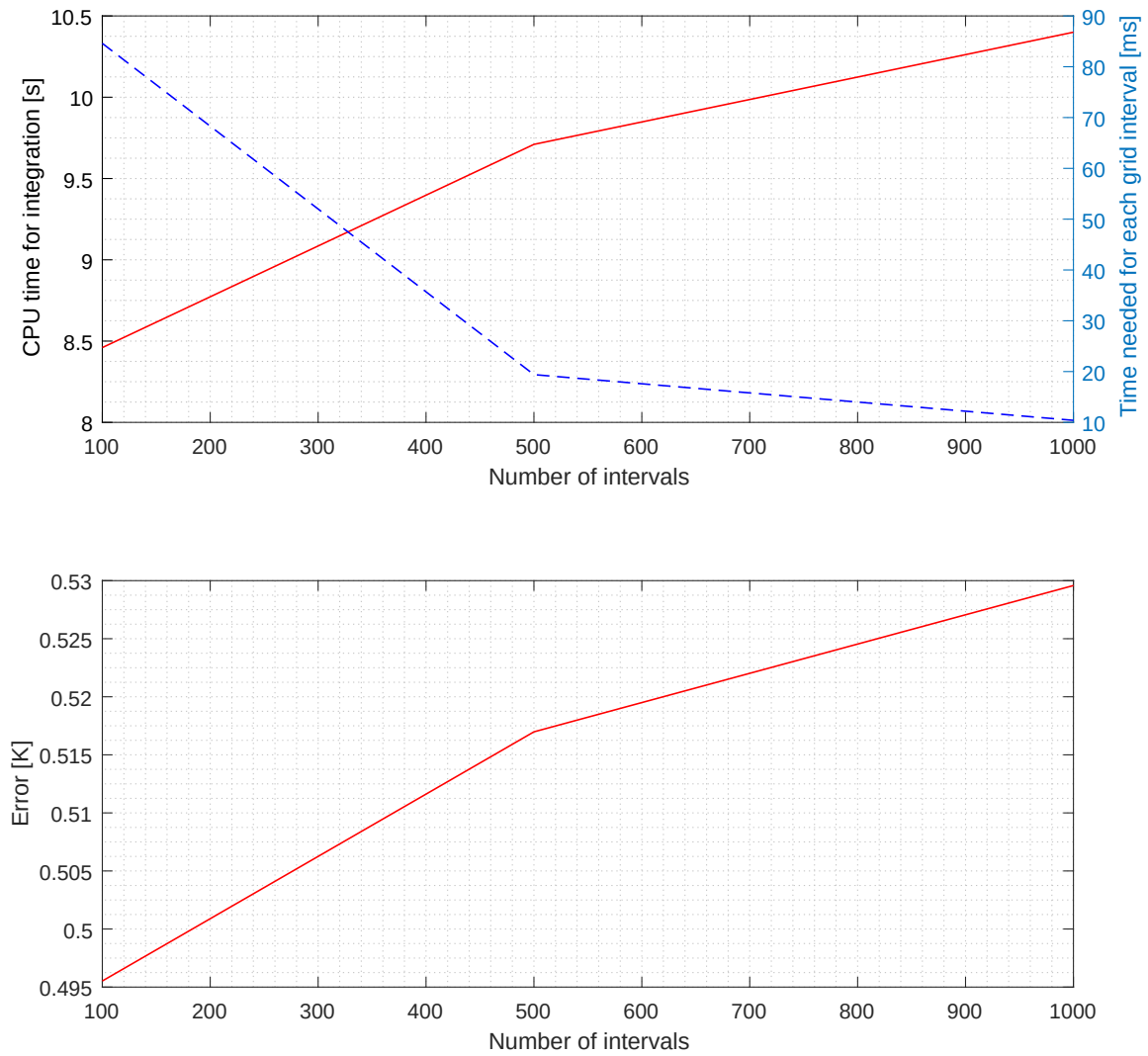


Figure 5.3: Computational performances and error at different numbers of discretising intervals.

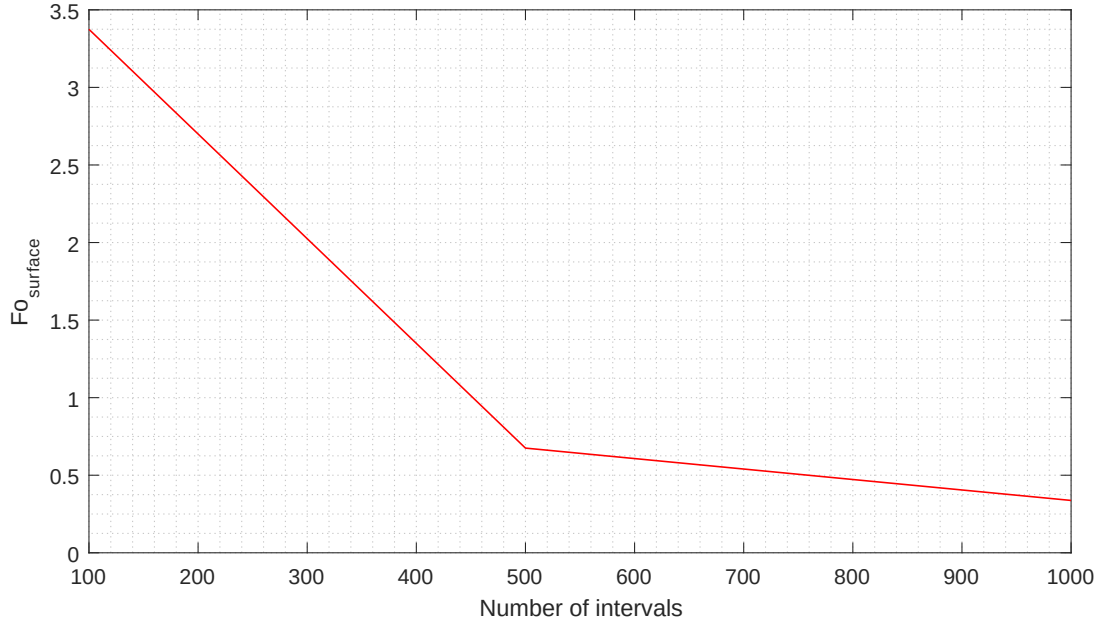


Figure 5.4: Fourier numbers at different discretisation intervals.

5.3.5 Experimental setup

The cell was positioned inside a supporting sled, three K-type thermocouples were mounted on a layer of electrically insulating tape on the external walls of the cell. Despite such a choice would inevitably have lead to an increase of sensor's thermal inertia, eventually adding uncertainty to the wall temperature measurement, it was necessary to electrically insulate the thermocouples, in order to effectively measure the temperature.

The cell was covered with a thermally insulating material and positioned in a thermal chamber, in order to conduct the tests in a condition of fully controlled thermal boundaries.

The layout of the single cell experiment, including thermocouple positioning is represented in Figure 5.5.

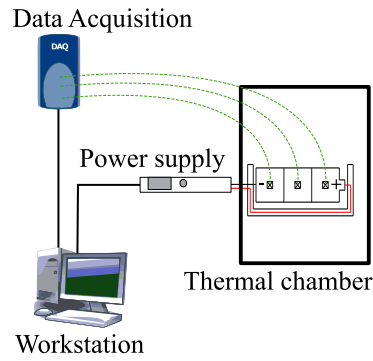


Figure 5.5: Experimental layout: bi-directional power supply and data acquisition platform, functional scheme.

Make	Kepeco
Model	BOP100-10MG
Power	1 kW
Voltage range	0 – 10 V
Current range	0 – 100 A

Table 5.6: Bi-directional power supply specifications.

Thermocouple temperature range	–40 to 1000°C
Uncertainty of thermocouples	$\pm 1.5^{\circ}\text{C}$ or $\pm 0.4\%$
Data acquisition uncertainty	$\pm 0.2\%$

Table 5.7: Uncertainty of K-type thermocouples and data acquisition system.

5.3.6 Optimising the parameters

A major issue in modelling is accurately representing the OCV and the ECM terms. Starting from different interpolation techniques for the OCV and from the range of ECM variables, an exhaustive search was run, comparing results with the experimental profile, in order to optimise the performance of the ECM. An initial 6th degree polynomial interpolation for the SOC-OCV correlation was tested, as previously mentioned in Chapter 3. It was compared with different polynomials and with a "hybrid" option, using a 4th degree polynomial below 10%, a 7th polynomial above 90% SOC and a 6th degree polynomial

in between. As it can be seen in Figure 5.6, the combined use of different polynomials, depending on the SOC, proved to be more effective and so the formula proposed in Chapter 3 was therefore adjusted accordingly. The benchmark was a 1C full discharge cycle at initial SOC of 100% and ambient temperature of 25°, data provided by the manufacturer [210].

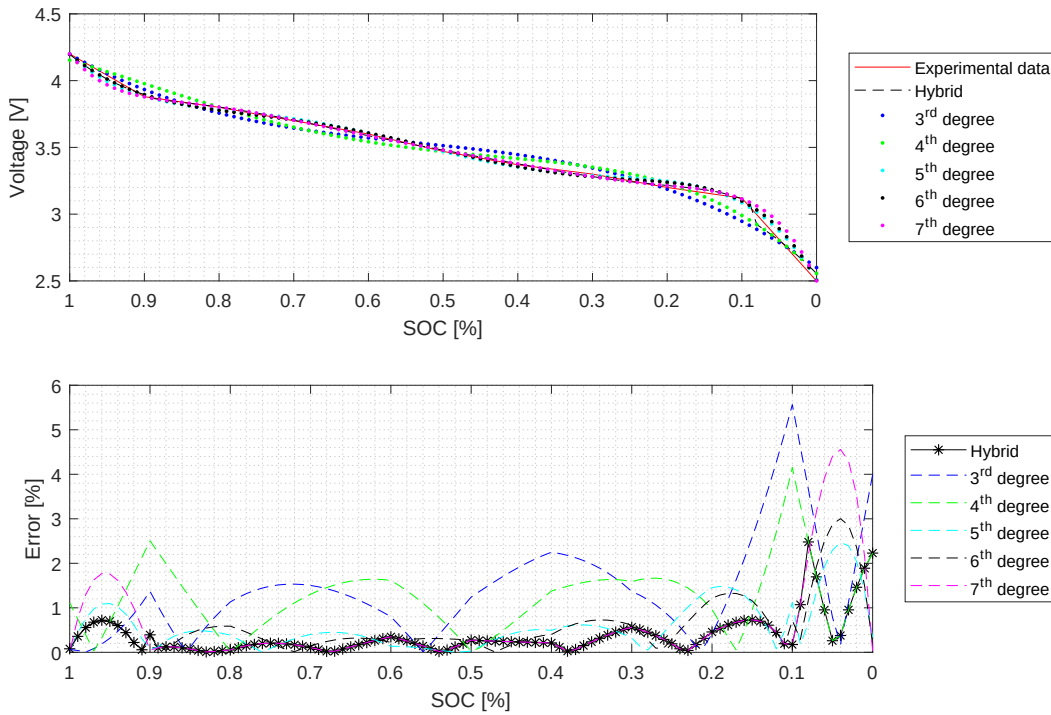


Figure 5.6: Comparison of different strategies for optimising the OCV interpolation strategy.

5.3.6.1 Discharge cycle

The equivalent direct current resistance of the cell varies with SOC and temperature as illustrated below, where the equivalent resistance obtained from the elements in the ECM is compared with that measured by the manufacturer. The cell was first discharged at continuous current at a rate of 1.5C, the temperature was sampled in different spots on the cell external wall and it was compared with the simulation. The model appears to be

effectively reproducing the cell's thermal behaviour. The voltage profile presents some remarkable discrepancies which will be dealt with in the next paragraph. The error is generally reduced and below 1°C , with the exception of the side wall towards the end of the cycle, when the error reaches 2°C for a duration of 1 min . Such an error, however, is only 4% of target temperature, while the error remains within 2% for most of the test. As shown above, such figures are better than those found in literature.

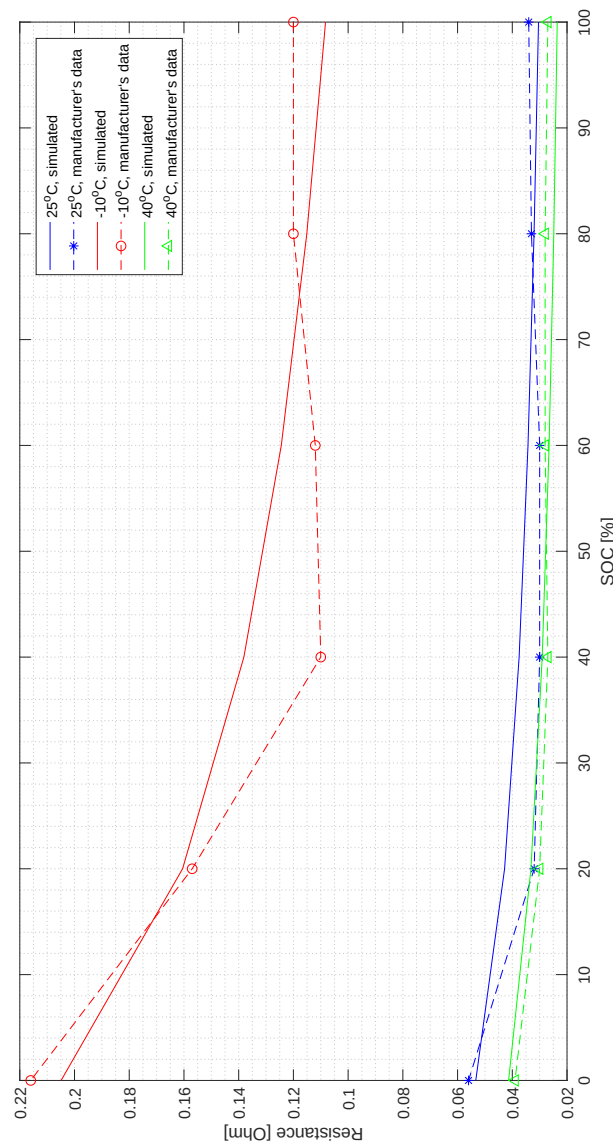


Figure 5.7: Equivalent resistance of cell vs. SOC: model versus manufacturer's data.

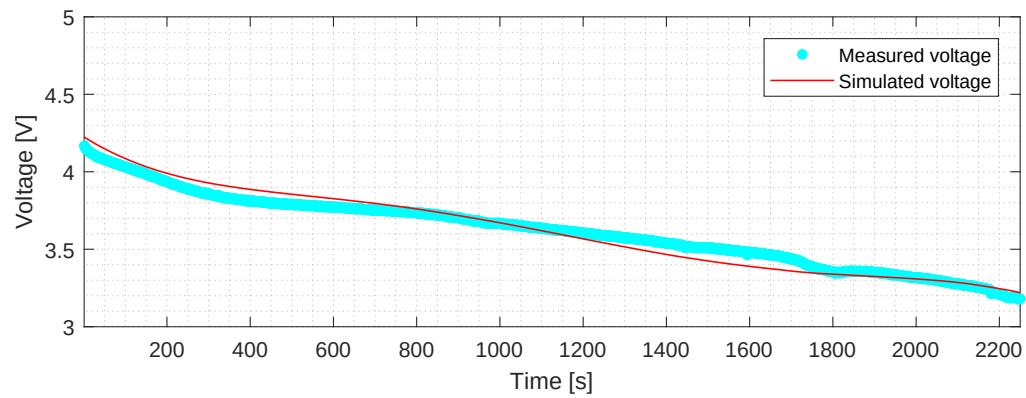


Figure 5.8: Voltage profile comparison at 1.5C current rate, initial SOC 100%.

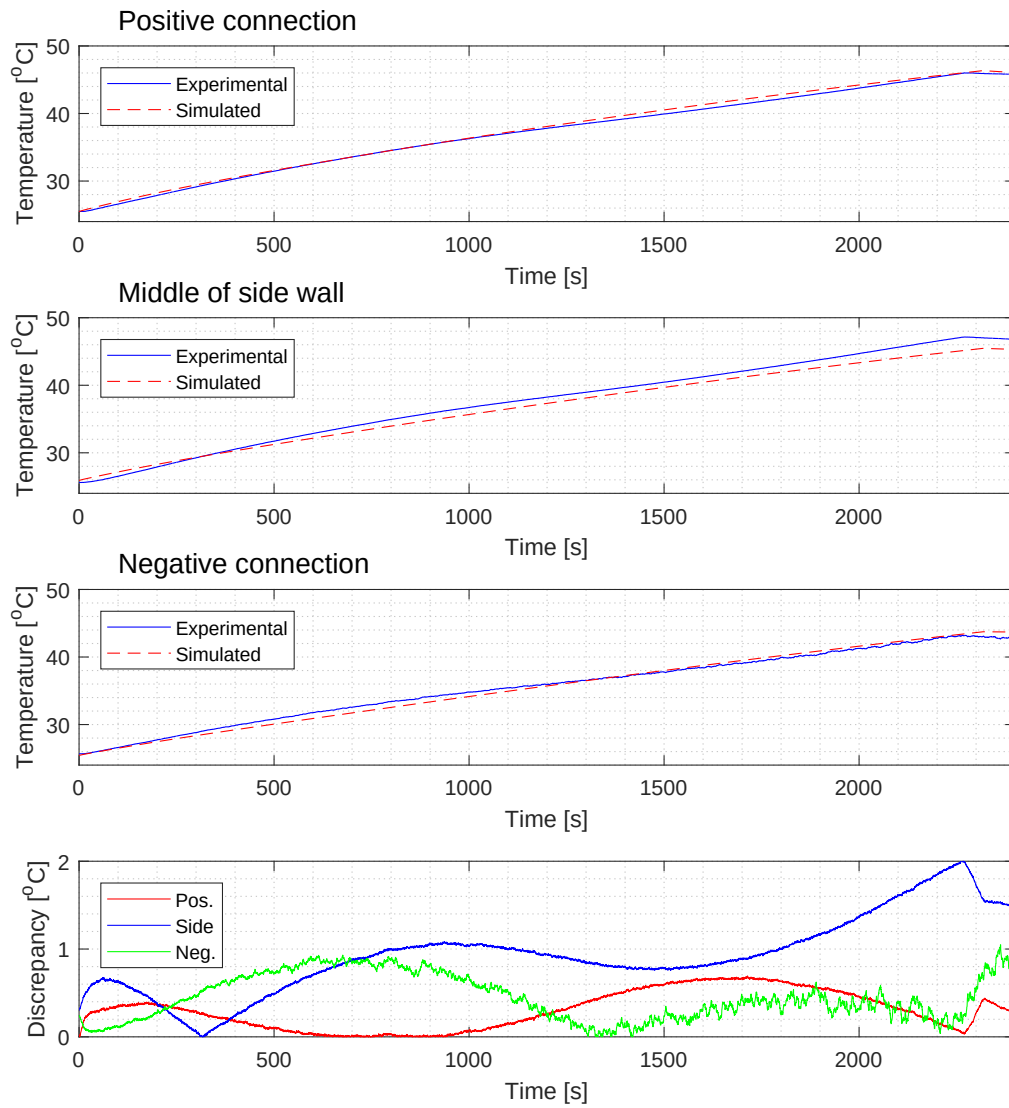


Figure 5.9: Constant current discharge cycle from 100% SOC, temperature profiles in different regions of the battery cell.

