

Impedance-based Battery Temperature Monitoring



Robert Richardson

Department of Engineering Science
University of Oxford

This dissertation is submitted for the degree of
Doctor of Philosophy

For A, B, C and M ...

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. Parts of the work have been presented at conferences and published in journal papers; these are specified in the text and referenced accordingly.

Robert Richardson
December 2016

Acknowledgements

I would like to begin by thanking my supervisor, David Howey, for his guidance and help over the last four years. I could not have imagined having a better supervisor and mentor for my DPhil study. On the academic side I would also like to thank Peter Ireland, Richard Stone, Ed Walsh, Robin Vincent, Vladimir Yufit, and the various other researchers and technical staff who provided assistance and valuable discussions. I recognize that this research would not have been possible without the financial assistance of the National University of Ireland (Travelling Studentship), the UK Engineering and Physical Sciences Research Council (Doctoral Training Award), Balliol College, University of Oxford (Foley-Bejar Scholarship), and Oxford University Press (John Fell Research Fund), and I express my gratitude to those agencies.

I'd like to thank my friends in and out of Oxford, in particular those in the Holder Group and the broader Energy and Power Group, in Balliol MCR, and on the football field, and everyone else whose helped make the last few years of my life an adventure. Finally, I would like to express my greatest gratitude to my loving parents, Marion and Bill, for their emotional and material support over the last twenty-six years; and to my brothers, Colin and Alastair, and the rest of my family for all the love I've received over the years. And to Katrien, for her love, companionship and unwavering support. This work would not have been possible without you.

Abstract

Accurate on-board temperature monitoring of lithium-ion batteries is important for safety and control purposes. Impedance temperature detection (ITD) is a promising approach for temperature estimation, whereby the internal cell temperature is directly inferred from online electrochemical impedance spectroscopy (EIS) measurements at a single frequency. Previously, ITD was used to infer the volume-average cell temperature; the present work focuses on extending ITD to enable estimation of the spatially-resolved temperature distribution of cells with internal temperature gradients.

Two novel hybrid methods for temperature monitoring are introduced, based on combining impedance measurements with (i) an additional surface temperature measurement, and (ii) a thermal model. These methods predict the temperature distribution of the cell in either 1-D or 2-D, and can therefore identify localised hot spots, and hence the global maximum cell temperature. In each case, the methods are experimentally validated using cylindrical LiFePO_4 cells (26650 for the 1-D experiments, 32113 for the 2-D experiments) monitored with periodic 215 Hz impedance measurements, and fitted with an internal thermocouple and one or more surface thermocouples for validation. Method (i) is shown to be more accurate than a standard ITD method based on impedance measurement only: $\bar{\varepsilon} = 0.6^\circ\text{C}$ vs. 2.6°C respectively, over a 3500 s drive cycle. In method (ii), the impedance measurement forms part of a state/parameter estimation algorithm; in this case, the performance of an extended Kalman filter using impedance measurement is shown to be comparable - although slightly inferior - to an equivalent Kalman Filter using a conventional surface temperature measurement.

This work also presents a novel low-order 2-D thermal model based on the spectral-Galerkin (SG) method. The model can be used in conjunction with the proposed hybrid methods or in a conventional temperature monitoring scheme. Time- and frequency-domain simulations show that the SG model using as few as 4 states is capable of accurately modelling the thermal dynamics of a large format cylindrical cell with a highly transient heat generation input. The model can account for different external

temperatures and/or convection coefficients at each surface - a generality which makes it suitable for simulating various battery cooling configurations.

Table of contents

List of figures	xv
List of tables	xix
Nomenclature	xxi
1 Introduction	1
1.1 Battery thermal management	1
1.1.1 Thermal issues in lithium-ion batteries	1
1.1.2 Battery thermal management system design	5
1.2 Electrochemical impedance spectroscopy	6
1.3 Battery temperature monitoring	7
1.3.1 Conventional method	8
1.3.2 Internal micro temperature sensors	9
1.3.3 Temperature estimation via impedance	10
1.4 Hybrid methods for non-uniform temperatures	13
1.5 Low-order modelling & state estimation	15
1.5.1 1-D assumption	16
1.5.2 Numerical methods	17
1.5.3 State estimation	21
1.6 Research focus and contributions	22
1.7 Outline of thesis	23
 I Temperature Monitoring in 1-D	 25
2 Impedance Temperature Detection in 1-D	27
2.1 Impedance for non-uniform temperature distributions	27
2.2 Calibration experiments	31

2.2.1	Setup	31
2.2.2	Procedure	32
2.2.3	Results	33
3	Hybrid Method I: ITD/T	37
3.1	Description of method	38
3.1.1	Steady-state thermal model	39
3.1.2	Constrained impedance model	40
3.2	Frequency analysis	40
3.2.1	Exact transient solution	41
3.2.2	Pseudo steady-state approximation	43
3.2.3	Results	44
3.3	Experimental validation	45
3.3.1	Procedure	45
3.3.2	Results and discussion	47
4	Hybrid Method II: ITD/TM	51
4.1	Description of method	52
4.1.1	Thermal model	53
4.1.2	Polynomial Approximation	54
4.1.3	Impedance measurement	57
4.2	Frequency analysis	57
4.3	Validation experiments: procedure	58
4.4	Model parameterisation & validation	59
4.5	State estimation	61
4.6	Results and discussion	63
4.6.1	Convection coefficient known	64
4.6.2	Convection coefficient unknown	65
4.7	Conclusions	67
II	Temperature Monitoring in 2-D	69
5	Spectral-Galerkin model	71
5.1	Toy problem	72
5.2	Thermal model	77
5.2.1	Overview	77
5.2.2	Model definition	78

5.2.3	Change of scale	79
5.2.4	Homogenization of the boundary conditions	80
5.2.5	Chebyshev-Galerkin approximation	81
5.2.6	Boundary lifting function	82
5.2.7	Solution algorithm	85
5.3	Results and discussion	87
5.3.1	Time domain	87
5.3.2	Frequency domain	93
5.4	Conclusions	94
6	Hybrid Method II (2-D)	97
6.1	Overview of method	98
6.2	Theory	100
6.2.1	2-D thermal model	100
6.2.2	State estimation	102
6.3	Experimental	103
6.3.1	Setup	103
6.3.2	Procedure: full spectrum impedance	104
6.3.3	Procedure: validation experiments	105
6.4	Full spectrum impedance	106
6.5	Parameterisation and validation	106
6.6	Test Set I: HEV drive cycles	110
6.6.1	Impedance calibration	110
6.6.2	Results and discussion	111
6.7	Test Set II: constant current discharge	116
6.7.1	Impedance calibration	116
6.7.2	Results and discussion	117
6.8	Conclusions	117
III	Conclusions	123
7	Conclusions and further work	125
7.1	Conclusions	125
7.1.1	Hybrid methods	125
7.1.2	Low order thermal models	126
7.2	Future work	127

7.2.1	Alternative thermal/electrochemical models	127
7.2.2	Further hybrid methods	128
7.2.3	Impedance calibration	128
7.2.4	Other factors affecting impedance	129
7.2.5	Multi-cell systems	129
7.2.6	On-board demonstration	130
References		133
Appendix A Polynomial Approximation: application to other geometries		145
A.1	1-D Cartesian	145
A.2	1-D annulus	152
Appendix B Polynomial Approximation: application to 2-D problems		157
Appendix C Modelling assumptions		165

List of figures

1.1	Thermal issues in lithium-ion batteries	2
1.2	Schematic impedance response of lithium-ion cells	7
1.3	Approaches to battery temperature monitoring	15
1.4	Battery cooling configurations resulting in 2-D thermal dynamics . . .	17
1.5	Thermal equivalent circuit network	19
1.6	Research areas related to impedance temperature detection	23
2.1	ITD for non-uniform temperatures	29
2.2	Experimental setup for calibration and validation experiments	32
2.3	Exemplary electrochemical impedance sepctrum at 10°C	33
2.4	Nyquist plots of full spectrum impedance at various temperatures . . .	34
2.5	Bode plots of full spectrum impedance at various temperatures	34
2.6	Arrhenius and polynomial fits to measured impedance	35
3.1	ITD/T schematic	37
3.2	ITD/T process flowchart	39
3.3	Frequency response analysis: PSS approximation	45
3.4	Experimental results: current pulses	48
3.5	Experimental results: HEV drive cycle	49
3.6	Artemis drive cycle error analysis	49
4.1	ITD/TM schematic	51
4.2	ITD/TM process flowchart	52
4.3	Schematic diagram of the 1D cylinder model	54
4.4	Frequency response analysis: PA thermal model	59
4.5	HEV-I drive cycle data: current, voltage and heat generation.	60
4.6	Model parameterisation and validation results	61
4.7	Results for EKF using Z' as measurement input	64
4.8	Results for DEKF using Z' as measurement input	65