5.3.7 Duty cycle description

Three different duty cycles were chosen: i) an aggressive validation duty, with an initial SOC of 85% and a final SOC of 75%, ii) a full drive cycle, with an initial SOC of 100% and a final SOC of 90% and iii) a duty cycle composed by two urban sections of a drive cycle with 1.0 C-rate charging in between, starting at a SOC of 70%, being discharged to 65%, recharged up to 75% and terminating the cycle again at 70% SOC. The latter is a plausible everyday scenario for urban vehicles. We previously presented the experiments in a publication [198].

5.3.8 Aggressive validation cycle

A current profile alternating 10 s of 1.5C discharging current to 10 s of 0.5C charging, as shown in Figure 5.10 (the figure shows the first 10 s only for reasons of clarity) was chosen for validation. The battery was cycled for 1000 s only in order to avoid safety concerns and permanent cell degradation, most prominently i) in order not to exceed the temperature safety limit of 60°C, and ii) putting most effort in examining the transient. Figure 5.11 shows the voltage profile at 25 °C whose error remains below 5% of the voltage range. Such discrepancies are mostly due to the difficulties in reproducing the connection resistances.

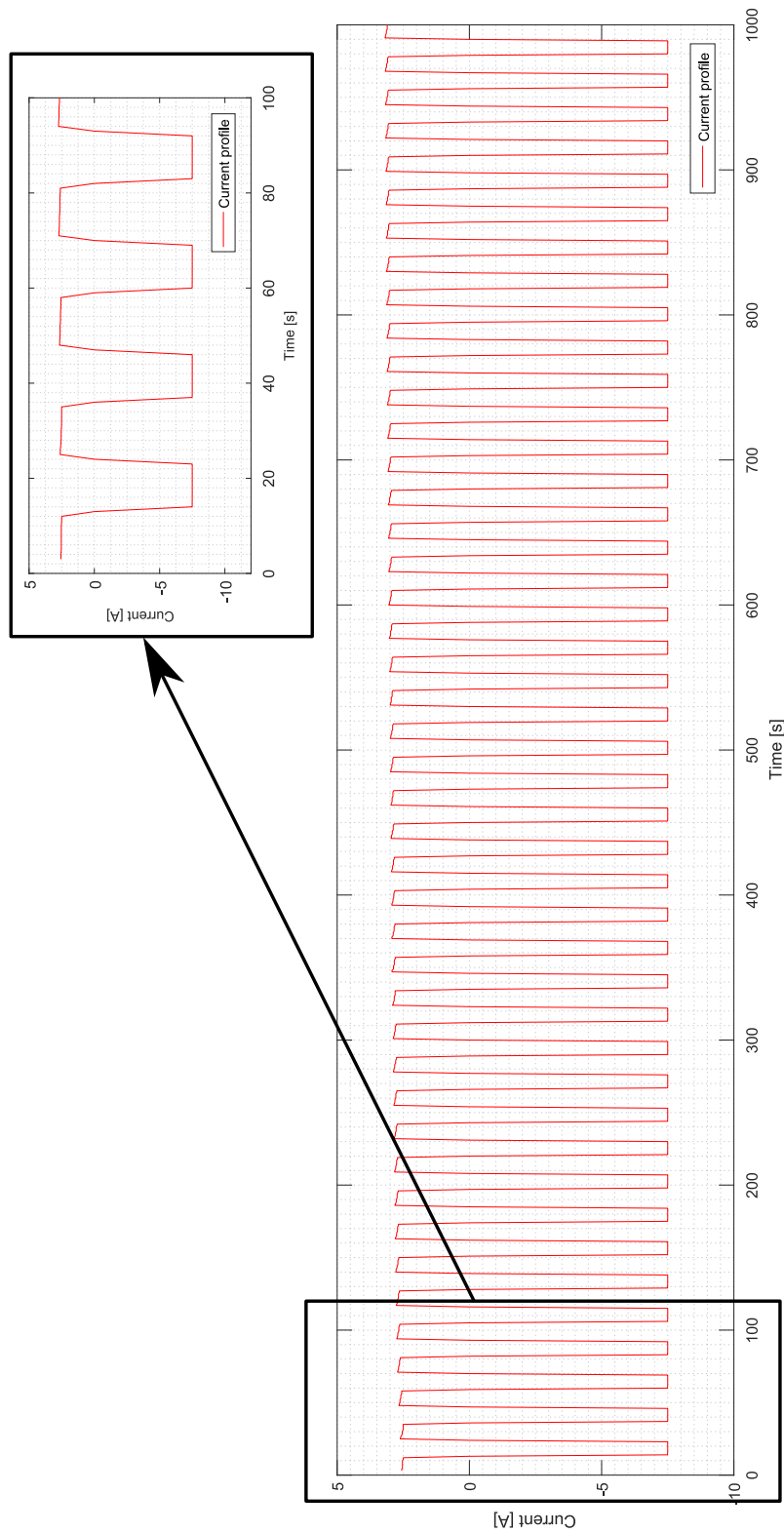


Figure 5.10: Current profile on the validation cycle, first 100 s only are represented in the picture for reasons of clarity, initial SOC is 85%, final SOC is 75%.

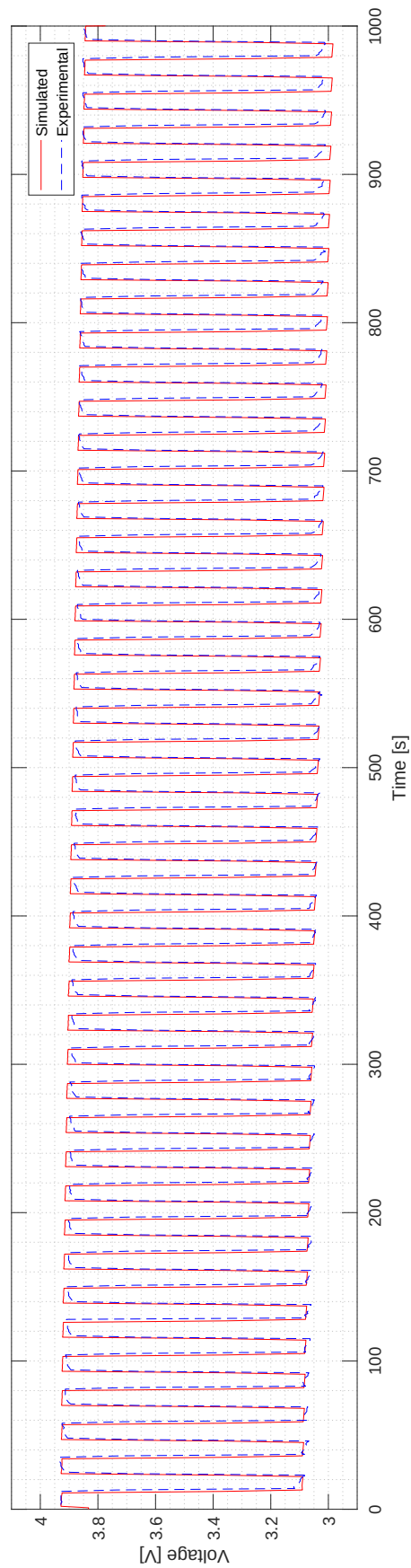


Figure 5.11: Simulated voltage versus experimentally measured voltage.

The duty cycle was run in a thermal chamber at -10 , 0 , 12 and 25 °C, with temperature profiles shown in Figures 5.12, 5.13, 5.14 and 5.15. Both tests and simulations were performed with an initial temperature difference between cell surface and ambient and an initial internal temperature gradient, in order to test the behaviour of the model in a transient, starting from non-uniform initial conditions.

Sub-zero tests required to gradually reduce the temperature of the thermal chamber and wait for the cell to reach the required temperature. The process required 24 hours in a ventilated and de-humidified thermal chamber.

The final gradient and the temperature value at each instant of time show a good accuracy of the model in predicting the thermal behaviour of the cell.

Ambient temperature	Initial cell average temperature	Initial internal temperature gradient
-10°C	-6°C	0.3°C
0°C	3°C	0.2°C
12°C	15°C	0.15°C
25°C	25°C	0.1°C

Table 5.8: Battery temperature, ambient temperature and internal temperature gradient under tested scenarios.

The model appears to be effectively dealing with the transient, the error appears to be greater on the side walls of the cell and at low temperatures. The definition of boundary conditions has a major impact on the magnitude of the error. Conduction heat exchange at the positive and negative connection is defined without major issues, since it deals with modelling a solid material whose properties are quite uniform. The side wall of the cell, however, poses more uncertainty in the modelling of the contact thermal resistance between the insulating material and the cell wall, which appears slightly overestimated in

the model. The error, after an initial overshooting, decreases, stabilizing when cell-wall temperature reaches 27°C , then diverging again after 35°C . The area around the negative connection is subject to a smaller error.

The magnitude of the error, compared with the uncertainty of the thermocouples allows us to conclude that assuming the thermal properties as linear within the operating temperature range is a plausible method.

The simulation error in temperature estimate subject to the largest variation, although being on average quite small, is that on the area near the positive connection. Reasons for such discrepancies can be the variation in contact resistance due to the expansion of the contact plate and the tolerances on dimensions and material properties.

The error on temperature estimation appears to be increasing over time due to the linearization of the temperature dependence of specific heat and thermal conductivity, leading to a greater error at the two ends of the temperature range, especially towards the end of the experiment.

Since the real increase of specific heat higher than predicted, the model tends to overestimate the temperature increase at the end of the experiment.

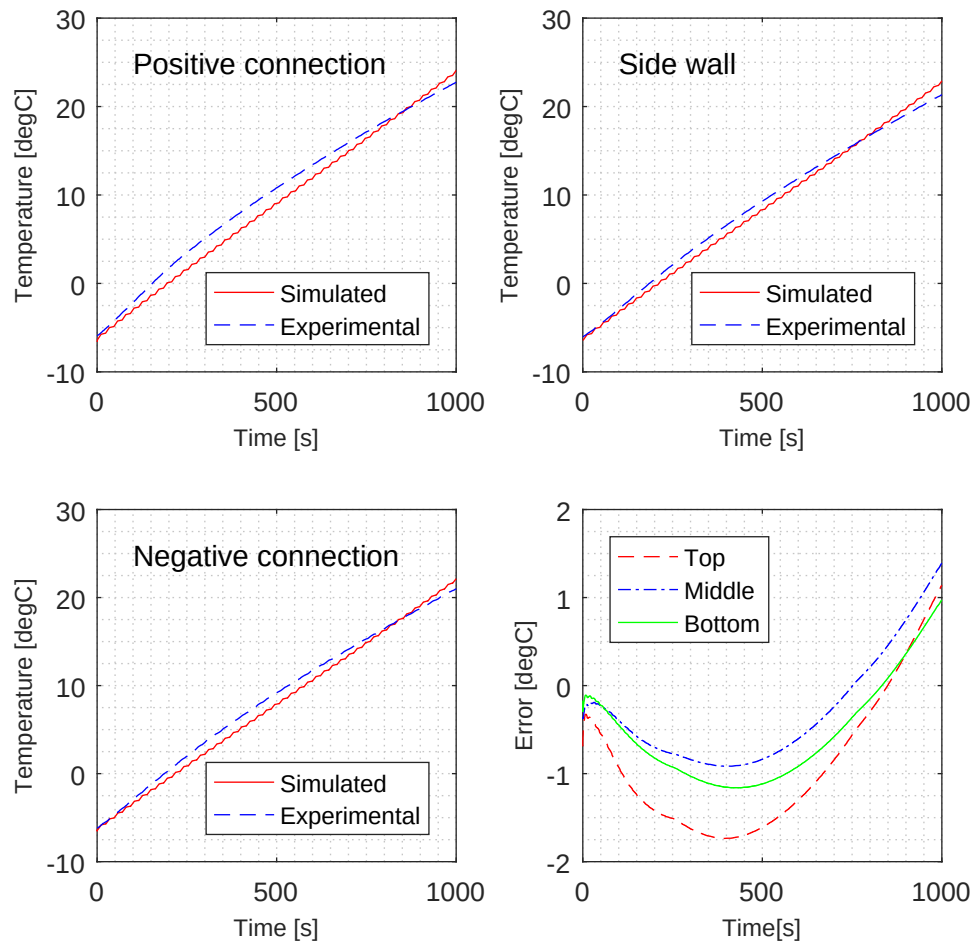


Figure 5.12: Temperature profile at -10°C ambient temperature.

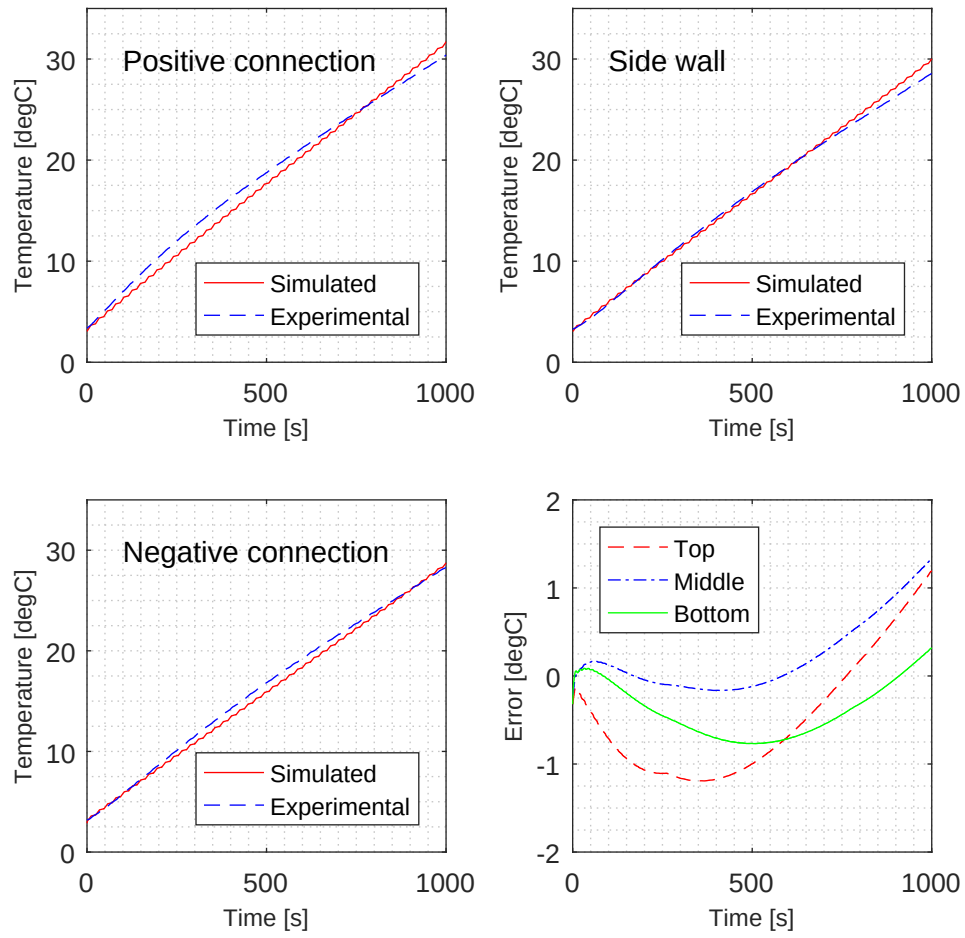


Figure 5.13: Temperature profile at 0°C ambient temperature.

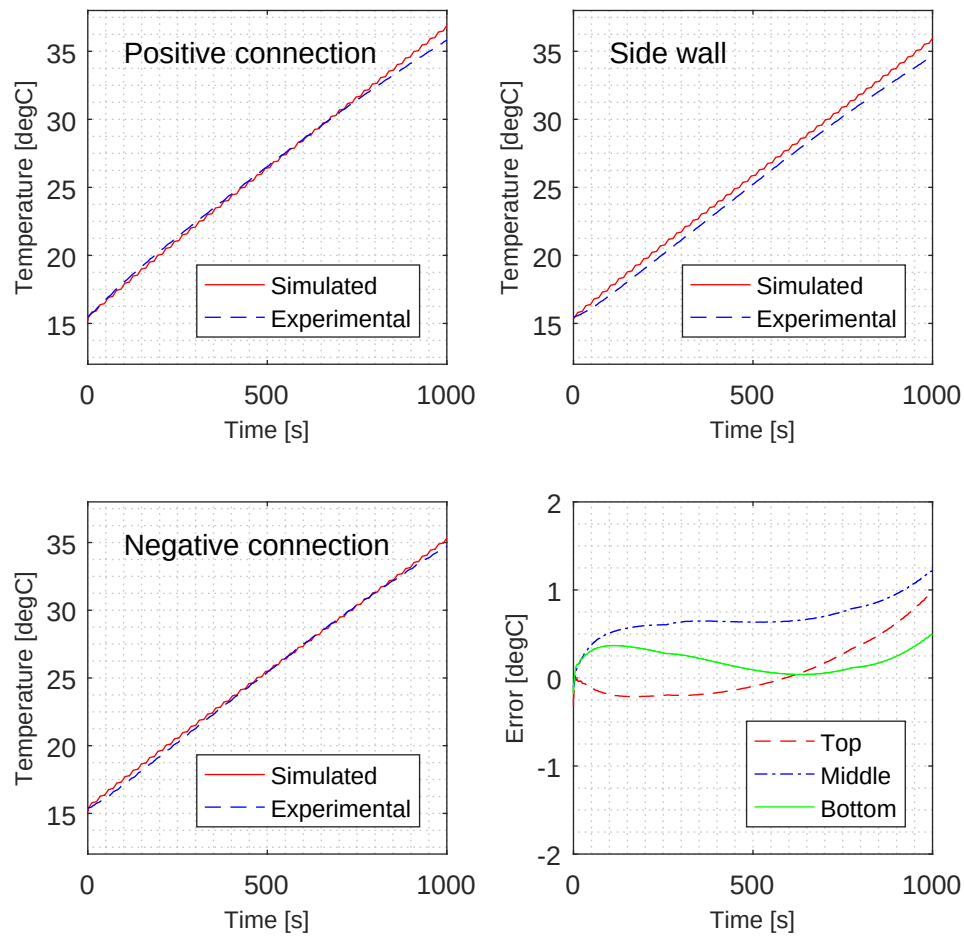


Figure 5.14: Temperature profile at 12°C ambient temperature.

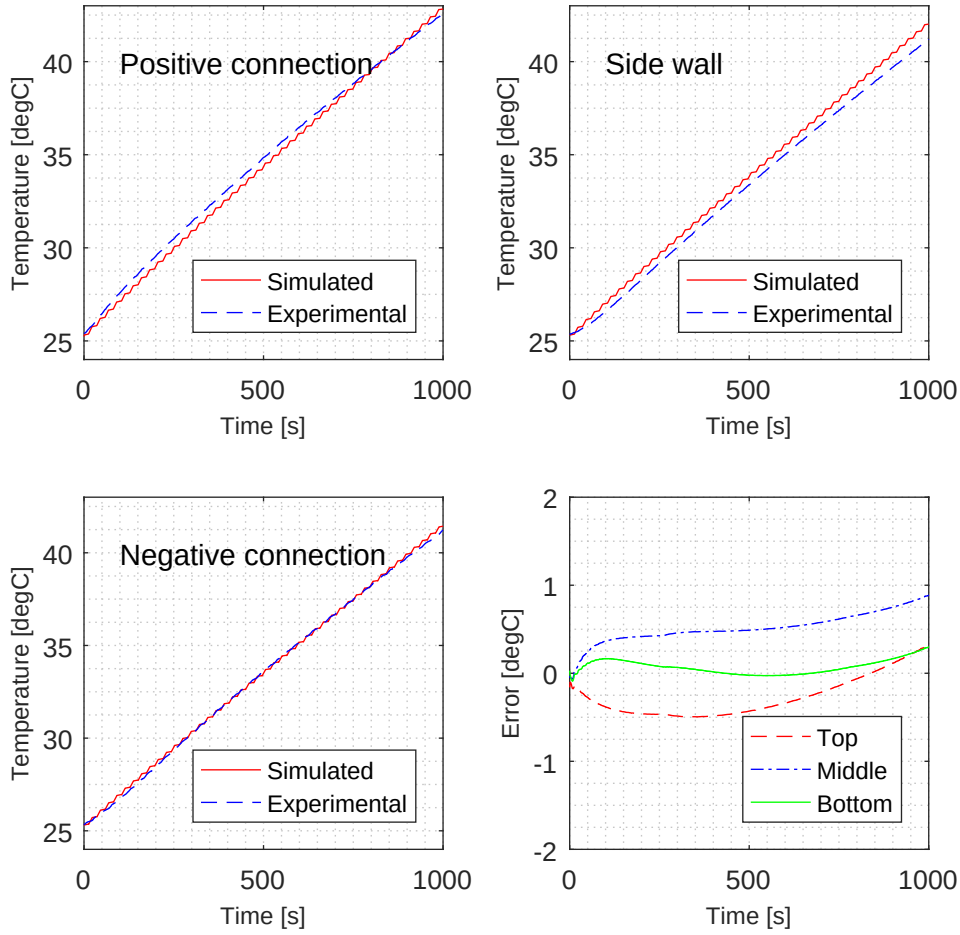


Figure 5.15: Temperature profile at 25°C ambient temperature.

The temperature increase after the experiments is high, especially at lower temperatures, as it is evident in Figure 5.12. Although such a result may seem counter-intuitive, since the difference in thermal potential is much higher, it is to be observed that the mass to surface ratio of the cells is very high, in addition the cell is covered with insulating material, in order to ensure a known thermal boundary. In addition, the insulating material was manually attached to the external walls of the cell, with a contact pressure that would still enable the gas release valve to correctly operate in case of cell failure. Clear access to the gas release valve is always a priority in the case of cylindrical cells. The error increases with the increase of the temperature range of the gradient between initial

averaged cell temperature and final averaged cell temperature. Such result is expected and it is the main drawback of linearising the thermal properties. The linear approximation does not capture the curvature of the properties in a large temperature range, this affecting temperature estimate and then resistance variation estimate and ultimately heat rejection. Heat rejection then is going to affect the temperature estimate at the following instant in time and the error is going to increase at each step. This happens especially in the neighbourhood of 0°C, where the maximum error is reached. However, within the considered temperature range, the error remains within tolerable limits, i.e. it is comparable with the uncertainty of the thermocouples. The model is therefore fit for an automotive use.

5.3.8.1 Discussion

It appears clear that most of the discrepancies are due to the uncertainties in modelling the cell boundaries. Boundaries are a key aspect in the model, in all domains. The model proves effective in reproducing the boundaries, however, it needs to be outlined that detailed information on the boundaries is still needed. Although the strategy allows some coarser discretisation of boundaries, with respect of traditional finite element models, without compromising results. Modelling and simulating the potting/supporting material is not a secondary issue. The materials used in the construction of a battery module are a bottleneck in thermal management that can be overcome either by over-sizing the battery, and therefore adding weight to the vehicle or by relying on direct cooling that would therefore require either a supply of cooled and dried air to the module or the use of a dielectric oil. Such options are not always feasible, especially in small vehicles, in which cost and weight are severe limitations to thermal management systems.

5.3.9 First case: WLTC duty cycle

On the first duty case, the behaviour of a battery cell within an oversized module was examined, under a at Worldwide Light-Vehicle Test Cycle (WLTC) 3rd class duty cycle, on a road with a 0% slope, at ambient temperatures of 0°C, 15°C and 25°C. The current profile per cell was calculated on the specifications of vehicle equipped with a battery pack described in Table 5.9 and without any cooling system or battery thermal management in general. The powertrain considered in the duty cycle calculation is presented in Table 5.10 and its power request is represented in Figure 5.16. The single-cell current profile obtained from such battery layout and power request is shown in Figure 5.17. Figure 5.18 compares experimentally measured voltage with simulated voltage at 15°C, errors is within the confidence interval of the multimeter integrated in the power supply and can be considered due to the uncertainties in the connection resistance estimation.

Cells capacity	5000 <i>mAh</i>
Cell nominal voltage when fully charged	4.25 <i>V</i>
Number of cells in parallel in a module	8
Number of cells in series in a module	12
Number of modules in series in a pack	8
Number of modules in parallel in a pack	3

Table 5.9: Battery layout in a WLTC 3rd class duty cycle.

Maximum torque	300 <i>Nm @ 1500 rpm</i>
Minimum efficiency	85% @ 1500 <i>rpm</i>
Maximum efficiency	97.3% @ 3000 <i>rpm</i>
Peak power	150 <i>kW @ 700 V</i>

Table 5.10: Arrival vehicle motor specifications [211].

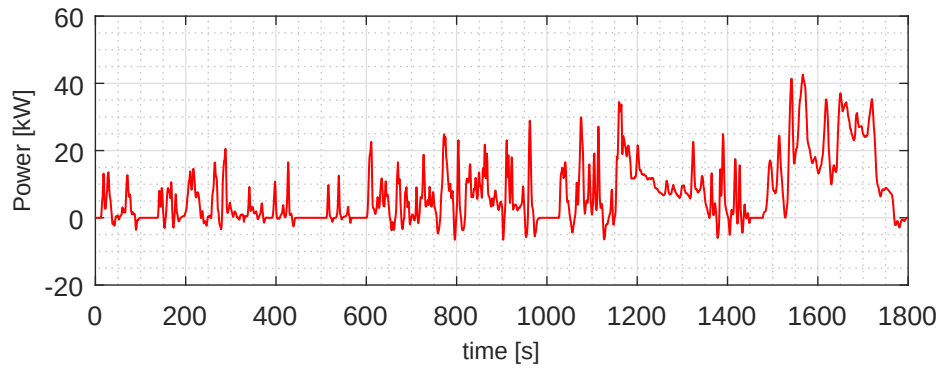


Figure 5.16: Resisting power profile in Case 1.

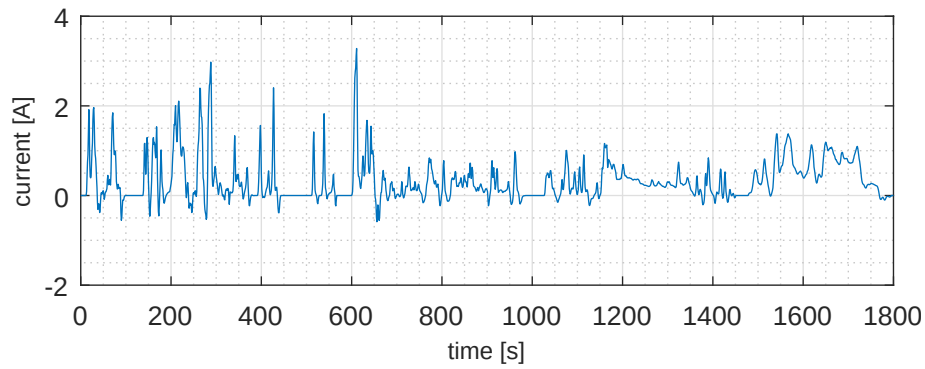
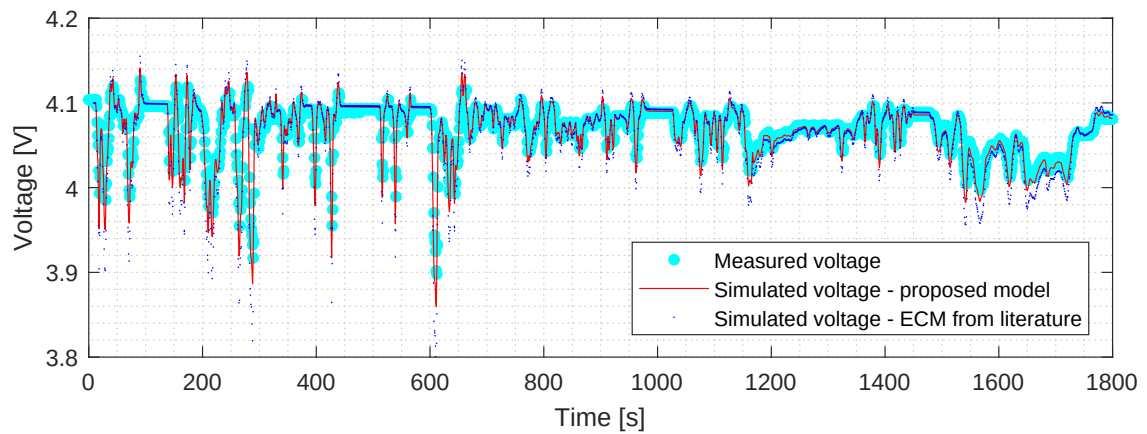
Figure 5.17: Current profile on a single cell on a WLTC 3rd class drive cycle.

Figure 5.18: Measured cell voltage versus simulated voltage, proposed model is compared with the Thévenin equivalent model proposed by other authors [212].

Figure 5.19 represents the temperature profile on the external wall of the cell in three different spots on the external walls at 0°C, while Figure 5.20 represents the same samplings at an ambient temperature of 15°C and Figure 5.21 the samplings at 25°C. Simulation and samplings were compared with the results from an ECM available in literature [212]. The temperature profiles show that the proposed strategy does not tend to diverge when temperature increases as the model from previous research.

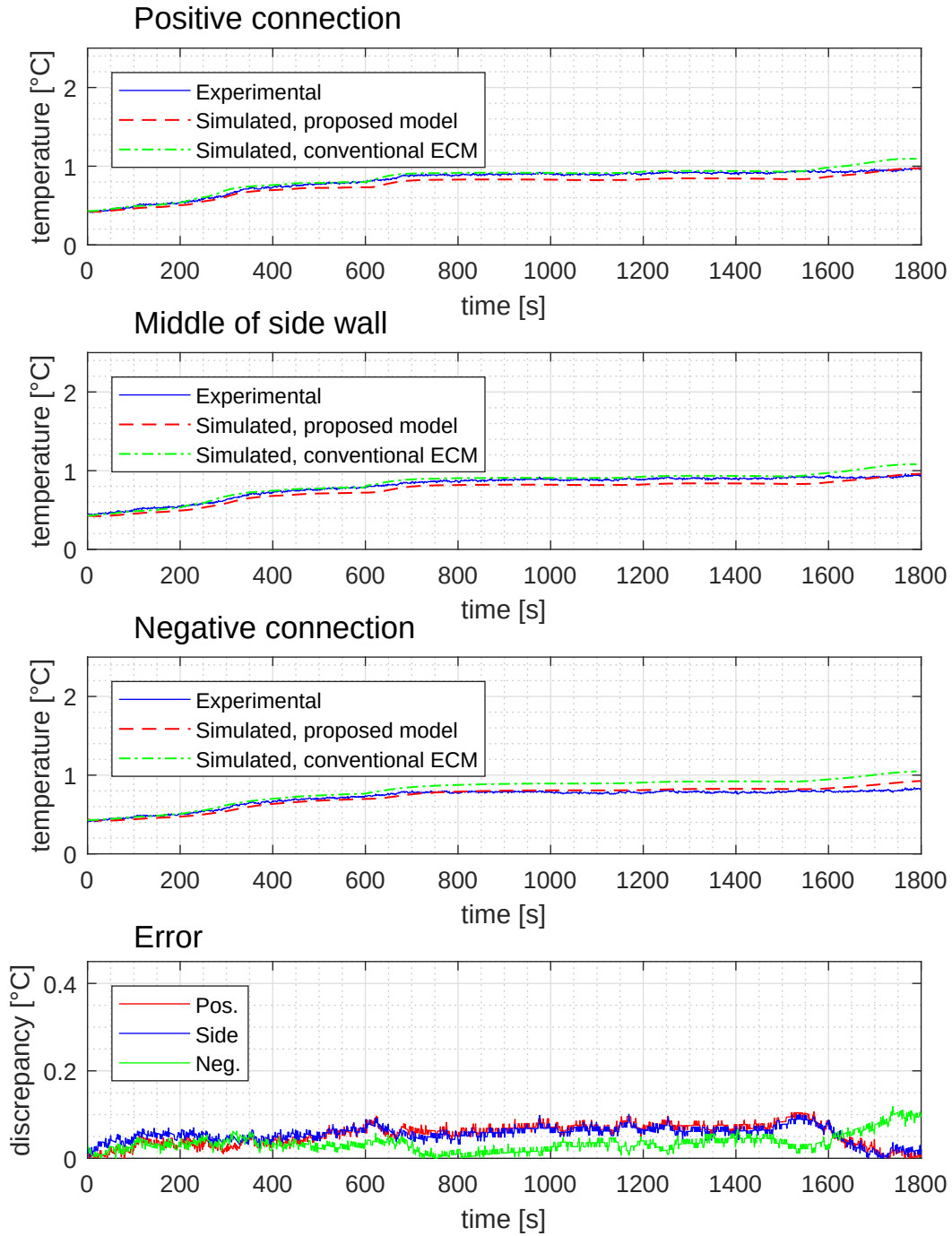


Figure 5.19: Temperature profile in different regions of the battery cell, at an ambient temperature of 0°C, WLTC duty.

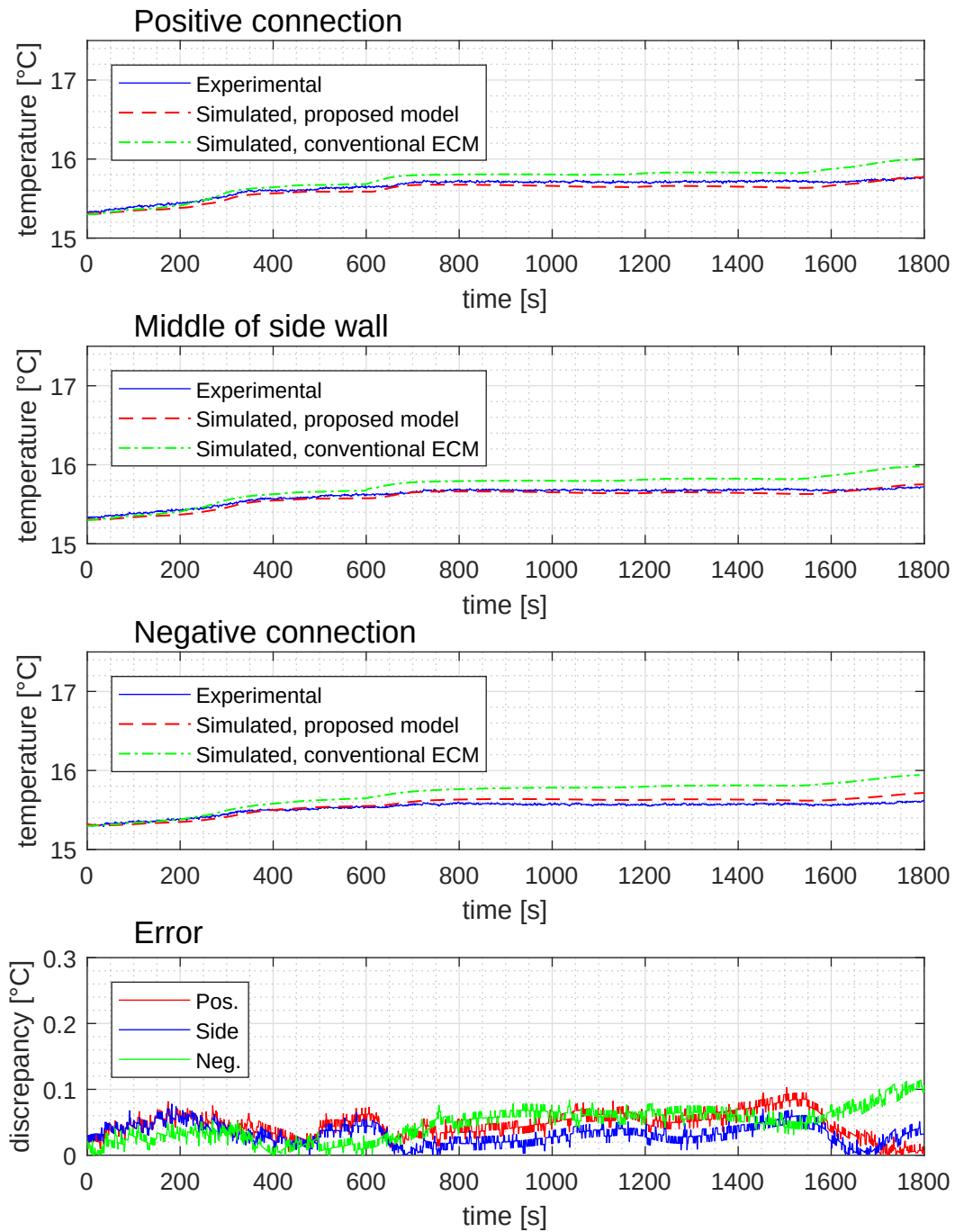


Figure 5.20: Temperature profile in different regions of the battery cel, at anambient temperature of 15°C, WLTC duty.