4.9	Results for DKF using T_{surf} as measurement input	67
5.1	Spectral-Galerkin model.	72
5.2	Composition of basis functions for Dirichlet boundary conditions	74
5.3	Composition of basis functions for Robin boundary conditions	75
5.4	Schematic of cylindrical cell geometry for the thermal model	78
5.5	Schematic of cell showing the model outputs	89
5.6	Comparison of SG vs. FEM results for Case 1: forced air convection . .	90
5.7	Comparison of SG vs. FEM results for Case 2: end-plate liquid cooling	91
5.8	Contour plots of SG and FEM methods for Case 1	92
5.9	Contour plots of SG and FEM methods for Case 2	92
5.10	Frequency response of the SG method for a range of model orders and Biot numbers	93
6.1	ITD/TM schematic (2-D)	97
6.2	ITD/TM process flowchart (2-D)	99
6.3	Schematic of cell showing the model outputs	101
6.4	Photos of experimental setup	104
6.5	Schematic diagram of experimental setup	105
6.6	Impedance spectra at 10°C and various SoCs	107
6.7	Model parameterisation and validation results	109
6.8	Identification of impedance-temperature polynomial fit for Test Set I .	110
6.9	Comparison of measured temperature vs. EKF/KF predictions for Config. 1	113
6.10	Comparison of measured temperature vs. EKF/KF predictions for Config. 2	114
6.11	Error analysis for Test Set I	115
6.12	Impedance-temperature polynomial fit for Test Set II	116
6.13	Measured temperature vs. EKF/KF predictions under 4 C currents . .	118
6.14	Measured temperature vs. EKF/KF predictions under 6 C currents . .	119
6.15	Error analysis for Test Set II	120
A.1	Schematic of prismatic cell geometry for the thermal model.	146
A.2	Frequency response of the Cartesian thermal model	151
A.3	Schematic of annular cell geometry for the thermal model.	153
A.4	Frequency response of the annular thermal model	156
B.1	Schematic of cylindrical cell geometry for the thermal model.	159

B.2	Frequency response of the 2-D PA model for a range of model orders and Biot numbers	163
-----	--	-----

List of tables

1.1	Comparison of ITD studies	12
1.2	Comparison of control-oriented/online temperature estimation studies.	14
2.1	Properties of the lithium-ion cell used for validation.	31
4.1	Comparison of reference and estimated parameters	60
4.2	RMSEs for core and surface temperatures with unknown convection . .	66
5.1	Thermophysical properties for model validation.	88
5.2	Convection coefficients for the two cooling scenarios.	88
6.1	Properties of the lithium-ion cell used for validation.	104
6.2	Thermal parameters for the two cooling configurations	108
6.3	RMS errors in the parameterisation and validation cycles	109

Nomenclature

Abbreviations

BTMS	Battery Thermal Management System
BVP	Boundary Value Problem
DEKF	Dual Extended Kalman Filter
EIS	Electrochemical Impedance Spectroscopy
EKF	Extended Kalman Filter
EV	Electric Vehicle
FDM	Finite Difference Method
FEM	Finite Element Method
GEIS	Galvanostatic Electrochemical Impedance Spectroscopy
HEV	Hybrid Electric Vehicle
ITD	Impedance Temperature Detection
KF	Kalman Filter
OCV	Open-Circuit Voltage
PA	Polynomial Approximation
PCM	Phase Change Material
PDE	Partial Differential Equation
PEIS	Potentiostatic Electrochemical Impedance Spectroscopy
PSS	Pseudo Steady-State
RMSE	Root-Mean-Square Error
SC	Spectral-Collocation
SG	Spectral-Galerkin
SEI	Solid Electrolyte Interface
SoC	State of Charge
SoH	State of Health

TEC	Thermal Equivalent Circuit
TM	Thermal Model

Roman

A, B, C, D	system matrices
a_i	impedance polynomial coefficients
c_p	specific heat capacity [J kg ⁻¹ K ⁻¹]
C_k	k th deg. Chebyshev poly. of 1 st kind
E_a	Activation energy
h	convection coefficient [W m ⁻²]
H	cell height
H	system transfer function
I	Current [A]
I	identity matrix
j	imaginary number
k_r	radial thermal conductivity [W m ⁻¹ K ⁻¹]
k_z	axial thermal conductivity [W m ⁻¹ K ⁻¹]
q	volumetric heat generation [W]
N_s	number of model states
r	radial coordinate [m]
$\hat{r}$	scaled radial coordinate [m]
r_{in}	inner radius [m]
r_{out}	outer radius [m]
s	Laplace variable
T	temperature [K]
$\bar{T}$	volume-average temperature [K]
$\bar{T}_{EIS}$	EIS-based volume-average temperature [K]
$\tilde{T}$	auxiliary temperature function [K]
T_e	boundary-lifting function [K]
t	time [s]
U_{OCV}	Open Circuit Voltage
V	Voltage
V_b	Cell volume

$\mathbf{x}$	system state
y	admittivity [S m^{-1}]
$\mathbf{y}$	system output
Y	admittance [S]
z	axial coordinate [m]
$\hat{z}$	scaled axial coordinate [m]
Z	impedance [Ω]

Greek

α	thermal diffusivity
γ	temperature gradient [K m^{-1}]
ϵ	error
ν	test function
ρ	density [kg m^{-3}]
σ	standard deviation
φ	azimuthal coordinate
ϕ	impedance phase shift ¹
ϕ	basis function ¹
Ψ	vector of basis functions
ω	frequency

Subscripts

est.	estimated
exp.	experimentally measured
b	bottom edge
l	left edge
r	right edge
t	top edge
∞	ambient condition
'	real part (of impedance/admittance)
"	imaginary part (of impedance/admittance)

¹Since the Greek symbol, ϕ , is conventionally used to indicate the impedance phase shift in the EIS literature but also the basis function in the spectral methods literature, I have chosen to use the same symbol for both in this thesis. It should be clear from the context which is meant in any instance.

Chapter 1

Introduction

The sustainable development of transportation relies on the widespread adoption of electric vehicle (EV) and hybrid electric vehicle (HEV) technology. Lithium-ion batteries are suitable for these applications due to their high specific energy and power density. However, their widespread deployment requires reliable on-board battery management systems to ensure safe and optimal performance. Since they must operate under a wide range of demanding conditions, including elevated temperatures and high charge/discharge rates, thermal issues are particularly significant [1]; hence, accurate on-board estimation of battery temperature is of critical importance.

This thesis focuses on a recently introduced method of estimating the temperature of a battery by measuring its electrochemical impedance. Significant improvements are made to this ‘impedance-based’ temperature estimation approach, by combining impedance measurements with on-line thermal models and control-oriented techniques. In particular, the improved methods presented in this thesis enable the spatially distributed temperature field of a battery to be estimated rather than just an average or uniform value. Since batteries exhibit large internal temperature non-uniformities during operation, the estimation of such distributed temperatures results in a significant improvement in the accuracy of local temperature estimation.

1.1 Battery thermal management

1.1.1 Thermal issues in lithium-ion batteries

Under typical operating conditions, such as an EV or HEV drive cycle, individual cells may experience temperature differences between surface and core of 20 °C or more [2], and during a rapid overheating event this discrepancy can be as large as 40-50 °C [3].

The temperatures of different cells within a pack may also diverge substantially [4, 5]. Non-optimal temperatures and temperature gradients can have a variety of deleterious effects on battery performance and safety, such as thermal runaway, accelerated aging, electrical imbalances and lithium plating. These effects are summarised in Fig. 1.1, and discussed in further detail below. These issues highlight the need for a reliable on-board thermal management system with accurate monitoring of cell temperatures and internal temperature distributions.

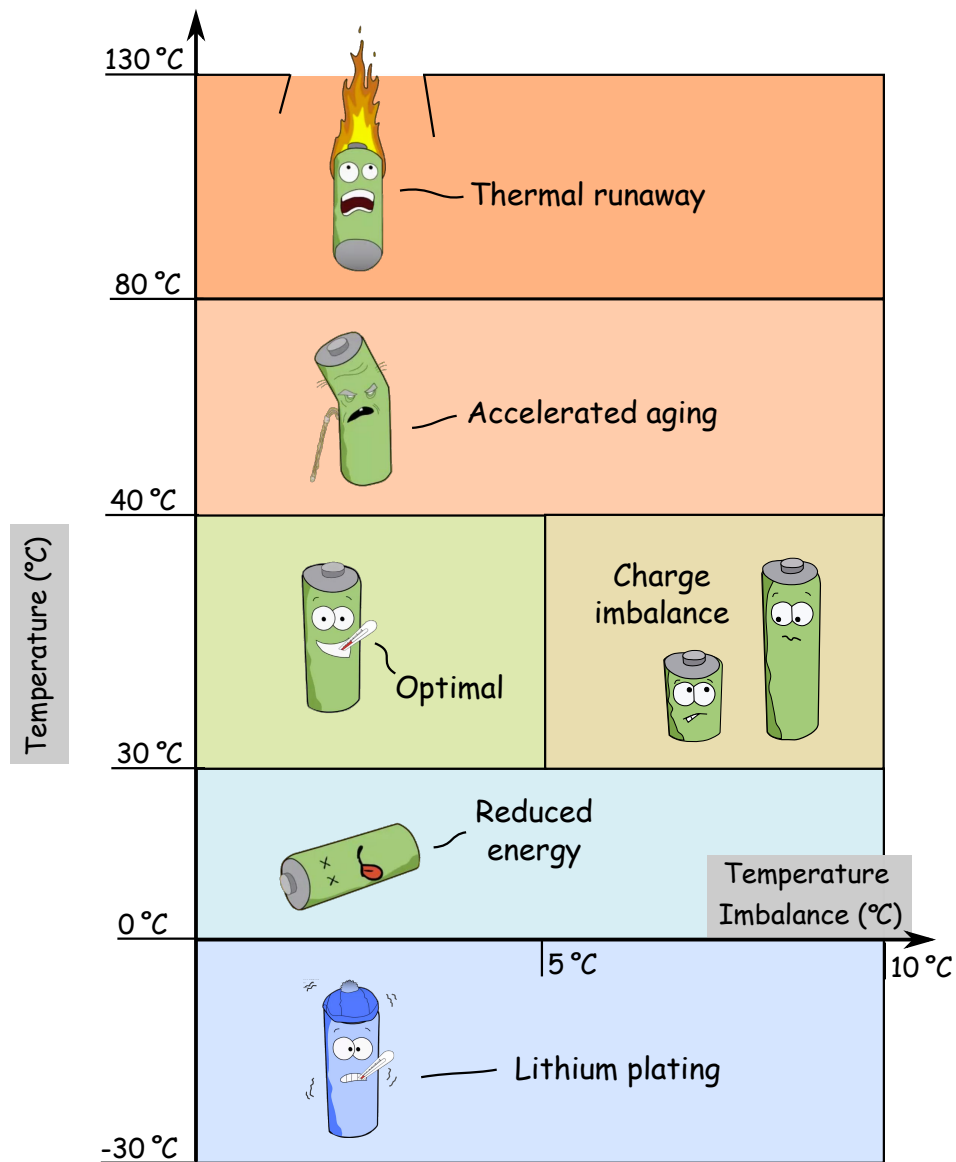


Fig. 1.1 Thermal issues in lithium-ion batteries associated with different temperature ranges. The y-axis represents the absolute temperature of the battery and the x-axis represents the temperature difference between different locations in a cell or pack.

Thermal runaway

Thermal runaway occurs when parts of the cell exceed a critical temperature and initiate exothermic reactions. The initial undesired temperature rise might be caused by electrical or mechanical abuse, or as a result of an external heat source. The general path to thermal runaway has been elucidated by several researchers and can be summarized as follows [6–8]: when the temperature of the cell rises to between 90 and 120°C, the Solid Electrolyte Interface (SEI) layer on the graphite anode decomposes exothermically. This results in further heat generation and gas evolution as reactions occur between the lithiated carbon and the electrolyte. The SEI layer continues to decompose exothermically up to temperatures of $\sim 220^\circ\text{C}$ at which stage the graphite phase begins to break down. The separator, which is typically made of materials based on polyethylene and polypropylene, starts to melt at above $\sim 130^\circ\text{C}$. A melted separator could cause the battery to short circuit, resulting in further heating. Common cathode materials such as LiFePO_4 begin to decompose at $\sim 300^\circ\text{C}$, resulting in further exothermic reactions. Without external intervention this process will continue until a catastrophic failure of the cell occurs, often resulting in fires, venting and electrolyte leakage.

Obviously thermal runaway events can be quite dangerous, and although such incidents are rare (occurring in one in one million to one in ten million batteries [6]), consequences include costly recalls and potential endangerment of human life. One pertinent example is the series of battery fires which occurred on board a number of Boeing 787 aircraft in January 2013 [9]; the subsequent airline groundings cost the company $\sim \text{£}393$ million [10].

The most common method of preventing thermal runaway involves the use of safety devices such as pressure relief valves or Positive Temperature Coefficient (PTC) devices. PTCs are connected in series with the cell and operate by increasing their electrical resistance in response to increased temperatures, in order to limit current flow and prevent continued heat generation. However, these devices add undesirable electrical resistance, and once they are triggered the cell is generally rendered unusable. Therefore, a correctly designed thermal management system is also essential for maintaining safe cell temperatures and minimizing internal temperature gradients which may lead to localized hot spots [11]. However, regardless of the thermal management system design, it is clear that methods of monitoring the cell temperature are also crucial for avoiding unanticipated excursions to high temperatures.

Aging

Battery aging or degradation is characterized by the loss of available energy (capacity) and/or power. Capacity loss occurs when the active material is transformed into inactive phases, and power loss arises when the battery impedance is increased. There are several mechanisms responsible for battery degradation, and as yet these are not all fully understood [12]. However, it is clear that temperature plays an important role. Specifically, cycling and/or storing a battery at elevated ($>45^{\circ}\text{C}$) or very low temperatures ($<0^{\circ}\text{C}$) is known to result in accelerated aging in terms of both capacity and power fade [13, 14].

Electrical imbalance

To achieve the voltage and power necessary for EVs and HEVs multiple lithium-ion cells must be connected in series and parallel. Since the weakest cell limits the capacity of the pack, batteries with mismatched capacities connected in series are unable to exploit all of the available energy. Charging the pack may then cause the weaker cells to be overcharged, which could trigger thermal runaway of the overcharged cells. Imbalances between parallel-connected cells are equally undesirable. If the open circuit voltages (OCV) of parallel-connected cells differ, superposed transfer currents will cause energy to be discharged from one cell to the other [15]. Temperature differences play a significant role in causing such electrical imbalances since (i) the usable capacity of the cell at a non-zero C-rate depends on its internal impedance, which in turn is dependent on temperature and (ii) the OCV is a function of temperature (it may increase or decrease with temperature depending on the sign of the entropy term; see Eq. 4.2 and the subsequent discussion). For instance, Fleckenstein et al. [15] showed that differences of 5.3% in SoC occurred between two cells with a difference in temperature of 20 K, after applying a SoC-neutral pulse cycle. Analogous issues can occur on the single cell level, whereby electrical imbalances are induced between regions of the cell of differing temperature. Such temperature gradients inevitably arise in a cell which generates heat throughout its volume whilst being cooled at its surface. Hence, it is an objective of the battery thermal management system to minimise such thermal imbalances between cells and within individual cells.

Low temperature performance

Low temperatures result in substantially reduced energy and power capabilities of lithium-ion batteries. The primary mechanism responsible for irreversible capacity loss

at low temperatures is lithium plating, although other degradation mechanisms play a minor role [16, 17]. In particular, the charging performance is affected more than the discharging performance. For instance, Fan et al. showed that a typical li-ion battery can discharge almost 90% at a C/5 rate at -20°C but cannot accept this on charging at the same rate and temperature [18]. These issues have led to research into efficient heating methods, such as internal self heating via applied alternating current pulses and external heating from, for instance, the waste heat from the combustion engine in a HEV [19, 20].

1.1.2 Battery thermal management system design

Battery thermal management systems (BTMS) must be designed to address the aforementioned issues whilst also taking into account practical considerations related to the cost and complexity of the system. The objectives of a BTMS can thus be summarised as:

- Ensure the maximum and minimum temperatures of the pack are kept within an optimum operating temperature range (this may require both cooling and, in cold climates, heating)
- Minimise temperature variations between cells within a module, and between modules within a pack
- Minimise temperature variation within each cell
- Minimise the overall volume and mass of the system
- Adhere to designs which can be easily manufactured, have low maintenance costs, and are easily serviceable

BTMS's can be divided into categories based on the type of heat transfer medium employed and whether latent heat effects are exploited. These choices have a significant impact on the performance and cost of the BTMS. The simplicity, low cost and light weight of air heat transfer makes it preferable to liquid heat transfer for cases where the former will suffice. However, for higher power densities, air cooling may not be sufficient to achieve the design requirements and it may be necessary to employ liquid cooling, Phase Change Materials (PCMs), or even evaporative cooling.

For each of these categories, there are various design choices regarding the configuration of the cooling system. For instance, air cooling may be applied via a transverse or axial flow, and the cells may be arranged in a staggered or in-line configuration. Similarly,

liquid cooling may be applied using liquid cooling plates between cells or via a plate at the base/head of a selection of cells. The choice of cooling configuration inevitably impacts the extent to which multidimensional temperature gradients arise during operation - an issue which is important when modeling thermal dynamics, as discussed in Section 1.5.

1.2 Electrochemical impedance spectroscopy

Electrochemical impedance spectroscopy (EIS) is a common analysis method in electrochemistry. The general principle of *galvanostatic* EIS is to apply a sinusoidal current signal and measure the corresponding voltage response from the cell, in order to determine its small signal frequency response. *Potentiostatic* EIS (whereby the input is the current and the output is the measured voltage) is also possible, although this approach is less common in battery applications and hence is not used in the present work.

Fig. 1.2a shows a theoretical typical EIS spectrum on a Nyquist plot. The spectrum shows characteristic behaviour represented by the five different sections illustrated in this plot. These sections have been related to particular kinetic processes as follows [21]:

1. *Inductive elements:* At very high frequencies the spectrum shows inductive behaviour caused by the reactances of metallic elements in the cell and wires.
2. *Ohmic resistance:* the ohmic resistance of the cell, represented by the intersection of the curve with the real axis, is the sum of the resistances of the current collectors, active material, electrolyte and separator.
3. *High frequency semicircle:* the high frequency semicircle is typically associated with the solid electrolyte interface (SEI) and is formed during cycling on the surface of the anode.
4. *Low frequency semicircle:* the low frequency semicircle represents the double layer capacity and charge transfer resistance at the electrodes.
5. *Low-frequency diffusion:* The very low frequency response consisting of a straight line in the impedance plot represents diffusion processes in the active material of the electrodes.

Measured spectra often show variations on this theoretical curve. Most notably, often the high and low frequency semicircles are indistinguishable from one another, as is

the case in the spectra obtained in the present work (see, for instance, Figures 2.3 and 6.6).

It should be noted that equivalent circuit models are often fitted to such impedance spectra in the literature, to facilitate dynamic modelling of the electrochemical behaviour of the cell [22]. Figure 1.2b shows a typical equivalent circuit model used to model the behaviour in the corresponding Nyquist plot. The Z_{arc} elements used to model the high frequency and low frequency semi-circles consist of a parallel connection of a resistor and a constant-phase-element (CPE). These circuit elements are necessary to capture the depressed semicircle feature. The Warburg element, Z_w , is defined by $\tanh(\sqrt{j\omega\theta})/j\omega\theta$ and shows a linear slope with an angle of 45° at low frequencies. Approximations are required for both the Z_{arc} and Warburg elements, since neither of these have an associated Laplace transform. Z_{arc} elements are typically approximated by a variable number of RC-elements, and the Warburg element by a series connection of a resistor and an RC element. The present work is focussed on thermal modelling and hence only considers the ohmic resistance term (for calculation of the heat generation; see Chapter 3) from such equivalent circuit models.