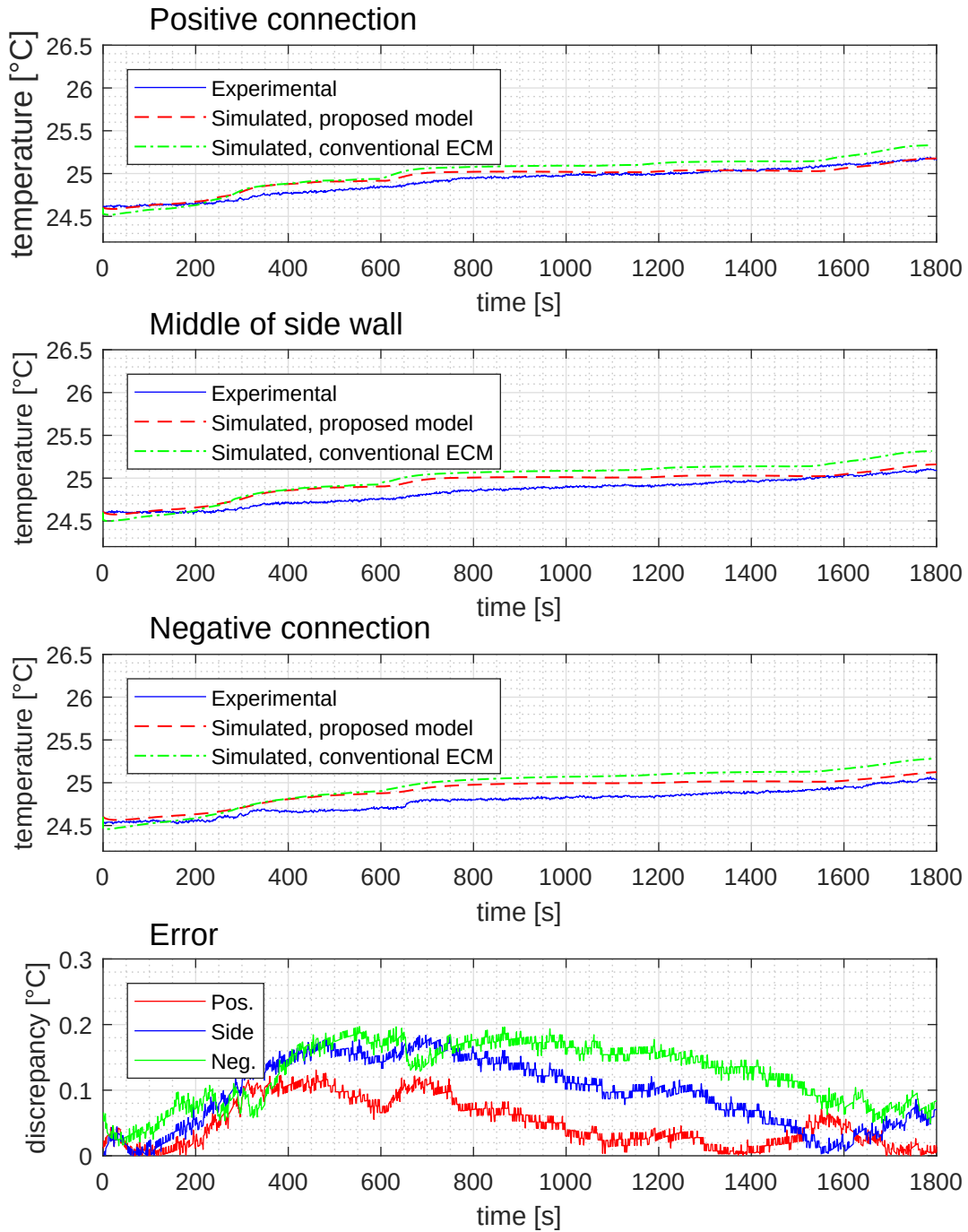


Figure 5.21: Temperature profile in different regions of the battery cell, at an ambient temperature of 25°C, WLTC duty.

The y-axis scale has been sized in order to allow the reader to magnify the difference between simulated and measured temperature. Such discrepancies always remain below

0.3°C, being even smaller than 0.2°C at an ambient temperature of 25°C, which means within the accuracy range of the thermocouples [213]. The discrepancy always lays in the confidence interval of the thermocouples. As expected, since most of the duty cycle consists of discharge, the positive connection is the hottest spot. The negative connection on the bottom effectively reduces collector resistance. Results provide detailed information about the temperature profile in different parts of the battery cell. In this battery configuration, current never exceeds a discharge rate of 0.5C with an increase of temperature of almost 0.5°C over a time of 1800 s. It is possible to observe an overshoot at the end of the duty cycle, when the current is subject to the last sudden increase. In general the profile appears to underestimate the temperature increase at lower ambient temperatures and overestimate it at higher ambient temperatures. In addition, the model tends to smooth fluctuations.

5.3.9.1 Discussion

Results show that oversizing a battery is an effective way of reducing thermal stress. The model allows a cell-by-cell investigation within a module model as it will be explained below. An oversized pack can result in cells being charged/discharged at a lower rate. By doing so, it is possible to drastically reduce ohmic heat, since the current's absolute value is lower and since it is possible to work at the minimum value of resistance. However, such an option would result in large and heavy battery packs. The combination of accuracy and computational lightness of the model allows a more precise sizing and can help in preventing exaggerated oversizing. A way of limiting oversizing while keeping some of its advantages could be implementing packs capable of varying the connections between each two modules in such a way that it would be possible to reconfigure them varying maximum voltage and capacity. A second conclusion that can be drawn is that the

model accuracy decreases with temperature. Such a result is expected and in line with the outcome of the validation cycle and confirms the initial conclusion that accuracy is higher in a range of temperatures between -10°C and 40°C . The model is capable of capturing internal temperature gradients and it is also computationally light to operate, but it is not designed to simulate the cell behaviour outside its safety boundaries.

The model predicts the temperature in different regions of the cell with a reduced error and requires a run time of less than 10 *min*, but it is not designed to simulate the cell behaviour outside its safety boundaries.

Such limit, however, is minor, since the purpose of the model is simplifying the battery module and battery thermal management system design procedure.

5.3.10 Duty 2

The second case featured an urban-oriented drive-cycle, based on two low-phase 3rd class WLTC, on a road with a 0% slope, with 5 minutes of 1C-rate charge in between, at an ambient temperature of 25°C .

Such a scenario is a plausible reconstruction of the duty cycle of a taxi. The battery layout for this case is presented in Table 5.11, powertrain data are still those introduced in Table 5.10. As in the previous duty case, the hypothesis of no cooling or thermal management system was taken.

Cells capacity	5000 <i>mAh</i>
Cell nominal voltage when fully charged	4.25 <i>V</i>
Number of cells in parallel in a module	8
Number of cells in series in a module	12
Module capacity	40 <i>Ah</i>
Module specific energy	175.2 <i>Wh · kg⁻¹</i>
Module voltage when fully charged	51 <i>V</i>
Number of modules in series in a pack	4
Number of modules in parallel in a pack	2
Pack capacity	80 <i>Ah</i>
Pack specific energy	156.7 <i>Wh · kg⁻¹</i>
Pack voltage when fully charged	204 <i>V</i>

Table 5.11: Battery layout in duty cycle 2.

Figure 5.22 shows the power profile, from which the single-cell current profile is obtained as it can be seen in Figure 5.23.

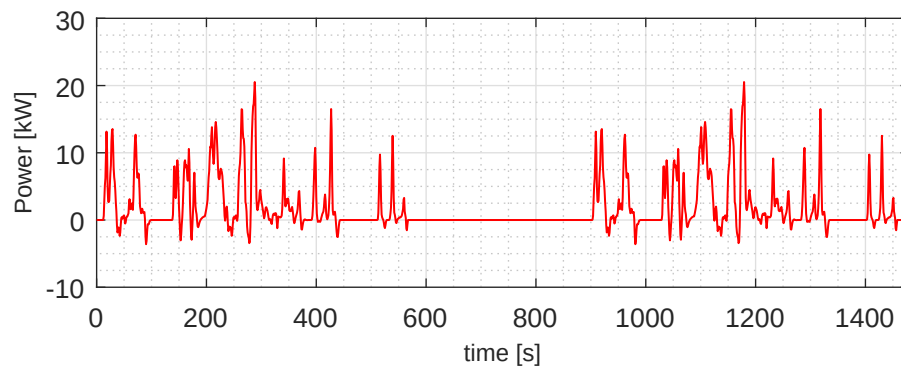


Figure 5.22: Resisting power profile in duty 2.

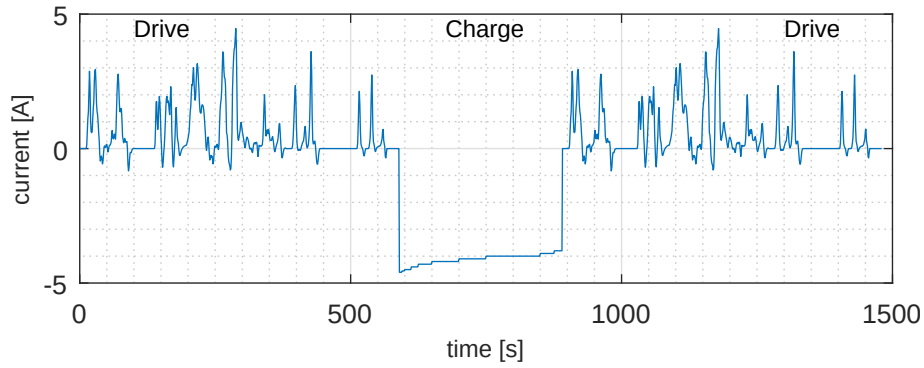


Figure 5.23: Current profile for duty 2.

Comparing simulation outcomes with experiments, the voltage appears to have a good degree of accuracy as in Figure 5.24

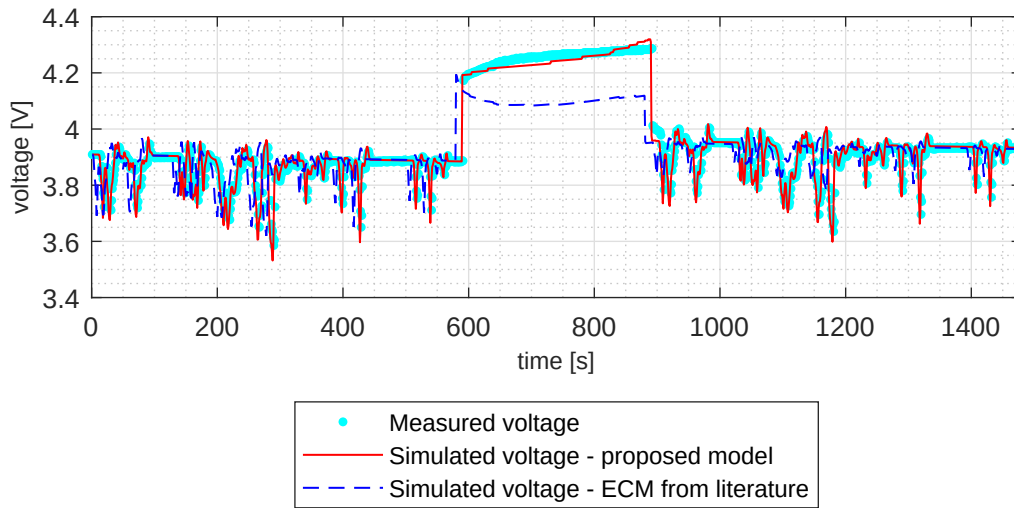


Figure 5.24: Measured cell voltage versus simulated voltage for duty 2, proposed model is compared with the Thévenin equivalent model proposed by other authors [212].

The temperature profiles are shown in Figure 5.25.

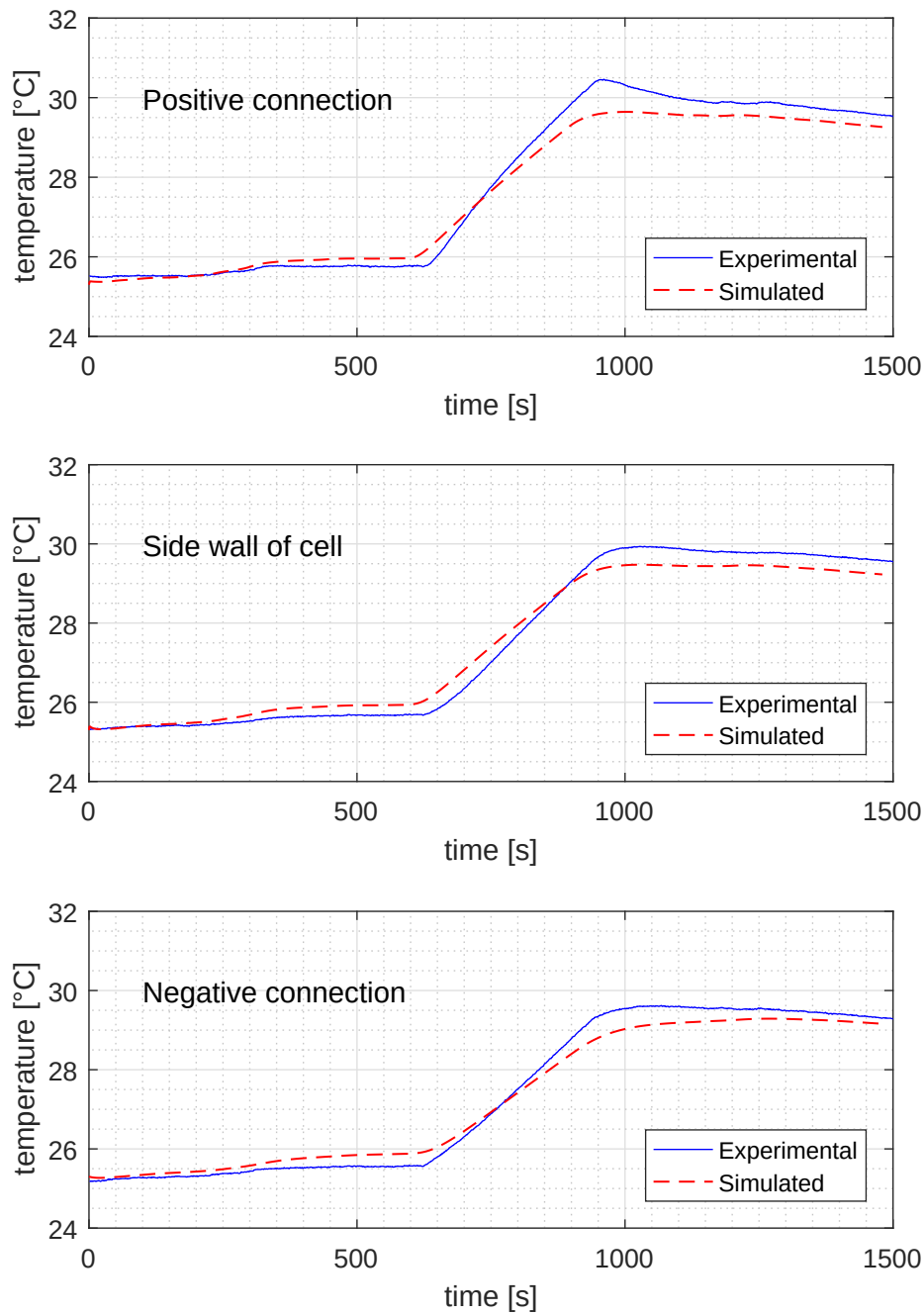


Figure 5.25: Temperature profiles in different regions of the cell, duty 2.

Discrepancies in temperature value still lay in the interval of confidence of the thermocouples. The sudden step increase in heat rejection is well reproduced, although the specific heat and the mass of the cell appear to be slightly overestimated and the model

presents therefore a higher thermal inertia in comparison with the experimental data. The model proves to be resilient to sudden changes in current profile. Results show a greater heat rejection while charging as expected, due to different factors: i) the higher current rate, ii) lower state of charge and higher temperature and therefore higher resistance. The positive connection is still the hottest spot on the cell.

5.3.10.1 Discussion

The proposed modelling strategy, when compared to experimental results appears to be reproducing the behaviour of the battery module during charging at high rate, with an error that is contained within the accuracy interval of the sensors. In addition, it is shown that a combination of urban cycles and fast-charging procedures provides a more realistic scenario for battery validation. Duty 2 outlines the importance of effect of fast charging. The charge rate has a major impact on the heat dissipation and therefore on the final temperature profile.

The main consequence of such finding is that fast-charging needs to be included in battery sizing. The experiments revealed an increase of temperature of almost 4°C throughout the process, mostly concentrated in the 10min of 2C charging, during which is consistent with the 5°C estimate provided by other authors for a similar cell [214]. It is evident that high-rate cycling without applying any cooling strategy would result in exceeding the safety temperature boundaries. Provided that a correct information about the boundaries is supplied, the model allows to examine which section of the cell would be subject to the greatest temperature increase. In such way it is possible to correctly size a thermal management system.

In the case of thermal management systems that rely on a controlled heat transfer mean circulation, the model can be used to spot the instant in time when the cooling system needs to be triggered in order to avoid a sudden increase in cell temperature. Beside the previously mentioned points, the model requires less than a minute to run.

5.3.11 Interim conclusions

The experiments on the single cell prove the model's robustness and adaptability to different boundary conditions and duty cycles. The model appears to be positively reacting to sudden changes in current direction.

The necessity of cooling during fast charge appears urgent. At this stage, a natural step forward, would be scaling up the cell model to a module level. In the next section a new cell geometry is explored and the model is used to generate a full-module model.

5.4 Battery module

The case-study module was a motorcycle battery. The module was charged and discharged at a rate of $2.0C$. The procedure featured a discharge to $95V$, followed by a recharge up to $110V$, setting $94V$ as lower cut-off voltage and $112V$ as upper cut-off voltage, as recommended by the manufacturer. A time of $6s$ was left between each charge and discharge cycle. The charge discharge cycle was repeated in two scenarios: no cooling and fluid circulation in the cold-plate and dual fan cooling.

The benefit of removable liquid-circulation cold-plate heat exchangers in motorbike battery charging is evident. Examining the different cases, it is possible to observe the following: i) the removable cold-plates are an effective mean of keeping the battery in its correct operating temperature range, and ii) such device could be integrated in recharging structures at a low cost. A second case study is the urban section of an Artemis drive cycle, followed by fast-charging (rate of 2.0C) bringing the voltage back to 100V and restoring part of the capacity.

5.4.1 Case study vehicle and powertrain

For testing purposes, we assumed the battery module is installed on a Zero Motorcycles ZF 2.8. The vehicle data are summarised in Table 5.12.

Vehicle data	
Mass	131 <i>kg</i>
Front section area	~0.7 <i>m</i> ²
Drag coefficient	0.65
Front wheel $\varnothing$	21 <i>in</i>
Rear wheel $\varnothing$	18 <i>in</i>
Final drive	3.33

Table 5.12: Specifications of the vehicle.

The powertrain specifications are summarised in Table 5.13.

Powertrain data			
Peak power	48	kW	600A supply
	29	kW	350A supply
Battery supply	100	V_{DC}	nominal
Continuous power	13	kW	
Peak current	600	A	
Continuous current	157	A	
Continuous torque	32	Nm	
Maximum torque	120	Nm	
Maximum speed	8000	rpm	

Table 5.13: Motorcycle powertrain data [215].

5.4.2 Battery specifications

The module specifications are summarised in Table 5.14. The module is assembled from 28 25Ah NMC pouch cell by Farasis, connected in series, through copper bus-bars. The whole block is then moulded into a block of thermally-conductive potting epoxy resin. Such module is then enclosed in an aluminium box with two copper screw terminals, surrounded by insulating polymer material enclosures. The structure was reconstructed by disassembling a module. Dimensions of the battery are summarised in Table 5.15.

Cell data	
Cell mass	0.485 <i>kg</i>
Cell capacity	25 <i>Ah</i>
Cell nominal voltage	3.65 <i>V</i>
Cell maximum voltage	4.15 <i>V</i>
Cell cut-off voltage	3.00 <i>V</i>
Cell specific energy	185 <i>Wh/kg</i>
Cells in parallel	1
Cells in series	28
Module data	
Mass	14.52 <i>kg</i>
Module capacity	25 <i>Ah</i>
Module nominal voltage	102 <i>V</i>
Module maximum voltage	116 <i>V</i>
Module cut-off voltage	84 <i>V</i>
Module specific energy	175 <i>Wh/kg</i>

Table 5.14: Battery module specifications [200].

Battery general dimensions	
Width	200 <i>mm</i>
Height	163 <i>mm</i>
Length	245 <i>mm</i>
Bus bars	
Thickness	3 <i>mm</i>
Width	14 <i>mm</i>
Aluminium cover	
Thickness	2 <i>mm</i>
Potting material	
Thickness	2 <i>mm</i>

Table 5.15: Size of the battery module.

5.4.3 Module discretisation and modelling

The battery was discretised by dividing it in longitudinal sections as presented in Figure 5.26, with the detail of a section outlined in Figure 5.27. Each section featured the pouch cell, the potting material, the Aluminium casing and an insulating rubber mat, the latter

on one side only. The sections were then joined in a loop in the Modelica code. By doing so the single cell model was scaled up to a whole module. The main advantage of such procedure is the reduction in computational cost. The outcome is a model that runs on a single solver, avoiding synchronisation issues and that can simulate a 28-cell layout, on a duty cycle of approximately $2h$ of duration in $2h$ simulation time. As quoted in Chapter 3, similar models, featuring smaller packs require up to $14h$ to run [190]. The boundaries were also modelled, including the heat exchanger and the surrounding enclosure box, as presented in Chapter 3.

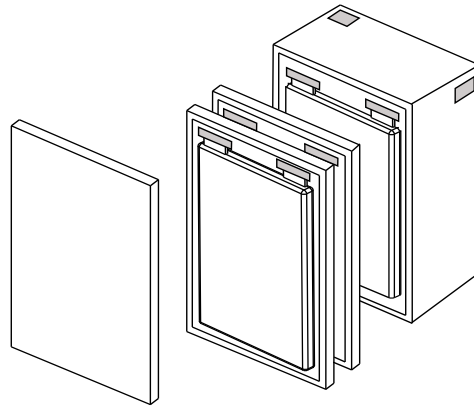


Figure 5.26: Module discretisation technique.

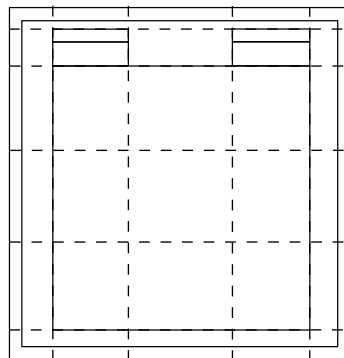


Figure 5.27: Discretising strategy applied to a section of the module.

5.4.4 Constant current discharging and charging

Constant current charge and discharge cycles were applied to the cell. This test allows evaluating performance under a highly stressful scenario for the module. The main outcome is analysing the thermal behaviour of the module under sudden current direction changes, especially at high rate. Each cycle was first performed without cooling and then with circulation of water-based coolant in a removable cold-plate heat exchanger attached underneath the battery. The aim of the tests was to evaluate the performance of the scaled-up model. The idea was to investigate the use of removable cold-plate heat exchangers on electric motorcycle batteries, since such case has a broad spectrum of applications and can be much beneficial over the next few decades. The battery was therefore tested with an operating indirect cooling system and without it. The specifications of the cooling system are summarised in Chapter 4, with further details in Table 5.16. Being the cooling system a removable cold-plate, no gluing material is used.

Coolant composition	25%	Ethylene glycol
	75%	De-ionised water
Flow rate	5 ± 0.85	l/min
Battery exchanging surface	0.04	m^2

Table 5.16: Properties of single-module cooling system.

Charge-discharge tests were conducted at a rate of 2, equivalent to 50A. Such current is representative of fast charge and aggressive discharge. The graphs in Figure 5.28 show that the experiments were conducted from the same starting voltage, in order to ensure repeatability of experiments and obtain results that could be compared with each other. Room temperature was regulated at 21°C. The temperature profiles are shown in Figures 5.29 and 5.30, overlapping the temperature sampling to the simulated temperature in both scenarios. Uncertainty is represented by a grey area around the sampling. The error

is represented in Figure 5.32. Figure 5.31, on the other hand, comparing the depleted capacity with the temperature increase at each time-step and representing the discrepancy of the estimated temperature increase with respect to the experimentally measured value.

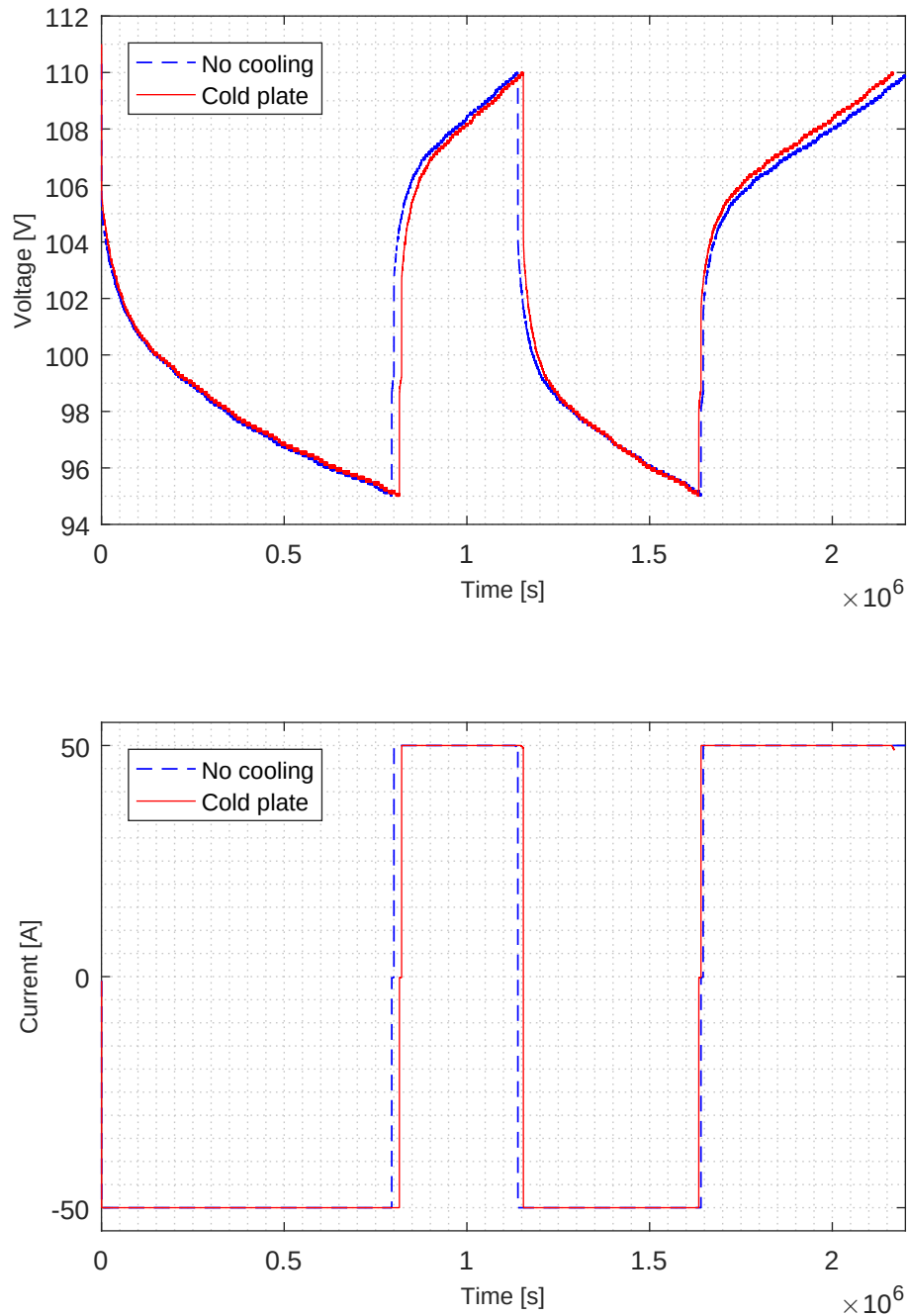


Figure 5.28: Measurements of voltage and current on the battery module during 2.0C charge-discharge duty cycle.

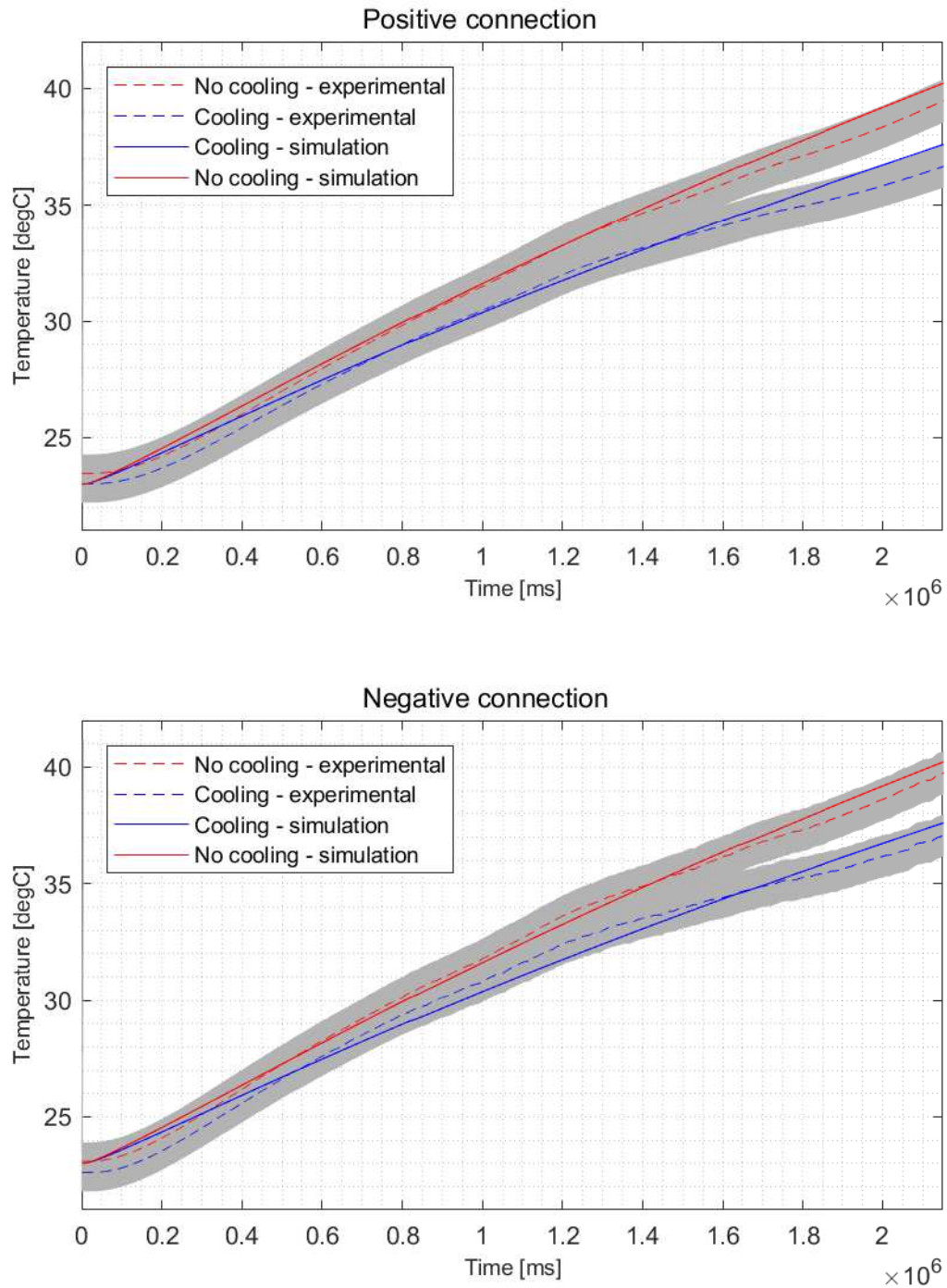


Figure 5.29: Temperature sampling versus simulated temperature near the positive and the negative connections of the battery, the grey area represents the interval of uncertainty.

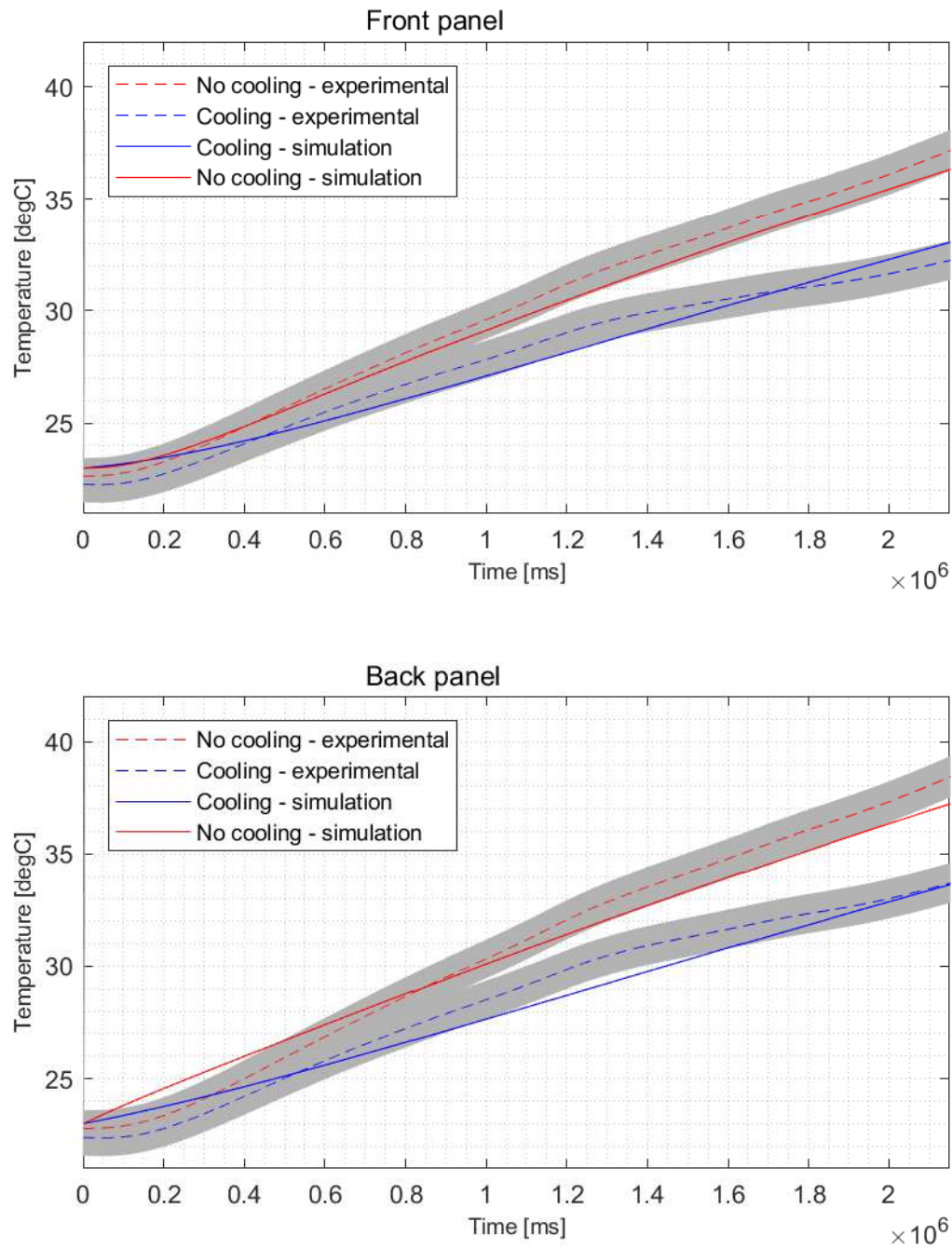


Figure 5.30: Temperature sampling versus simulated temperature on the front and back panels of the battery, the grey area represents the interval of uncertainty.