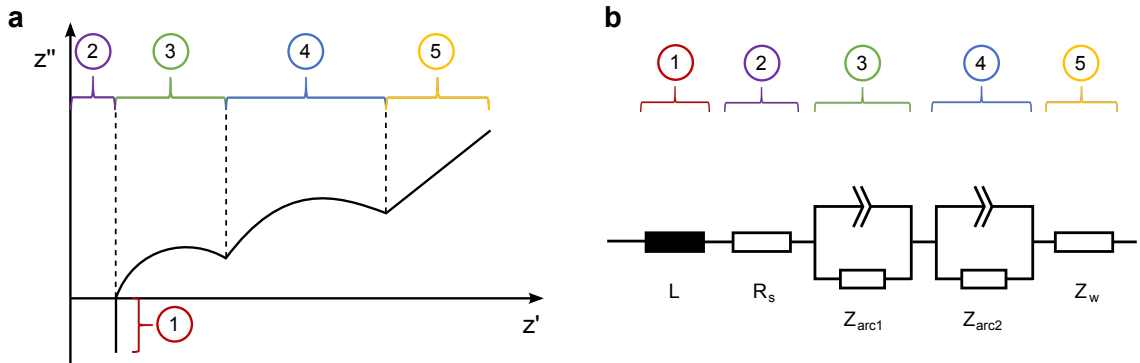


Fig. 1.2 Schematic impedance response of lithium-ion cells. (a) Nyquist plot, (b) equivalent circuit model.

1.3 Battery temperature monitoring

Regardless of the type of BTMS employed, it is clear that methods of monitoring the cell temperature are also crucial for ensuring safe and efficient operation. Below, the main approaches to temperature monitoring are described.

1.3.1 Conventional method

The conventional approach to temperature estimation is to use numerical electrical-thermal models coupled with online measurements of the cell surface temperature and/or the temperature of the heat transfer medium [23]. I refer to this as ‘Temperature (measurement) with a Thermal Model’ (T/TM). Using this method in conjunction with state estimation techniques such as Kalman filtering, the cell internal temperature may be estimated with high accuracy [24–27] (e.g. with RMS errors of $\sim 0.4^\circ\text{C}$ on the core temperature estimate for a HEV drive cycle which generates a temperature difference between the surface and core of up to 5°C [24]). However, there are three primary problems with this method, discussed below.

Measuring thermal properties

Thermal-electrical models rely on knowledge of the cell properties, heat generation rates and thermal boundary conditions, which can be difficult to measure in practice. The heat generation term is normally approximated as the product of the current squared, I^2 , and the internal resistance, R_e (along with other secondary source terms; see Eq. 4.2 and the subsequent discussion). The value of R_e is difficult to estimate since it is a function of temperature, state of charge (SoC) and state of health (SoH). The thermal properties of the cell are also difficult to measure, since cells consist of many different materials combined into a layered structure, and there are unknown thermal contact resistances between the layers [28]. Recently, novel methods have been introduced for estimating thermal properties in cells, including specific heat capacity and anisotropic thermal conductivity, based on electrothermal impedance spectroscopy (ETIS) [28–33]. ETIS examines the transfer function between a heat generation input and a surface temperature output in the frequency domain. An ETIS spectrum is typically obtained by applying modulated heat generation inputs of varying frequencies to the cell and measuring the output temperature. The steady state magnitude and phase shift at various frequencies are then used to build up a full spectrum. The resulting spectra can be used to identify the values of thermal parameters assuming the thermal structure of the cell is known or can be estimated. Early attempts at this method assumed a 1-D cell structure although recently it has been extended to 2-D [33]. Although it has been proven to be a useful technique, ETIS has some disadvantages. For instance, it is time intensive, and cell-to-cell variability may reduce its accuracy. Hence, the issue of uncertain thermal property estimation remains a challenge.

Instrumentation cost

Large battery packs may contain several thousand cells [11], and so the requirement for surface temperature sensors on every cell represents substantial instrumentation cost. As a result, EV manufacturers often use fewer temperature sensors in their battery packs than are required to achieve full observability of each cell. Observability is a measure of how well internal states of the system can be inferred from knowledge of its outputs. A system is said to be fully observable if the initial state vector can be determined by processing the input to the system and the output of the system. What constitute states in a battery pack depends on the modelling methodology used. For lumped parameter models, the states may consist of the nodal cell temperatures; for polynomial approximation methods, they consist of volume averaged temperatures and temperature gradients for each cell (Chapter 4), and for spectral-Galerkin methods, the states are the coefficients of the spectral basis functions (Chapter 5).

In practice full observability is difficult to achieve, and instead various measures of the degree of observability can be used [34]. For example, Lin et al. [35] found that for a series string of 10 cells, at least 4 sensors are needed to give full observability. However, the available sensors in commercial battery packs are typically much less than this, e.g. 16 for 288 cells in the Chevrolet Volt and 42 for 288 cells in the Toyota plug-in Prius [35].

Detecting rapid internal fluctuations

Rapid fluctuations in internal temperature may not be registered by surface mounted temperature sensors, regardless of the sampling frequency. This may mean thermal runaway cannot be detected, since associated timescales are often shorter than timescales associated with heat conduction through the cell [36]. Consequently, surface mounted temperature sensors even when used with a thermal model may be insufficient to track internal temperature to predict thermal runaway.

1.3.2 Internal micro temperature sensors

One approach to overcome these problems is to embed micro- temperature sensors within the cell [37, 38]. In these studies, flexible thin film thermocouples were fabricated and transferred onto the battery current collector, which was then embedded in a lithium-ion cell to enable in-situ internal temperature measurement. Lee et al. developed improved versions of these sensors which included additional measurements of voltage and current [39, 40]. Martiny et al. introduced a spatially distributed internal

temperature sensor which used a Kapton-based thermocouple matrix consisting of measurement points distributed over an area of the cell that could facilitate spatially resolved temperature monitoring [41]. Although these approaches have some obvious advantages, they also introduce additional manufacturing challenges and instrumentation requirements which would significantly increase the cost and complexity of the system.

1.3.3 Temperature estimation via impedance

Another alternative approach to temperature estimation uses EIS measurements at one or several frequencies to directly infer the internal cell temperature, without using a thermal model [42–46]. This exploits the fact that impedance is related to a type of volume averaged cell temperature, which is defined later (see Chapter 2). I refer to the use of impedance to infer such a volume-averaged temperature as Impedance-Temperature Detection (ITD).

The use of EIS measurements for the purpose of ITD was originally proposed by Srinivasan et al.¹ [42]. Their work experimentally demonstrated an intrinsic relationship between electrochemical impedance (specifically impedance phase shift ϕ at a single frequency between 40-100 Hz) and internal temperature between -20 and 66°C. They argued that their chosen frequency range was suitable for tracking cell temperature because: (1) the impedance of various types of li-ion cells at high frequencies (>30 Hz) is dominated by the anode [47], therefore impedance measurements in this range are unaffected by changes to the cathode structure; (2) the degradation of li-ion cells under normal conditions is primarily at the cathode [48], and so the anode structure may remain stable even after several thousand cycles [49]; and (3) the impedance due to the SEI layer is approximately independent of SoC, but highly dependent on temperature [47]. They later showed that with calibration, ϕ can be used as a type of cell temperature measurement under an applied load cycle [43], although they tacitly assumed a uniform internal temperature distribution, and they did not validate the predicted temperature against other sensor measurements.

The effect of temperature non-uniformity on electrochemical impedance was studied by Troxler et al. [50] who showed that the effective impedance of a cell with a temperature gradient applied could be accurately modelled by treating the cell as a parallel electrical

¹Although they didn't refer to it as ITD; they used the acronym "Battery Internal Temperature Sensor" (BITS). There are various creative names for this method in the literature but for consistency I use the expression ITD throughout. This is acceptable since they all predict an impedance-based volume averaged temperature, and the associated analyses for non-uniform temperature distributions are equivalent (see Section 2.1).

connection of individual electrodes. Schmidt et al. [44] showed that, based on this principle, ITD can be used for accurate estimation of mean internal temperature in a prismatic LiPo pouch cell. They used the real part of the impedance, rather than the phase shift, as the impedance-based metric to infer the average cell temperature. They also used a higher excitation frequency (10.3 kHz), than Srinivasan's studies: they chose this frequency based on their empirical analysis of the full-spectrum impedance data, which showed that very high frequencies were needed to mitigate the dependence on SoC for this particular cell. Under isothermal conditions, the internal temperature was determined as precisely as 0.17 °C with SOC known and 2.5 °C when the SOC is unknown. Since they did not use a fitted internal thermocouple they could not validate the transient internal temperature during the thermal cool-down.

More recently, advancements have been made towards identifying the optimal impedance metric for temperature inference, and to extend the range of temperatures at which it can be applied. Raijmakers et al. [45] proposed the use of the intercept frequency, f_0 . They presented a mathematical analysis showing that the intercept frequency, defined as the frequency at which the imaginary part of the impedance is zero ($Z' = 0$), decreases with increasing temperature. Furthermore, they demonstrated experimentally that f_0 is strongly dependent on temperature and independent of SoC and SoH for a LiFePO₄ cell. Spinner et al. demonstrated ITD up to higher temperatures on a LiCoO₂ cell by using a secondary, empirical fit applied to the range, $68 < T < 95$ °C [3]. Prior to their work, ITD had only been demonstrated for cell temperatures up to ~ 66 °C, above which the accuracy became unsatisfactory. However, tracking to temperatures beyond this range is desirable since lithium-ion cells may remain stable up to ~ 100 °C [7, 44, 51–53]. Koch and Jossen [54] investigated the performance of various impedance metrics with respect to sensitivity to temperature variation and to other parameters such as SoC, SoH and DC-offset currents (e.g. due to an applied drive cycle) for a LiFePO₄ cell. They found that the real part and absolute value of the impedance have a relatively strong dependency on SoC and DC-offset compared to the imaginary part and phase shift, and so the latter two metrics were recommended for temperature monitoring. They also evaluated and selected optimal frequency ranges based on similar criteria.

Table 1.1 lists the existing ITD studies, and the impedance metrics and excitation frequencies used in each case. Although some of these studies have argued in favour of one metric or another, there is not yet a general consensus on which is optimal. This is partly due to a variability in the performance of each metric depending on the cell

Table 1.1 Comparison of ITD studies. Impedance metrics: ϕ = phase shift, Z' = real part, Z'' = imaginary part, $|Z|$ = magnitude, f_0 = intercept frequency.

Study	Chemistry	Metric	f (Hz)	T (°C)	Notes
Srinivasan et al. [42]	LiFePO ₄	ϕ	0.04 – 0.1	-20 – 66	Demonstrated relationship between ϕ and T . Proposed ITD.
Srinivasan et al. [43]	LiFePO ₄	ϕ	0.04 – 0.1	-20 – 66	Used ITD to monitor $T_{uniform}$ (no validation sensor).
Schmidt et al. [44]	LiPo	Z'	10.3	-40 – 40	Used ITD to monitor $\bar{T}$ under iso-thermal conditions and during cool-down (validated with thermocouple under iso-thermal).
Raijmakers et al. [45]	LiFePO ₄ / Li(NCA)O ₂	f_0	0.3 – 6.0	-20 – 50	Proposed f_0 as metric based on theoretical analysis.
Richardson et al. [56]	LiFePO ₄	Z'	0.215	-20 – 45	Used ITD + thermocouple to monitor $T(r)$ during drive-cycle.
Zhu et al. [46]	LiFePO ₄	$\phi, Z $	10 – 0.1	-20 – 50	Investigated optimal frequency range for ITD.
Koch and Jossen [54]	LiPo	ϕ, Z''	42 – 0.42	10 – 45	Compared ITD metrics and frequencies based on sensitivities to SoC, SoH and DC-currents.
Richardson et al. [57]	LiFePO ₄	Z'	0.215	-20 – 45	Used ITD + thermal model to monitor $T(r)$ during drive-cycle.
Spinner et al. [3]	LiCoO ₂	Z''	0.3	-20 – 95	Demonstrated ITD up to higher T using secondary fit.
Richardson et al. [58]	LiFePO ₄	Z''	0.215	8 – 30	Used ITD + 2-D thermal model to monitor $T(r, z)$.
Raijmakers et al. [55]	LiFePO ₄	$f_{0.65}$	1.6 – 2.0	-20 – 50	Demonstrated ITD using $f_{0.65}$ in vehicle application.

chemistry. In my own published work, which is discussed in detail later, the real or imaginary part of the impedance at a single frequency is used as the impedance-metric.

The practical implementation of ITD-based methods relies on the ability to rapidly measure EIS spectra online in an electric vehicle or other application. This is an area of research which has received attention in recent years since EIS spectra may be useful for the identification of other important battery parameters such as SoC and SoH [59–63]. Howey et al. demonstrated a method of measuring EIS spectra between 1 Hz and 2 kHz using existing power electronics available in a vehicle [64, 65]. Moreover, accurate impedance measurements were even obtained using a passive approach whereby the noise excitation signal generated by a motor controller was used as the perturbation signal. Various studies have since demonstrated online impedance measurements in a range of applications [66–70]. Recently, Raijmakers et al. demonstrated online impedance measurement for the purpose of ITD [55]. In that study, they used an intercept frequency approach (similar to their earlier work), but a non-zero intercept frequency ($Z'' = 0.65 \text{ m}\Omega$) was chosen in order to minimise the noise arising from currents flowing through the battery pack under operating conditions. This was shown to give an accurate temperature measurement which closely matched the temperature of the negative electrode (which was measured using a thermocouple fixed to the tab), although exact accuracies over the entire cycle are not reported. This work highlighted the fact that issues arise in practical applications that may not be identified by laboratory experiments.

It is apparent from the foregoing discussion that most of the research on ITD has focused on the identification of the optimal impedance metric for a given chemistry and validation of its accuracy, and the development of methods for online implementation. Prior to the work outlined in this thesis (including that which has already been published), ITD had only been used to infer the volume average, or assumed uniform, temperature. However, under typical operating conditions cells exhibit large internal temperature non-uniformities and the average internal temperature may differ greatly from local temperatures, and so an improvement on the existing techniques is required.

1.4 Hybrid methods for non-uniform temperatures

Similar to a conventional surface temperature measurement, ITD alone does not provide a unique solution for the temperature distribution within the cell. In this thesis I propose two novel "hybrid methods" to overcome this issue: (i) combining ITD with an

additional surface temperature measurement (ITD/T), as shown Fig. 1.3c, and (ii) combining ITD with a thermal model (ITD/TM), as shown in Fig. 1.3d.

Each of these methods has unique advantages and disadvantages. ITD/T does not rely on knowledge of the cell thermal properties, heat generation rates or thermal boundary conditions, and so overcomes many of the aforementioned issues relating to thermal parameter estimation. However, it requires both a thermocouple and impedance measurement on each cell and so its instrumentation cost may be prohibitive. Moreover, although it overcomes the requirement for a thermal model, it still relies on an approximation based on assuming the temperature distribution is a second-order polynomial, which (as shown in Section 3.2) may affect the accuracy of the solution when the temperature of the heat transfer fluid varies rapidly. On the other hand, ITD/TM relies on knowledge of the cell electrical/thermal properties and heat generation rates. However, as shown in Section 4.6, some of the thermal parameters may be estimated online; and once these properties have been identified, the cell temperature may be estimated to high accuracy. Moreover, it requires only a single measurement input - the impedance metric - and thus has the potential to substantially reduce instrumentation costs.

Fig. 1.3 and Table 1.2 show the present study in the context of existing temperature estimation techniques, both conventional and impedance-based. Fig. 1.3 shows four different approaches to battery temperature monitoring: (a) and (b) are the conventional method and the impedance-based method, respectively, whereas (c) and (d) are the two hybrid methods proposed in this thesis. Table 1.2 lists a range of studies based on each of these methods, and highlights the chapters corresponding to the novel methods presented in this thesis.

Table 1.2 Comparison of control-oriented/online temperature estimation studies.

Method	Figure	Studies	Model		Measurement	
			1-D	2-D	T_{surf}	ITD
T/TM (1-D)	1.3a	[23–27]	✓		✓	
ITD	1.3b	[42–45]				✓
ITD/T	1.3c	Chapter 3 [56]			✓	✓
ITD/TM (1-D)	1.3d	Chapter 4 [57]	✓			✓
T/TM (2-D)	1.3a	Chapter 6 (Section 6.6) [58]		✓	✓	
ITD/TM (2-D)	1.3d	Chapter 6 (Section 6.7) [58]		✓		✓