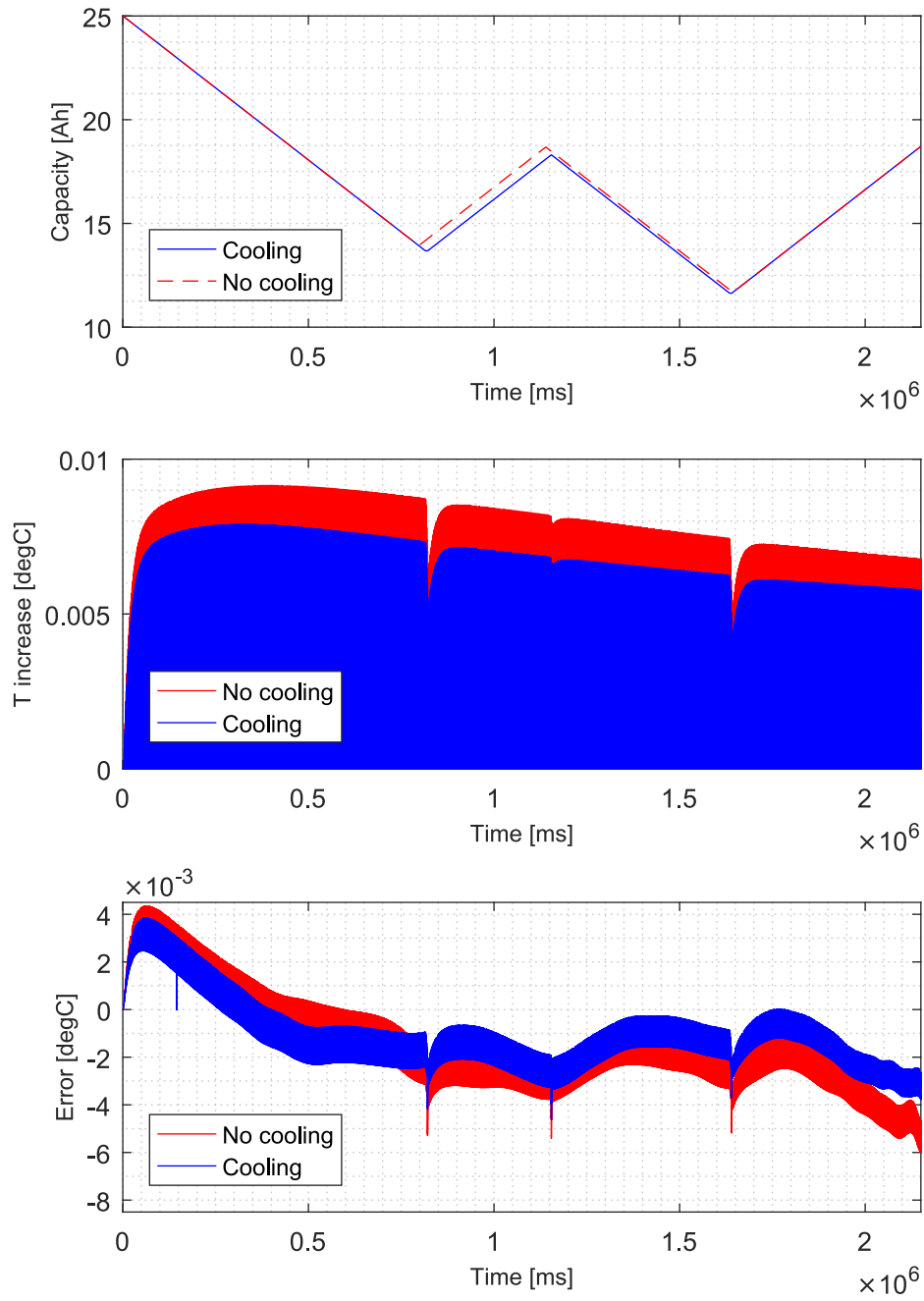


Figure 5.31: Capacity drop throughout the cycle (top), temperature increase at each time step (middle) and error in temperature estimation with respect to experiments, compared with capacity drop, for the positive connection (bottom).

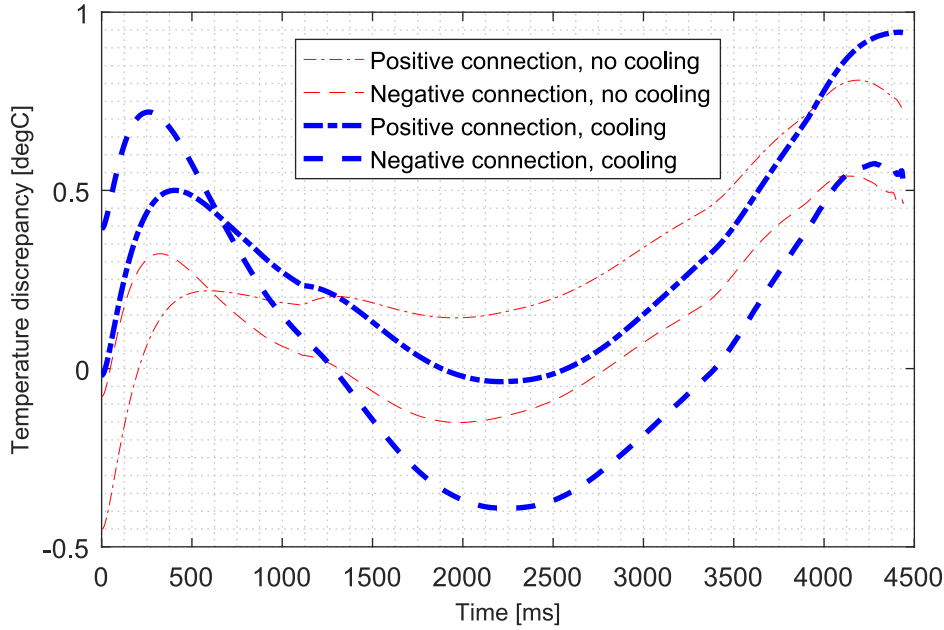


Figure 5.32: Discrepancy between simulated and experimental temperature on positive and negative connections.

5.4.4.1 Results and discussion

The addition of the cooling plate significantly stabilised the temperature, especially in the long term. In the initial stage of the experiment the difference between the two cases still lies within the interval of confidence. The trend, however is already evident and, after 100ms, it is evident that the cold plate provides a major benefit by containing the temperature during high-current-rate cycling. The established model accurately reproduces the variations of temperature. It is however remarkable that sudden temperature variations are smoothed, resulting in a more regular temperature curve, in comparison with measured values. Discrepancies still lay in the confidence interval of the test-rig sensors. However, it is important to notice that the error reaches its maximum shortly before the end of the simulation, and then stabilises. Despite still being within the confidence interval, the difference between measured and simulated values, in the case of the module model, appears greater than in the case of the single-cell model. Such outcome is expected when

scaling up models. The overall behaviour of the error is similar to that found in the single cell case. The model provides therefore a reliable representation of the thermal behaviour of the battery. The initial overshoot and the general behaviour of the curve are due to errors in the estimation of the mass percentage of the different materials and they reproduce, on a larger scale the behaviour of the single cell model. The error is greater on the back panel of the battery module. This is possibly due to an underestimation of the effect of the proximity of the connections, more specifically to an overestimation of the heat transfer resistance of the insulating material surrounding the connections. The model however predicts well the difference in behaviour between the simple layout and the one integrating a cold-plate heat exchanger. As mentioned, in early stages of the experiment, the effect of the cold plate is not pronounced. There is however a clear indication that this methodology of cooling contributes in maintaining the battery module within its safety temperature range, particularly when dealing with high-current-rate cycling. Removable cold-plate heat exchangers can therefore be a feasible application, allowing fast charging of electric motorcycles or any other vehicle without on-board BTMS and with exposed battery enclosures. From Figure 5.32, it is possible to observe that the battery, when cycled without operating the cooling system, is subject to a much higher temperature increase than when cycling it with a cooling system. This means that, without running a cooling system, the battery sees a greater increase of the temperature over the same interval of time, which ultimately means more thermal stress is posed on cells, potting material and enclosure. Another observation that can be made is that the increase of temperature is greater at the beginning of the cycle, then it tends to drop, this is a reasonable result for the materials involved and outlines the necessity of triggering the cooling system from the very beginning of cycling when operating at high current rates.

The model proves to accurately capture the behaviour of the module. Despite not

reproducing very small temperature oscillations, the trend is accurately reproduced and matches the experimental outcome within the confidence level of the sensors used. The battery is subject to greater heat rejection during charging. The removable cold plate heat exchanger enhances heat exchange but requires additional power. The battery is kept in its safe operating temperature range, with an additional power consumption of approximately 300 W. Such a power request is acceptable in fast charging operations. At a rate of 2, charging the battery from 20% to 80% requires approximately 25 min, the energy required by the cooling would therefore be equal to 450 kJ, while the battery would be charged with 3.975 MJ. With an 11.3% energy consumption increase, it is therefore possible to contain the temperature increase during fast charge operations. It would be possible to integrate such systems in recharging stations at a low cost and the resulting system would be quite similar to the test-rig layout. The increase in energy consumption at the charging station would be justified by preventing the battery from reaching temperatures that would undermine it functioning correctly, eventually resulting in permanent damage. Beside this, we can observe that, even without an optimal heat-transfer interface and with only 16.4% of the battery surface in contact with the cold-plate, the effect of indirect liquid cooling is relevant and can prevent the battery from exceeding the safety temperature limits at high rates. The model appears to be capable of capturing the difference. It is therefore possible to use it to determine the effect of different cooling strategies with the model. This marks a breakthrough in reducing computational expense of multi-domain battery-module models. The novelty of this work lies in the re-scalability of the model and in exploiting acausal, object-oriented modelling to implement a module model that runs on a single solver, without using a different solver for each domain, removing therefore the problem of synchronising different solvers. Representing ECMs and IHTMs of each single cell as arrays of modelling objects describing the physical behaviour of each cell and the interaction between each two cells allows the user to implement different

module models from the same cell components by only varying the size of the arrays. All these features result in a lean and re-configurable modelling library that were previously missing from the literary landscape. It is possible to observe that the model is capable of capturing the temperature difference between the cooled and the non-cooled layout on a long time-scale, which allows outlining the benefits of cooling during prolonged high-rate charge/discharge cycles.

5.4.5 Artemis and fast charging

This case was chosen to provide a duty cycle that reproduces the behaviour of small-sized motorcycles in an urban scenario, where they travel for short distances and are charged at high rates for short periods of time. The duty includes an Artemis drive cycle followed by a re-charge duty at 2C, restoring 2Ah of capacity. The battery was cooled at a rate of $5 \pm 0.85 \text{ l/min}$.

Figures 5.34 and 5.35 represents the temperature profiles, while Figure 5.33 represents the error where it appears to be larger: on the positive and negative connections. In this case too, capacity drop is compared with the increase of temperature at each time step, also providing account of the error in temperature increase estimation, as it can be seen in Figures 5.36.

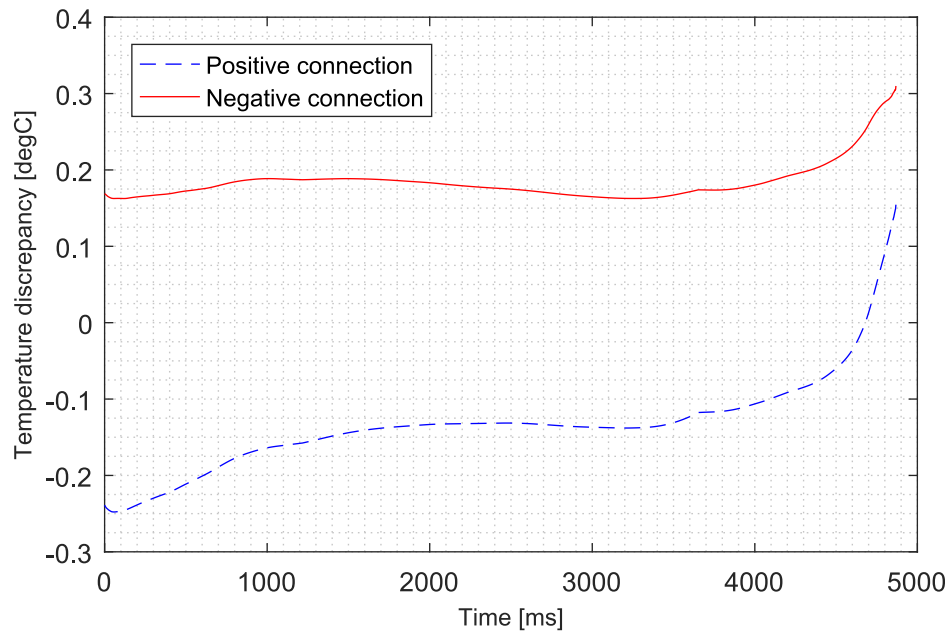


Figure 5.33: Error in temperature estimation on the positive and negative connection.

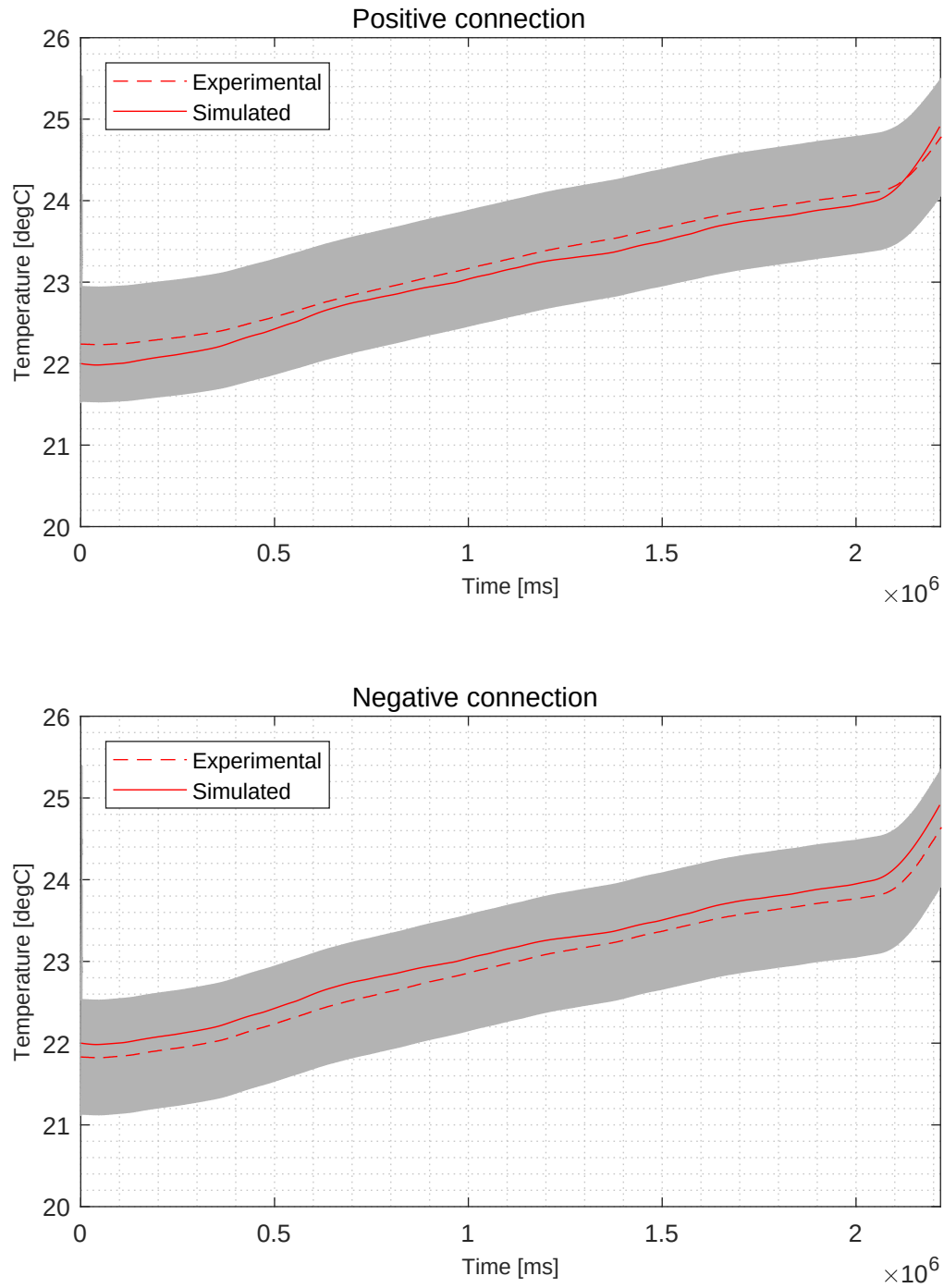


Figure 5.34: Artemis urban and fast charging, temperature on positive and negative connection.