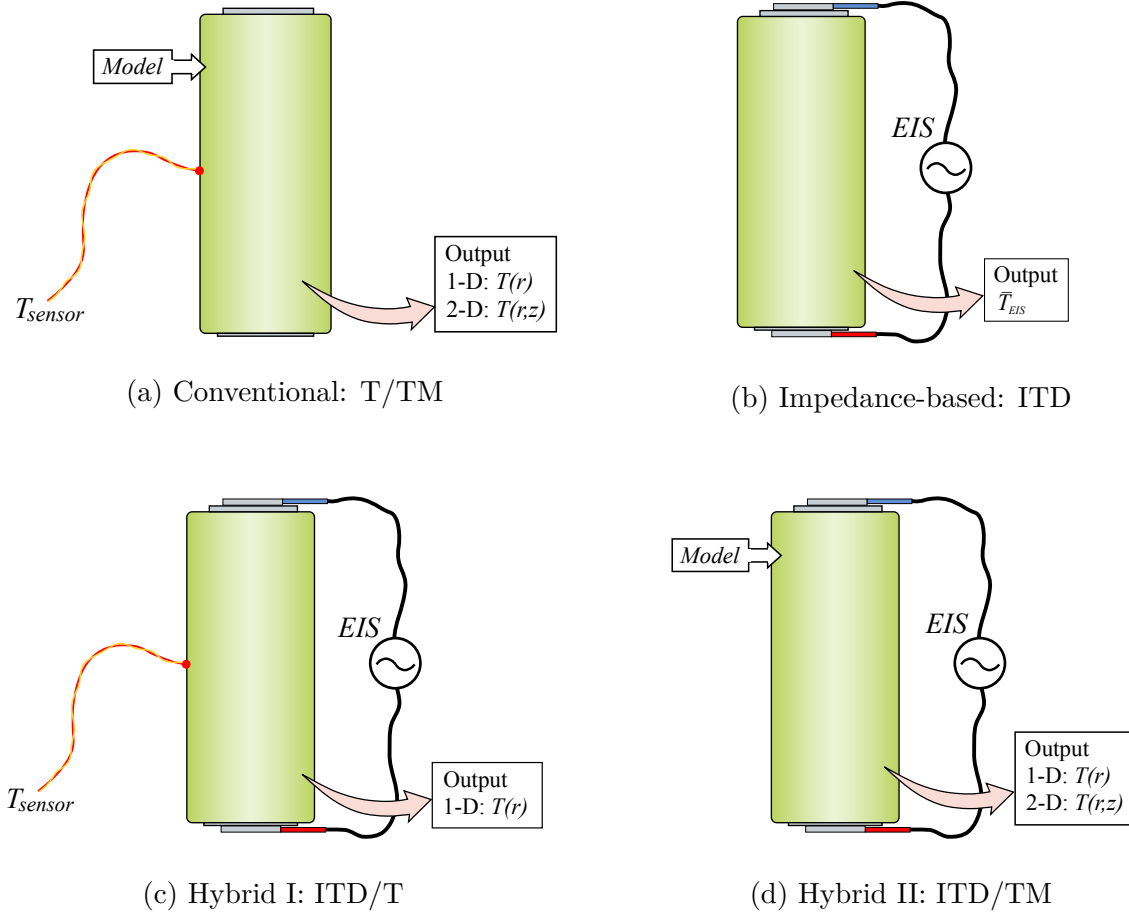


Fig. 1.3 Approaches to battery temperature monitoring. TM = Thermal Model; T = Temperature (measurement); ITD = Impedance Temperature Detection (measurement). Novel contributions of this thesis include the introduction of the hybrid methods, (c) and (d), and an application of the conventional method (a) in 2-D.

1.5 Low-order modelling & state estimation

It is apparent from the foregoing discussion that online thermal modeling is an important consideration for modern battery temperature monitoring schemes², both conventional and impedance-based. The issue of low-order thermal modeling is par-

²Although I should emphasise that not all BMSs include a thermal model. For less demanding applications where thermal effects are less significant, such modelling may not be indispensable. Ultimately, the decision to include a model or not, and how sophisticated that model should be, comes down to a cost-benefit analysis. However, with modern EV and HEV applications temperature estimation is increasingly important. In view of the discussion in Section 1.1.1, an error of about 5 °C would be considered acceptable in typical vehicle applications. Errors greater than this could give rise to unsafe conditions (the maximum temperature of the cell exceeding safety thresholds) or significantly accelerated aging.

ticularly important: a model must be efficient enough to be implementable using a low-cost micro-controller with limited computational power. It is therefore important to identify the most suitable numerical method for the task, and to exploit potential simplifications, for instance by assuming 1-D conditions. Such models are also more amenable to the application of state and parameter estimation techniques, which are necessary for robust online monitoring and control. These issues are discussed in detail below.

1.5.1 1-D assumption

The assumption of 1-D is acceptable for cases in which thermal gradients predominantly arise in one direction. This may occur in practice in cylindrical cells since (i) the thermal conductivity of the cell in the axial direction is often an order of magnitude greater than that in the radial direction since the imperfect contact between layers of the jelly roll structure gives rise to relatively large through plane thermal resistances and (ii) the tabs connecting the current collector to the casing at either end have small cross sections, giving rise to relatively high thermal resistances compared to the radial path. Hence, in some situations the heat transfer from the top and bottom ends may be significantly less than the radial, and so the axial temperature distribution may remain relatively uniform whilst the radial temperature gradient dominates. It may also be applicable to cells connected in series with identical cells on either end - a configuration which may apply to the majority of cells in a large battery pack - since the temperatures of adjacent cells in such a scenario will be similar, provided they receive equal cooling, and so there should be minimal temperature gradient to drive axial heat flux.

As a result of the above characteristics, the 1-D assumption has been used successfully in various studies, although only for small form factor (e.g. 18650 or 26650) cells, cooled via natural convection or transverse forced convection to air [24, 25, 28, 71, 72]. In many other cases of interest, non-negligible 2-D or 3-D temperature gradients may arise. For instance, larger cells inevitably have a greater propensity for thermal gradients in multiple directions. Recent studies have used 45 Ah cylindrical cells with a diameter of 64 mm and height of 198 mm [73]. Such dimensions give rise to much larger Biot numbers and hence more significant thermal gradients. Moreover, certain cooling configurations, such as end cooling via cooling plates, are more likely to give rise to axial thermal dynamics. Fig. 1.4a shows an exemplary case with forced convection via a liquid coolant at the base of the cell and natural convection to the air at the other surfaces. Fig. 1.4b shows another scenario in which unequal cooling of multiple

cells can result in 2-D thermal dynamics as heat is transferred axially through the tabs from one cell to a neighbouring cell.

There are also scenarios in which azimuthal temperature gradients may develop - for instance, if cells are cooled via transverse air cooling, the side of the cell facing the air stream may receive stronger cooling than the side facing away. However, the resulting temperature gradients are likely to be less significant than the axial gradients arising from the examples described above. Hence, for the 2-D examples studied in the present thesis (Chapter 5), the axial component is selected to be incorporated as the second dimension.

The choice of 1-D vs. a higher dimensionality should therefore be made on a case by case basis; the simplicity and efficiency of 1-D makes it an ideal choice if it will suffice, but in more complex cases models capable of capturing 2-D or 3-D thermal dynamics may be necessary. This choice will also inevitably affect the choice of numerical method since certain methods may only be suitable for 1-D simulations, as discussed below.

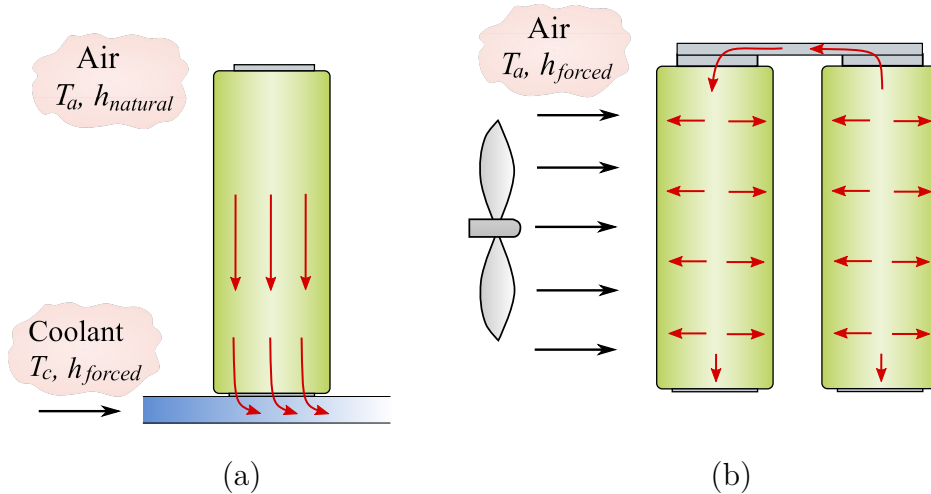


Fig. 1.4 Battery cooling configurations resulting in 2-D thermal dynamics: (a) Plate cooling, (b) unequal cooling with intercell heat transfer

1.5.2 Numerical methods

Conventional numerical methods - such as Finite Difference Methods (FDM) or Finite Element Methods (FEM) - can achieve arbitrary accuracies and are generally applicable to a broad range of problems. Since they solve the underlying diffusion partial differential equation (PDE) governing the cell, their outputs can include the full temperature field throughout the domain of interest. Several studies have presented 2-D or 3-D thermal simulations of battery cells using these approaches [74–77]. However,

these methods are computationally intensive and so their potential for application in control systems is limited. Below, the main alternative methods for efficient/control-oriented battery thermal modelling are discussed³. In this section, a qualitative overview of these methods is provided. For the methods employed in this thesis (notably Polynomial Approximation and Spectral-Galerkin), the quantitative description is delayed until the respective sections.

Thermal equivalent circuits

Lumped parameter thermal equivalent circuit (TEC) models (based on the analogy between electrical and thermal equivalent circuit networks) are perhaps the most popular approach for efficient thermal modelling. These methods have been used extensively for low-order and control-oriented modelling of battery cells and packs [4, 23, 27, 79–83]. A more detailed description can be found in the aforementioned references, however Fig. 1.5 shows two examples of TECs, which are typical of those used in battery thermal modelling. The main advantages of these approaches are that they are simple to implement, and they can easily be applied to multi-dimensional problems. However, they are unable to predict the full temperature field throughout the domain of interest since their outputs merely consist of nodal values representing the average surface temperatures. This is a particular limitation when comparison with temperature measurements at discrete locations is necessary for online state or parameter estimation. Moreover, whilst the parameters of the model do have a physical meaning, their values are lumped and hence do not necessarily reflect the fundamental material properties. This is particularly detrimental to their performance when there is internal heat generation [84]. Although some modified TEC models have been developed to overcome this [85, 84, 86], these are known to have poor performance for large Biot number simulations, whilst increasing the number of elements to improve accuracy comes at the expense of increased computational complexity [87, 88].

Analytical methods

Analytical solutions to battery thermal models have also been developed. Shah et al. introduced fully time-dependent battery thermal models for a 2-D solid cylinder [89] and a 2-D annulus [90]. However these are inappropriate for on-line applications since

³Note that there are various other low-order approaches for modelling heat transfer [78], some of which have been applied to batteries. For instance, Muratori et al. used techniques such as balanced truncation [71, 72] to simulate 1-D battery thermal dynamics. I have chosen to discuss only the most relevant ones here since a detailed discussion of all of these methods is beyond the scope of this work.