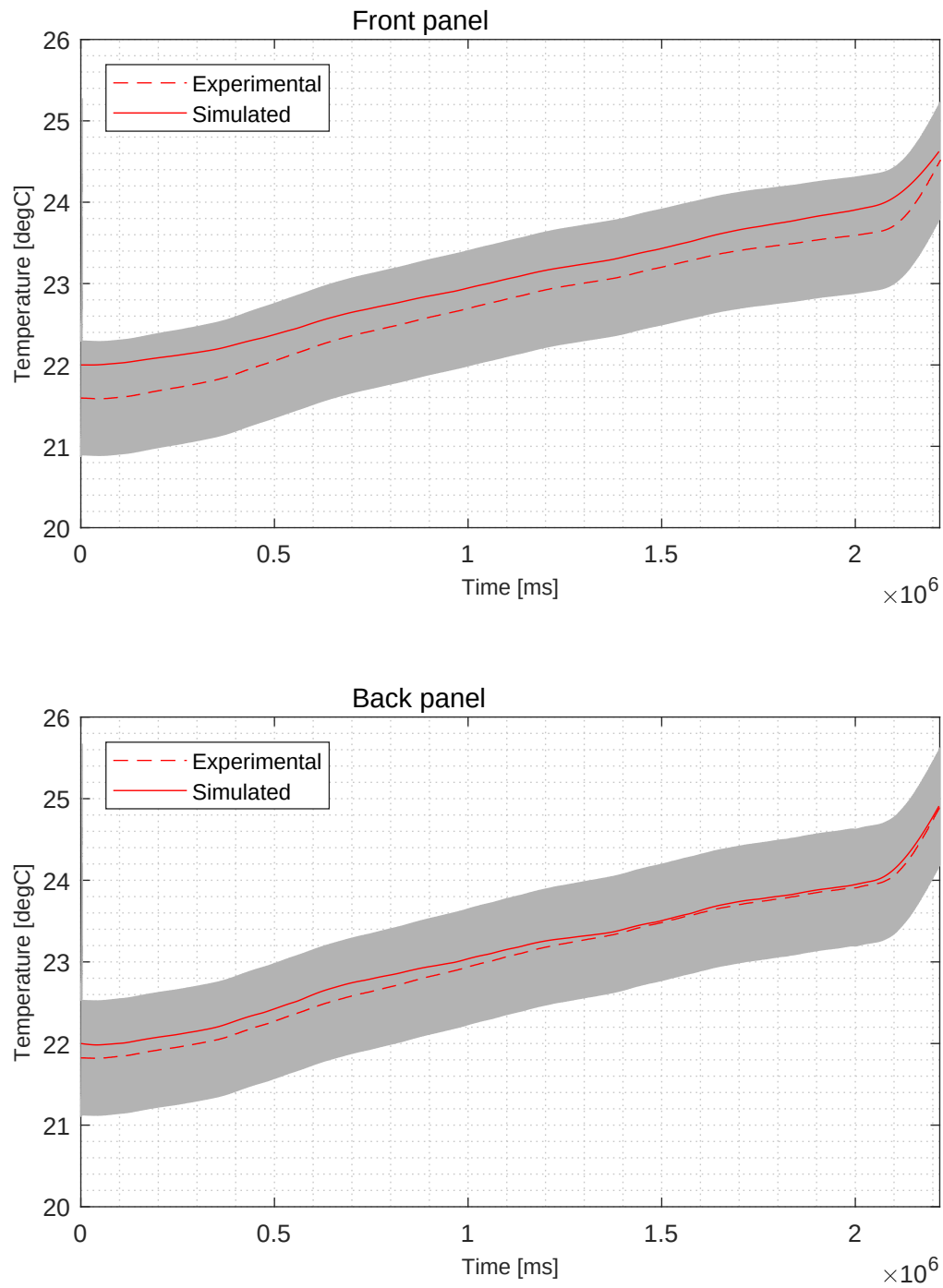


Figure 5.35: Artemis urban and fast charging, temperature on front and back panels.

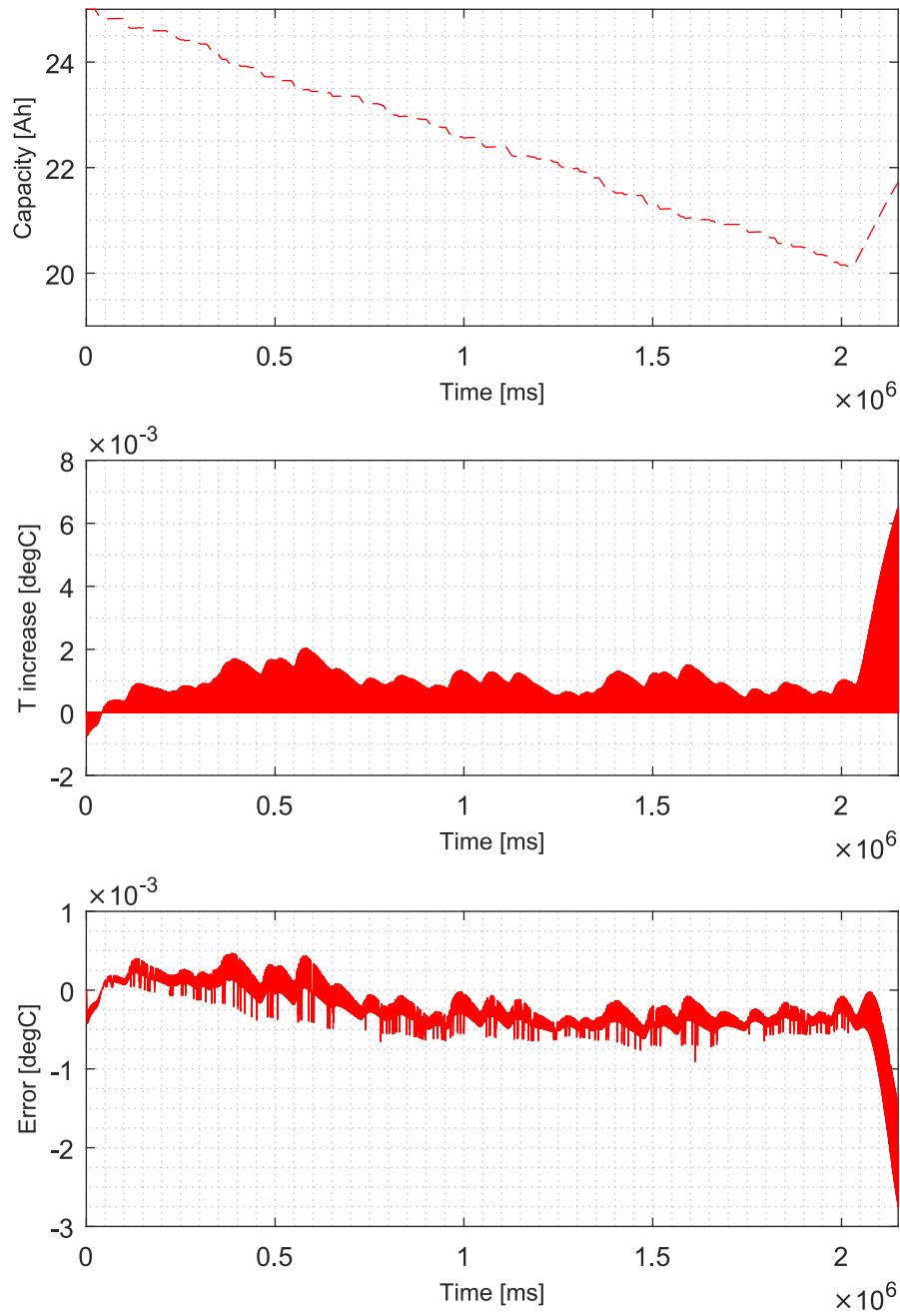


Figure 5.36: Temperature increase from one time-step to the following one and error with respect to experiments, compared with capacity drop.

5.4.5.1 Repeatability of experiments

The tests were run multiple times and the initial temperature and the voltage were observed. It is possible to observe in Figure 5.38 that the voltage sampling is subject to variations equivalent to 2.2% of the voltage range, similar, or even lower than the discrepancies found in literature [216, 128]. The temperature sampling shows a contained dispersion and the variance falls within the uncertainty range of the temperature sensors as per Figure 5.37.

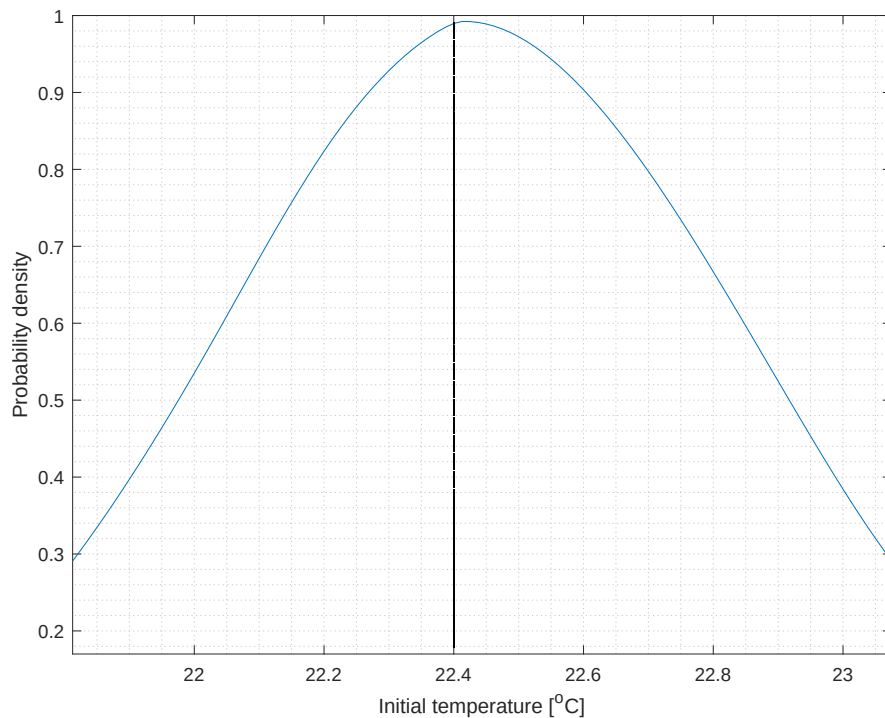


Figure 5.37: Range of initial temperatures throughout the experiment runs and their probability distribution.

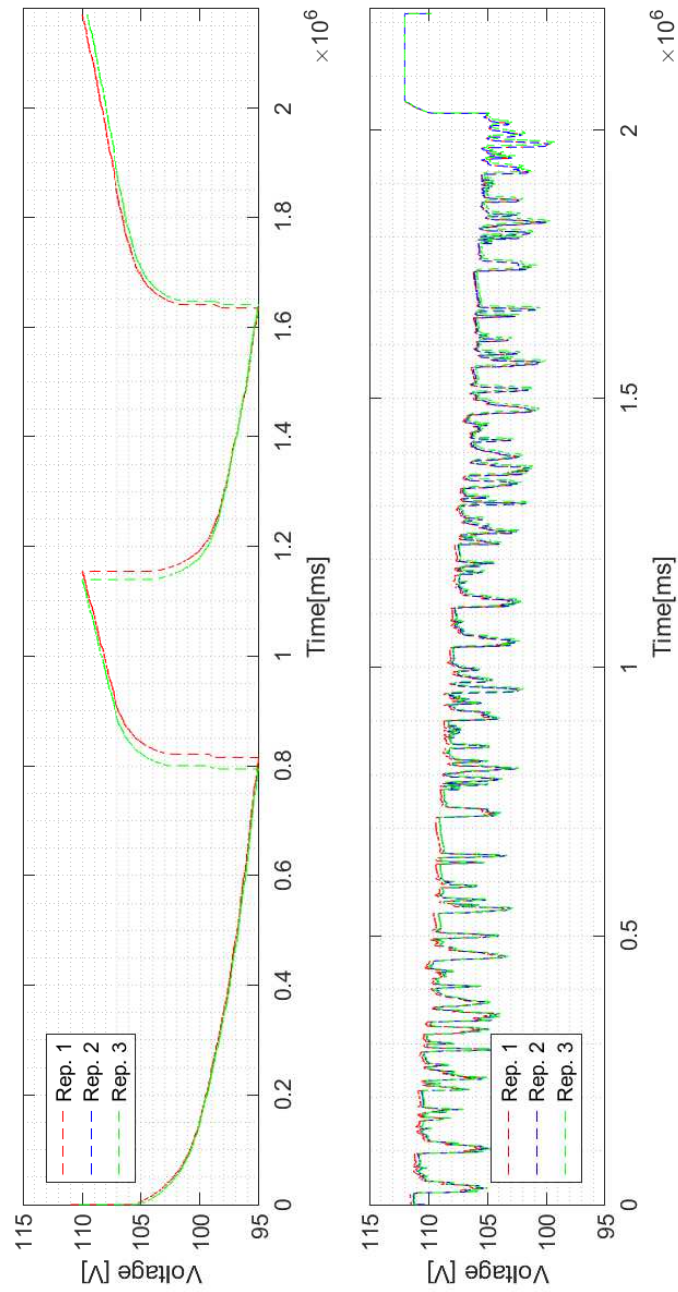


Figure 5.38: Voltage profile in different experiment runs for the two different duties.

5.4.5.2 Results and discussion

The model reproduces accurately the temperature profile. The error is smaller than in the constant current experiment. The reason for that is the lower current rate. The error, as per Figure 5.33, remains within the confidence interval of the measurement, allowing therefore a reliable estimation of the temperature profile. It needs to be noted, however, that homologation drive-cycles appear not to be ideal in terms of thermal analysis. In fact, the battery seems not to be subject to major temperature increase during this duty cycle. As it can be noticed in Figure 5.36, there is a correlation between the current rate and the temperature increase, mostly due to the high contribution of ohmic heat. Despite the absolute error being much higher at high rates, it is possible to also outline that fast charge causes a much higher temperature increase. In addition, the overshoot of temperature during the fast-charge process can be related to the initial overshoot during the high-rate charge/discharge cycle.

As discussed above, the model reproduces the behaviour of the battery module accurately, but oscillations appear to be smoothed. In addition, the drive cycle seems not to be causing a remarkable temperature increase. Such result is expected, since battery modules are designed to pass homologation duty cycles. The cycle is more representative of a real-life scenario than traditional drive cycles. The model appears to be correctly reproducing the abrupt change in current.

5.4.6 Interim conclusions

Simulations and experiments on the battery module proved the rescalability of the single cell model. In addition, test-rig experiments provided reliable and repeatable results that were used to validate the simulation. It can be concluded that the error is larger in the

case of module simulation, but the outcome still lies in the interval of uncertainty of measurements. It is also relevant to note that, at high rate, an initial overestimation of temperature takes place, subsequently, the error decreases as the model gets more stable iteration after iteration. The model allows the correlation of different physics domains at a low computational cost, it is rescalable from single cell to module and, despite not being as accurate as more complex finite element models, still provides a good level of accuracy. Most prominently, thanks to this model it is possible to correlate the duty profile with the temperature profile, with a decent level of discretisation. Flexibility is proven by simulating different cell topologies, rescalability by generating a module model from the single cell. The framework can effectively reduce the time for simulation in battery development.

5.5 Summary of chapter

In this chapter the optimisation of model and simulation parameters was first introduced. Then different case studies were presented for a single cell: a discharge cycle, an aggressive cycle, a WLTP and a cycle alternating urban duties and fast charging. Results of simulation were compared to voltage and temperature samplings. After the single cell experiments, module experiments were run and compared to simulation for a 2C charge-discharge cycle and the urban section of an Artemis cycle, combined with fast charging. The model proved effective and rescalable from cell to module level. The next chapter will draw conclusions and outline future work.

Chapter 6

Conclusions

This work started questioning how the design procedure of battery modules could be more systematic, standardised, and cheaper, taking into account thermal issues from early stages. In order to answer such research questions, this work introduced a re-scalable, multi-domain, battery modelling framework, coupled with a re-configurable battery module thermal management test rig. It was shown that such methodology can provide more insight on the battery by correlating the electrical and the thermal behaviour, in such a way that it is possible to simulate a battery cell's temperature profile in different regions of its volume. In addition, the model included a portion of its boundaries allowing therefore the implementation of a module model as an array of cell models.

The need for a more cross-domain methodology that featured chemical, electrical and thermal modelling was successfully addressed. On a modelling side, such approach enables the generation of different module and pack layouts from a single cell model. With the implemented simulation library it is possible to start from a single-cell model and implement a whole module model. The model is computationally lean and takes short time to compute (approximately 2 hours for a 28-cell module). And since the level of

discretisation is higher than that of a lumped model, the proposed strategy represents a more accurate representation in space of the cell thermal behaviour. The model represents a good trade-off between accuracy and reduction of computational effort. The model was validated both against single-cell and module experimental data. Different duty cycles were examined and a specific cooling scenario was analysed. After a full characterisation materials, initial conditions and boundaries, simulations and experiments were run on different current profiles.

The methodology makes a novel use of acausal object-oriented modelling, generating a re-scalable multi-domain battery modelling library. Previously existing re-scalable models were not developed in acausal object-oriented platforms. In addition, a discretising technique previously used for the modelling of air ducts has been successfully applied to the case of battery internal heat transfer models, relying on a network of lumped masses. Each of which represented with a physical properties modelling technique that has never been used in combination with such discretisation strategy. Furthermore, the model is not only re-scalable, but it provides a full-three-dimensional volume of the cell and it allows the implementation of different cell geometries. In addition, a different scale can be set by the user in each physics domain, which is a novelty in acausal multi-domain modelling. The final delivery of this work is a Modelica simulation library that can be deployed in Dymola or OpenModelica software, which previously lacked from the market. A further innovation is found in the combined use of a re-configurable battery-module thermal test-rig with the simulation library, which adds robustness to the technique.

Comparison of outcomes with single-cell models shows that discrepancies with experimental data generally do not exceed 1 K in a range of 20 K temperature difference, within the operating temperature range of automotive batteries. The re-scalable model,

required a specific experimental layout for validation.

The developed test-rig is highly reconfigurable and can host different battery packs and thermal management systems. The test-rig allows an effective, accurate and low-cost model validation, resulting in considerable reductions in research, development and prototyping costs. Researchers have estimated the cost of research and development to affect the cost of Lithium-ion batteries at pack level by 10% of total battery module development cost [217]. The estimated cost of battery packs has been estimated to currently be between $500\text{USD}/\text{kWh}$ and $300\text{USD}/\text{kWh}$, declining at a pace of -8% per year over the past 20 years [218]. Considering that a finite element models for battery cell heat conduction simulation of a single pouch cell, which is limited to a single cell, does not include an electrochemical model takes approximately 3000s to simulate a steady-state constant heat generation case on 4 processors in parallel [158]. The proposed library runs in a time which is one order of magnitude lower on a similar hardware and provides a transient simulation. This would mean, for a single cell case, cutting the simulation hours by 90% and reduce therefore the research and development costs, contributing to a further speed-up of battery cost decrease over the next few years. Discrepancies of simulations outcome with experimental measurements were larger in the case of the module than in the case of single cell, however they are still lying in an interval of confidence of 5%.

As a specific case study, external and removable cold-plate heat exchangers with circulation of a 25 – 75% mix of Ethylene Glycol and de-ionised water were analysed. The heat exchanger provides a benefit at high charge/discharge current rates, ensuring battery modules are kept within their operating temperature range, allowing a more aggressive use. Such a system has a minor impact on the energy consumption, i.e. 0.3 kW per module and therefore less than 1 kW on the examined motorcycle battery module. Liter-

ature suggests a cooling-system power consumption of approximately $4.1kW$ for a $9kWh$ battery pack [219]. Other authors have found a battery thermal management system consumption ranging from $0.5kW$ up to $1.5kW$ for an air cooled $280V$ and $1.9kWh$ module, with an air flow rate ranging from 0.4 to $1.4m^3 \cdot s$ [220]. Other authors suggested that the quote of energy consumption due to a refrigerant-based cooling battery system ranges between 9.8% and 11.2% of total energy consumption on the urban section of an Artemis drive cycle for a $2000kg$ hybrid-electric vehicle equipped with a $6.5Ah$ and $120V$ battery pack [221]. The energy consumption of the proposed layout is therefore in line with that of in-built systems.

The largest temperature increase is observed at high current rates and the model captures it with a good level of accuracy. Such results mean that most of the effort in designing a battery thermal management system should be concentrated on high-current-rate operations, particularly fast charging. Additional removable cold plates, more specifically, allows fast charging on electric motorcycles or other small-size vehicle that do not feature any battery thermal management system.

A new modelling technique has been introduced and its effectiveness has been validated. The modelling and testing framework developed, enabled to examine cases that previously would have needed much more computational effort.

It was shown that the developed strategy can be re-scaled from a single cell to a module, enabling much flexibility in battery design. Different charge and discharge cycles, in both transient and steady state can be examined and thermal management options evaluated for each case.

In addition, error never exceeds $1K$ in a temperature range of 0 to $45^{\circ}C$, and never exceeds $2K$ below $0^{\circ}C$ on the single cell model and never exceeds $1.5K$ on the module model. In addition, compared to the models quoted in literature, the model provides a finer discretisation than reduced order models and shorter computational times than electrochemical models presented in Chapter 2, which is beneficial in battery as explained few lines above. The sensitivity to temperature variation trends is good since the error remains within the aforementioned range during different duty cycles and the temperature. The model is also computationally light as we showed few lines above computational times are much lower than its competitors. Although at early stages uncertainty of sensors may overlap, when different experiment start from the same initial temperature, there is no doubt that the combination of model and test rig can provide an effective and accurate prediction of the temperature profile in time.

6.1 Future work

The current model will be extended with an Arrhenius-based ageing model in order to account for capacity fading due to cycling and calendar ageing. In addition, multi-particle layers reproducing the solid-electrolyte interface with a higher accuracy will be implemented. In addition, the model will be applied to different battery chemistries, examining more case studies and benchmarking the behaviour of different cells.

Further developments in the chemical model will allow the extension of the equivalent circuit model with the addition of a triple-species element, to improve the representation of the variation of Lithium-ion concentration, further increasing the accuracy of the model. In addition, the current path within the cell will be examined through the implementation of a bunch of equivalent circuits connected in parallel, representing the

different regions of the battery cell and ultimately resulting in a more detailed local heat generation model, and local ageing model. The thermal model will be further developed by examining other case studies, such as different electrode-coating chemistries, different base materials and different electrolytes, including solid-state electrolytes and gel electrolytes. Future more detailed models will be compared to the current version and the trade-off between accuracy and computational expense will provide a guideline in the selection of the fittest option, depending on the case study.

A further step in the boundary modelling is the integration of the model in an algorithm that, by generating different Dymola scripts in an external software such as a Matlab script that would run different simulations, examines different potting materials in order to optimise the battery architecture by minimising the mass and optimise heat dissipation towards the external environment.

A more in-depth proof of concept of the test rig will be provided, analysing the capability of the test rig to work with different heat exchangers and different cooling fluids. A range of heat exchangers will be tested, coupled with different coolants. The capability of the test rig to reproduce the desired working conditions: i.e. removed heat and battery enclosure internal temperature will be examined. The range of scenarios the test-rig layout can simulate will therefore be defined more in detail, providing the final user with a guidance in terms of sizes of heat exchangers that can be installed and how much heat they can remove before the enclosure internal temperature is subject to variations greater than the tolerance of the instruments and what range of fluids can be used in the test rig. Furthermore, the test-rig layout needs to be re-assembled in a thermal chamber to prove it can work at different ambient temperatures.

The experimental layout will be used in the future to examine a different range of cooling fluids. A major topic that will be investigated in future work are dielectric oils, comparing different fluids in terms of dissipated heat, power consumption of the system, mass and component cost.

A further implementation of the test-rig will be the addition of proportioning valves and heaters to simulate different pressure drops and heat rejection spots on the cooling loop, simulating the presence of other devices on the system. Such devices will be assembled upstream and downstream of the battery module cooling system, in order to compare different cooling system arrangements and define the performance of each one in terms of how capable each layout is of keeping the components in their required operating temperature range. The test rig will be further developed by direct liquid cooling. The battery enclosure allows the installation of different heat exchangers and battery module, including immersion direct cooling modules. According to the current plan, the test-rig will be used to examine different battery cooling heat exchangers over the next semester and the next academic year.

The test rig would be extended by adding a simulation of the road resistance and road thermal boundaries under the vehicle. The addition will be implemented by adding an enclosure with a ventilation system under the table level of the test rig. The test-rig layout can be fully disassembled and re-built. A further step will therefore be re-assembling it inside a thermal chamber.

A further case study to be examined will be the new Arrival Ltd. battery module. First WLTP cycles will be tested on a single module on the test-rig and then simulation and module test-rig outcomes will be compared with road tests on the Arrival T4 vehicle.

A Matlab version of the modelling library is currently being developed. In the most immediate future, the test-rig and the result obtained so far will be used for a proposal issued by the university about battery thermal management testing standards.

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Appendix A

Modelica code

A.1 Modelica code

The Modelica code was organised into a main script, featuring two subscripts. The two subscripts are the ECM and the IHTM. In the case of the single cell, they are linked as represented in Figure A.1. Each submodel is organised into different sections: i) model definition ii) unit definition, iii) constants definition, iv) variable definition v) additional components definition, vi) equation statement (which can eventually be split into a) initial equations and b) equations) vii) model end. Sections i), ii), iii), iv) and v) are represented in Figure A.2. After the enunciation of the model name, the initialisation definition block is imported into the model, to allow the user to select the type of initialisation required. Subsequently the units are defined and the variables are enunciated. Finally electrical connection ports and thermal connection ports are added. Sections vi) and vii) are showed in Figure A.3. The first step was defining the SOC and the OCV the former being calculated from initial capacity and the integral of current (Coulomb count), the former being obtained from a polynomial from manufacturer's data and the SOC and being re-corrected depending on temperature and charge/discharge rate. The IHTM code

is similar to the ECM code in its initial section. However, section vi) differs quite a lot, since it is used to generate elements of the different layers of materials and define the correlations between each other. First material properties are define element by element, as a parallel of a solid element, a liquid element and a series of liquid and solid elements, then the internal heat transfer is defined, linking the ECM with the IHTM, as in Figure A.4. In order to scale up the model from a single cell to a whole module, arrays of single-cell ECMs and single-cell IHTMs were generated as shown in Figure A.5 and linked in a series of 28 cells. In addition, bus bars and potting material were added to the model by means of resistive elements between each two ECM and additional materials around cells through which heat is conducted and which are subject to conduction and convection at their external interfaces.

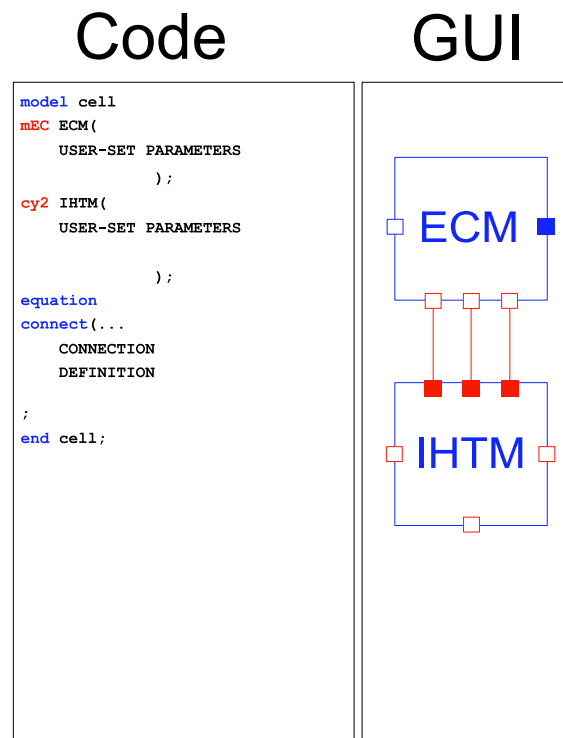


Figure A.1: Representation of domain coupling.

```

model mEC "EQUIVALENT CIRCUIT MODEL"
//PARTIAL MODELS IMPORT
import Modelica.Blocks.Types.Init;
//UNITS
type Time = Real(unit="s", min=0);
...
//CONSTANTS
parameterResistance rAcc = 0.2 "Resistance of anode current collector";
...
//VARIABLES
Resistance RA;
Resistance RS;
Resistance RC;
Capacitance CdlA;
Capacitance CelA;
Capacitance CelS;
Capacitance CelC;
Capacitance CdlC;
...
//INTERFACES
Modelica.Electrical.Analog.Interfaces.PositivePin pinP;
Modelica.Electrical.Analog.Interfaces.NegativePin pinN;
...

```

Figure A.2: First section of the Modelica code for the equivalent circuit.

```

equation
  pinP.i+pinN.i = 0;
  ...
  //Capacity, Open Circuit Voltage and State of Charge
  der(iInt) = pinP.i;
  ...
  //SOC
  SOC = iSOC-(((iInt)/3600)/cellCapIn)*100;
  ...

  //Circuit parameters
  R_A = ... ;
  R_S = ... ;
  R_C = ... ;
  CelA = ... ;
  ...
  CdlA = ...
  ...
  //Definition of circuit connections
  i_CdlC = pinN.i;
  ...
  QAphach = ...; //Phase change heat
  ...
  portAnd.Q_flow = -(QAohmic+QAreac+QAphach); //Total heat rejection
  ...
end mEC;

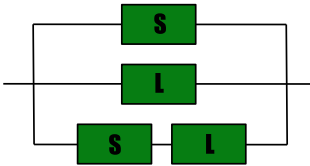
```

Figure A.3: Equation and final part of ECM Modelica code.

```

equation
    ...

    //                                     -MATERIAL PROPERTIES-
    meland = rhoank*(xank*yank*zank)+rhoanc*(xanc*yanc*zanc);
    ...
    //Cathode
    for iiii in 1:2 loop
        for iji in 1:3 loop
            for iij in 1:3 loop
                PROPERTIES DEFINED AS FOR A PARALLEL OF DIFFERENT MATERIALS


                ...

                end for;
            end for;
        end for;
    //Anode
    ...
    //                                     Anode
    Cand*der(T_and[1,1,1]) = -Gxand[1,1,1]*(T_and[1,1,1]-T_and[1,2,1])-Gyand...;
    ...
    //                                     Current collectors
    ...
    rhoal*xacc*yacc*zacc*cpal*der(T_acc[3,1]) = aGEN.Q_flow- ... ;
    ...

```

Figure A.4: Equation section of IHTM.

Code

```

model module
mEC ecm[cells] (
    USER-SET VARIABLES
    ...);
cy2 ihtm[cells] (
    USER-SET VARIABLES
    ...);
...
equation
for i in 1:cells-1 loop
    connect(ecm[i].pinN,res[i].p);
    DEFINE ELECTRICAL CONNECTIONS
    ...;
end for;
for j in 1:cells loop
    connect(ecm[j].portAnd,ihtm[j].aGEN);
    DEFINE ELECTRICAL CONNECTIONS
    ...;
end for;
...
end module;

```

GUI

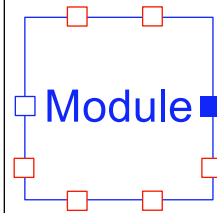


Figure A.5: Scaling up of the single-cell model into a module model.

Appendix B

Additional details on boundary modelling

With reference to Equation 3.35, the function $f(Re_D)$ is determined by the value of Re and by the geometry and A is a corrective coefficient which depends on the heat transfer fluid as follows:

$$A = 1 \quad \text{for gases}$$

$$A = (Pr/Pr_w)^{1/4} \quad \text{for liquids} \quad .$$

In the presented model, non-uniformity of wall temperature and wall effect on velocity are taken into account. Such model was implemented in Modelica code, with a Dymola GUI-interface and fed with a simplified velocity profile. In the case of the single cell, a model of thermal contact resistance was coupled with a model of convection within the thermal chamber.

Appendix C

Test-rig layout

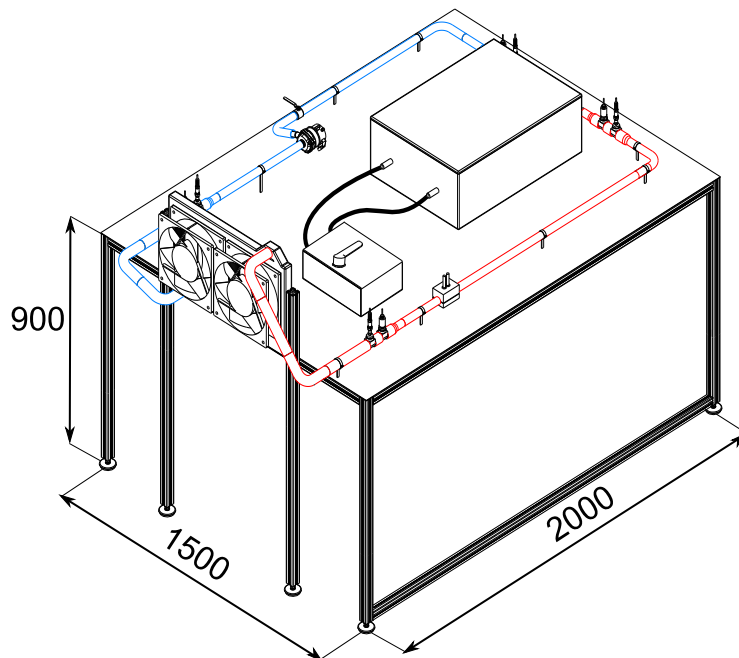


Figure C.1: Dimensions of test rig.

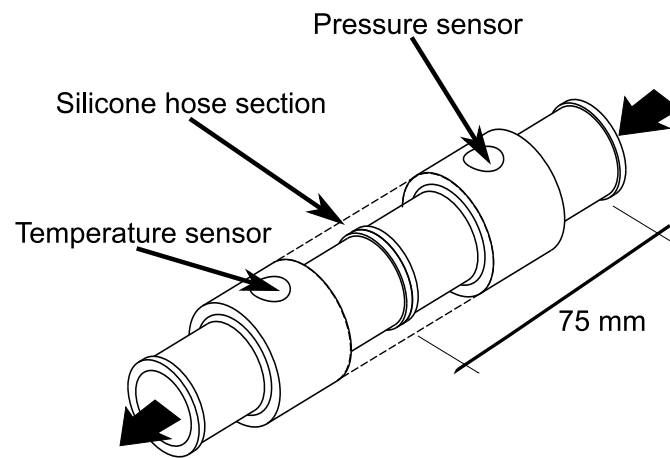


Figure C.2: Cooling-loop sensor adaptors arrangement.

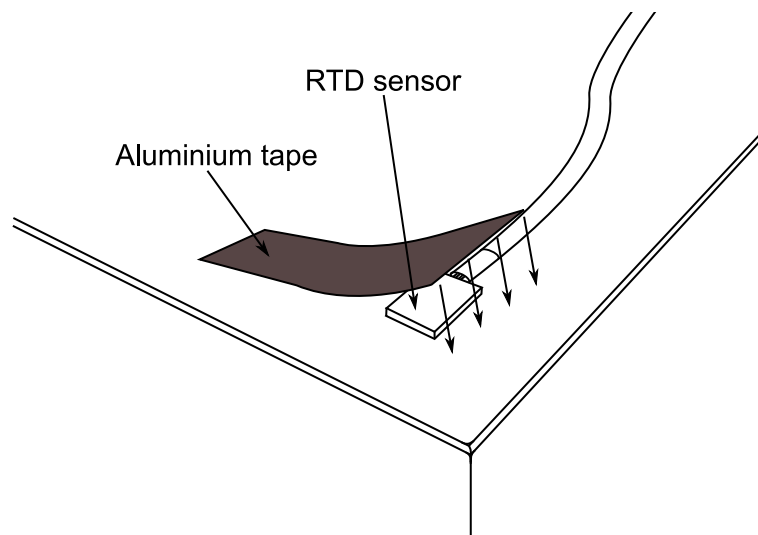


Figure C.3: Positioning of RTD sensors on the external wall of the battery.