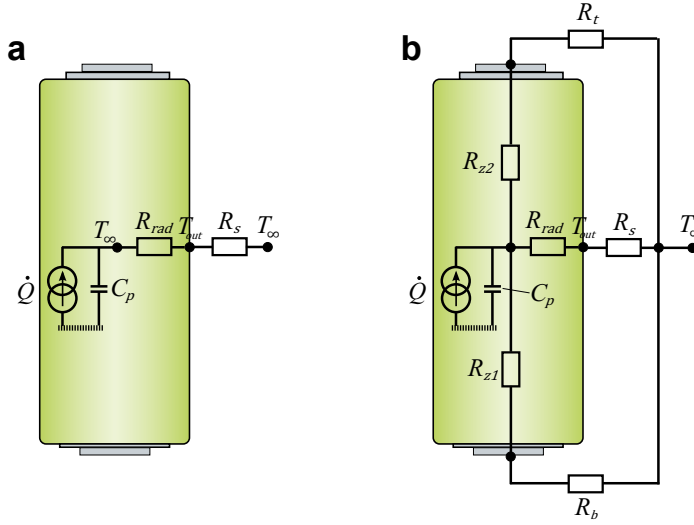


Fig. 1.5 Thermal equivalent circuit (TEC) models based on the analogy between electrical and thermal networks. a) a 1-D TEC model of a cylindrical cell equivalent to that employed in several studies [4, 23, 27, 79, 80]. b) A more sophisticated TEC of the same cell accounting for 2-D effects.

time domain solutions rely on computationally intensive integral transforms. Shah et al. also developed steady-state analytical battery thermal models [91], although these are of little practical use for control-oriented modelling. On the other hand, my work introduced a "pseudo steady-state" method, which combines a pre-calculated analytical steady-state solution with online measurements of impedance and surface temperature. This enables efficient computation of the 1-D temperature distribution, which is suitable for online computation [56]. This method is discussed in detail in Chapter 3.

Polynomial approximation

Polynomial approximation (PA) is a low-order modelling method which is commonly used in heat transfer problems [92]. It is also sometimes referred to as the integral method [93] or the integral heat balance method [94]. PA consists of integrating the governing equation over some domain, and assuming a given form of the solution (usually a polynomial) applies over this domain. Since basic laws are adhered to in an average sense, the resulting model is inherently approximate [92]; however the resulting accuracy is generally satisfactory for engineering applications, even for models with as few as two states. PA is relatively easy for a non-specialist to understand and implement, compared with, for instance, spectral methods; however, it does not have guaranteed convergence properties, and so its accuracy depends on the specific problem under consideration. In general it is only suited to 1-D problems involving infinite or semi-infinite domains, or symmetric boundary conditions [92]; although it has also been used for some steady-state 2-D problems [94].

Recently, PA has been used for battery thermal modelling. Kim et al. presented a 1-D cylindrical battery thermal model based on PA, which was then used in an online state/parameter estimation scheme [24, 25]. For the demonstration of the second hybrid method (ITD/TM) in 1-D, I incorporate the PA from [25] into a thermal-impedance model, as discussed in Chapter 4. I also derive and validate additional PA models for 1-D Cartesian coordinates and a 1-D annulus (Appendix A), which may be used for ITD/TM in their respective geometries. However, for transient 2-D problems PA models are unsuitable (as demonstrated in Appendix B), and so it is necessary to use more advanced numerical methods.

Spectral methods

Spectral methods are an alternative numerical method for solving PDEs. The primary difference between them and conventional methods such as FDM and FEM is that the spatial discretization is carried out using global rather than local approximating functions [95, 96]. For finite domains, this function will typically be a Legendre or Chebyshev polynomial. In general, FDM and FEM are suitable for complex geometries, whereas spectral methods provide greater computational efficiency at the expense of model flexibility.

Spectral methods are a type of weighted residual method - a group of approximation techniques in which the solution errors are minimized in a certain way - and they are classified according to the minimization technique employed. The most common two techniques are spectral-collocation (SC) and spectral-Galerkin (SG). In an SC method, the solution is obtained by interpolating an approximating function at a set of domain nodes, whereas in an SG method, the solution is obtained by forcing the residual of an integral multiplied by a test function to zero. A quantitative introduction to spectral methods is given - by means of a toy example - in Section 5.1.

Spectral methods have been used in previous studies for low-order battery modelling [97–99, 63], and recently they have even been applied to 2-D problems [100]. However, to the best of my knowledge, no study has applied an SG method to 2-D battery thermal problems. This is perhaps due to the complexity of accounting for non-homogeneous boundary conditions, in particular convection boundary conditions, using an SG method. For instance, in the scenario depicted in Fig. 1.4a it is possible for each surface of the cell to be in contact with a different cooling fluid with a different free stream temperature and/or convection coefficient; and this makes the SG method non-trivial to implement.

Chapter 5 presents a novel 2-D model of a cylindrical battery cell based on a Chebyshev spectral-Galerkin method. The model accounts for transient heat generation, anisotropic heat conduction, and non-homogeneous convection boundary conditions, with different convection coefficients and external temperatures at each surface. This generality makes it suitable for simulating the aforementioned cooling configurations, and could not have been achieved using PA methods. Accurate results were obtained using as few as four states, which means that the model can be implemented as efficiently as a typical lumped parameter TEC. Moreover, the accuracy can be improved arbitrarily by increasing the number of basis functions in either dimension.

The SG model is suitable for use in an ITD/TM scheme in 2-D, as demonstrated in Chapter 6; although its use in a conventional temperature monitoring scheme (e.g. an application in 2-D of the conventional T/TM scheme discussed in Section 1.3.1) is also demonstrated in the same chapter. Chapters 5 and 6 are primarily based on our work published in [101] and [58] respectively.

1.5.3 State estimation

As discussed in Section 1.3, state/parameter estimation techniques can be an important element of battery temperature monitoring methods. A state estimator is a system that provides an estimate of the internal state of a dynamic system, from measurements of the input and output of the system. The Kalman filter provides an efficient computational (recursive) means to achieve this for a system perturbed by white noise, in a way that minimizes the mean of the squared error between the measurement and the prediction (see ref. [102] for further information on Kalman filtering). Kalman filters have been applied extensively to battery problems, primarily for the estimation of SoC and SoH [103–110]. Most of these studies followed from Plett’s seminal work on extended Kalman filtering (EKF) and dual extended Kalman Filtering (DEKF) for estimating the SoC and SoH respectively of a LiPB cell [108–110].

Relatively fewer studies have used Kalman filtering techniques for temperature monitoring. The first such studies to the authors knowledge are those of Lin et al. [26, 27] and Kim et al. [24, 25], which consider estimation of temperature in a thermal equivalent circuit and of the volume average temperature and temperature gradient in a polynomial approximation model, respectively. Recently, there have been many further studies which consider similar approaches for different thermal models and cell chemistries, e.g. [111–113]. However, with the exception of the work presented in this thesis, there are no impedance-based temperature monitoring studies which use Kalman filtering or

state estimation, or which combine impedance measurements with a thermal model. This is one of the key novel aspects of the present work.

1.6 Research focus and contributions

The focus of this research is on the application of ITD to non-uniform temperatures. Its purpose is to answer the question:

How can the (possibly non-uniform) temperature distribution of a cell be estimated using measurements of the EIS-based volume average temperature?

Broadly speaking, addressing this question has involved: (i) introducing novel hybrid methods to battery monitoring (as discussed in Section 1.4) and (ii) developing low-order modeling methods to use with these hybrid methods (as discussed in Section 1.5). Fig. 1.6 shows some of the main areas of ITD-based research; the subfields highlighted in green are the focus of the present work. Specific contributions of this thesis are summarised as follows:

1. Proposed novel conceptual approaches to battery temperature monitoring, based on combining impedance-based methods with a thermal model and/or discrete temperature measurements. (Chapters 3 and 4)
2. Experimentally demonstrated ITD/T under laboratory conditions with imposed 1-D thermal dynamics. This was the first time an ITD-based method was validated experimentally against internal thermocouple measurements. (Chapter 3)
3. Experimentally demonstrated ITD/TM under laboratory conditions with imposed 1-D thermal dynamics. (Chapter 4)
4. Derived and validated PA thermal models for a 1-D annulus and for a 1-D cartesian geometry with symmetric boundary conditions. These models are suitable for ITD/TM in their respective geometries. (Appendix A)
5. Demonstrated that PA is suitable for a limited class of 2-D problems involving symmetric boundary conditions, but unsuitable in general for transient 2-D modelling. (Appendix B)
6. Developed a novel low-order 2-D thermal model based on a spectral-Galerkin method. The model is capable of predicting arbitrary temperature fields to high accuracy with as few as 4 states, and is therefore suitable for ITD/TM (or other online temperature monitoring techniques) in 2-D. (Chapter 5)

7. Experimentally demonstrated ITD/TM under conditions involving 2-D thermal dynamics. (Chapter 6)

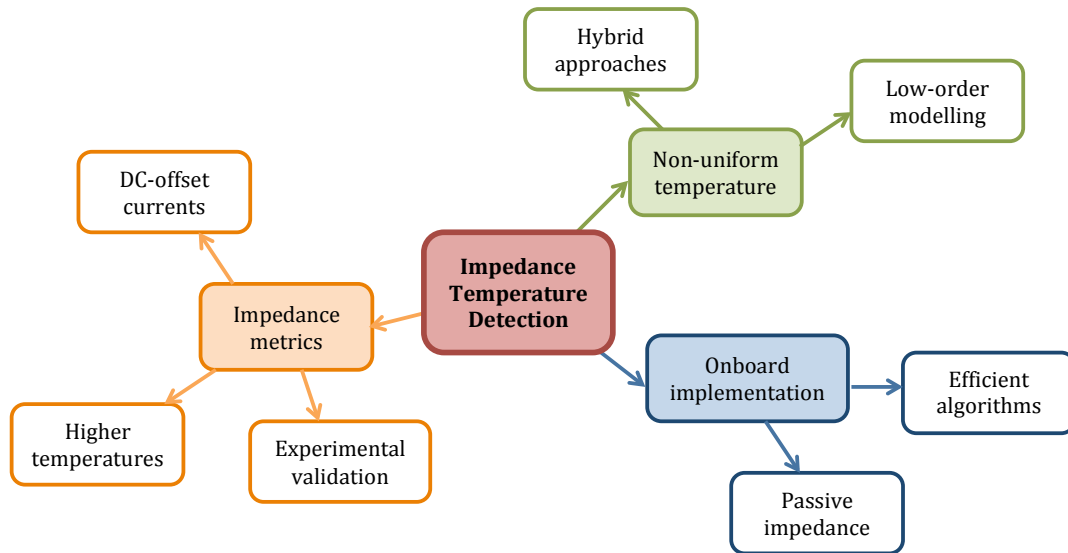


Fig. 1.6 Research areas related to impedance temperature detection. The box labeled “Non-uniform temperature” and its associated subfields are the focus of this thesis.

1.7 Outline of thesis

Chapter 1 (Introduction) has introduced the importance of thermal aspects of lithium-ion batteries, described the conventional and impedance-based approaches to battery temperature monitoring and highlighted the contributions of the present work towards applying the ITD method to problems with non-uniform temperature distributions.

Chapter 2 (Impedance Temperature Detection in 1-D) presents a mathematical analysis of impedance measurement for non-uniform temperatures under 1-D conditions, and describes the experimental procedure for calibrating the EIS-metric against temperature for the experiments in the first part of the thesis.

Chapter 3 (Hybrid Method I: ITD/T) presents the first of the two hybrid methods to temperature estimation considered in this thesis, ITD/T, including the results of validation experiments with an EV drive cycle.

Chapter 4 (Hybrid Method II: ITD/TM) presents the second method, ITD/TM, including results of validation experiments, along with the application of state and

parameter estimation techniques for robust temperature monitoring when the convection coefficient is unknown.

Chapter 5 (Spectral-Galerkin model) presents a low-order 2-D thermal model based on a spectral-Galerkin method, including its validation against a high fidelity finite element method.

Chapter 6 (Hybrid Method II (2-D)) presents ITD/TM in 2-D using the aforementioned spectral-Galerkin model, including experimental validation and state estimation.

Chapter 7 (Conclusions and further work) summarises the work undertaken in this thesis and makes suggestions for future work.

Appendix A (Polynomial Approximation: application to other geometries) presents the derivation and validation of two additional PA models: 1-D Cartesian coordinates and a 1-D annulus, which are suitable for ITD/TM in their respective geometries.

Appendix B (Polynomial Approximation: application to 2-D problems) presents a PA model for a 2-D cylinder, demonstrating the limitations of PA for transient 2-D problems.

Part I

Temperature Monitoring in 1-D

Chapter 2

Impedance Temperature Detection in 1-D

This chapter presents some preliminary material on ITD, which is relevant to the subsequent analysis in Chapters 3 and 4. Section 2.1 presents an analysis of impedance under non-uniform temperatures in 1-D, resulting in an expression relating the overall cell impedance to the temperature distribution. Section 2.2 describes the experimental setup (Section 2.2.1) and procedure (Section 2.2.2) for calibrating the EIS-metric against temperature, and discusses the results of these experiments (Section 2.2.3). The results show that the impedance at 215 Hz is highly dependent on temperature but approximately independent of SoC, and that the corresponding impedance-temperature relationship can be approximated by a second-order polynomial fit.

In Chapters 3 and 4, the real part of the impedance, Z' , is used as the temperature dependent parameter, and so the mathematical treatment presented in the next section is applied to Z' . However, it should be noted that similar relationships exist for other impedance parameters (such as the imaginary part of impedance, the phase shift etc.), and so these could also be used as the impedance-based inputs to the model.

2.1 Impedance for non-uniform temperature distributions

As discussed in Chapter 1, the principle of galvanostatic EIS is to apply a small single-frequency sinusoidal current signal and measure the voltage response from a cell, which depends on the impedance. The impedance, Z , is then defined as the transfer

function of the voltage U with respect to the current I :

$$Z(j\omega) = \frac{U(j\omega)}{I(j\omega)} = Z'(\omega) + jZ''(\omega), \quad (2.1)$$

with $\omega = 2\pi f$, where j is the imaginary number and f is the frequency, and Z' and Z'' are the real and imaginary parts of the impedance, respectively. The inverse of cell impedance is the admittance, given by

$$Y(j\omega) = \frac{1}{Z(j\omega)} = Y'(\omega) + jY''(\omega). \quad (2.2)$$

Since admittances in parallel are additive, it is more straightforward to use admittance than impedance in the following analysis. The specific admittance (or admittivity), denoted y in this study, is the admittance per unit area, in analogy to conductance and conductivity in a resistive circuit. If the admittance throughout a cell is uniform, the admittivity is given by

$$y(j\omega) = \frac{Y(j\omega)}{A} = y'(\omega) + jy''(\omega), \quad (2.3)$$

where A is the cross sectional area and $y'(\omega)$ and $y''(\omega)$ are the real and imaginary parts of the local admittivity respectively. A cylindrical cell with a continuous temperature distribution in the radial direction is equivalent to an infinite number of concentric annuli, each of which has radius r , thickness dr , and height H , as shown in Fig. 2.1.

Since admittivity varies with temperature (as discussed below), the admittance of each infinitesimal annulus depends on the temperature at that radius. Since each of the elements are electrically connected in parallel, and admittances in parallel are additive, the admittance of the entire cell is therefore

$$Y(j\omega) = \int_A y(r, j\omega) dA, \quad (2.4)$$

provided that the admittivity varies in the radial direction only. Substituting A with $\pi(r_{out}^2 - r_{in}^2)$ and dA with $2\pi r dr$, and simplifying, yields

$$Y(j\omega) = 2\pi \int_{r_{in}}^{r_{out}} r y(r, j\omega) dr, \quad (2.5)$$

where r_{in} and r_{out} are the inner and outer radii of the cell active material. It follows that the real part of the admittance at a single frequency is related to the real part of

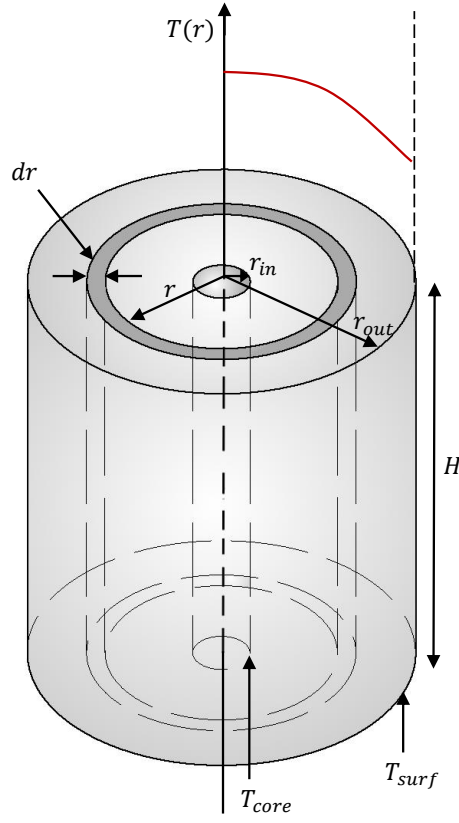


Fig. 2.1 The cell jelly-roll with a continuous temperature distribution in the radial direction modelled as an infinite number of radially arranged volumetric elements of radius r , thickness dr , and height H .

the admittivity at that frequency by

$$Y'_{\omega_1} = 2\pi \int_{r_{in}}^{r_{out}} r y'_{\omega_1}(r) dr, \quad (2.6)$$

where the subscript ω_1 denotes admittance at the frequency ω_1 . The relationship between Y'_{ω_1} and uniform cell temperature can be approximated by a second order polynomial fit from experimental data:

$$Y'_{\omega_1} = a_1 + a_2 T_{uniform} + a_3 T_{uniform}^2, \quad (2.7)$$

where $T_{uniform}$ is the uniform cell temperature and a_1 , a_2 and a_3 are the fitting coefficients. Note that Eq. (2.7) is only valid when the cell temperature is actually uniform (and Y'_{ω_1} is a monotonic function of T in the range of interest). If the temperature distribution is non-uniform, then ITD can be viewed as identifying an EIS-

based volume average temperature $\bar{T}_{EIS}$, which I define as the uniform cell temperature that would give rise to the measured EIS:

$$Y'_{\omega_1} = a_1 + a_2 \bar{T}_{EIS} + a_3 \bar{T}_{EIS}^2. \quad (2.8)$$

As discussed in Section 2.2, an Arrhenius fit was also obtained; however, the second order polynomial fit is used in this analysis since it closely matches the Arrhenius fit but facilitates a less complex analytical solution, and thus faster online computation.

We now wish to obtain an expression involving the local radially resolved temperature. Dividing Eq. (2.7) by A , we get the following expression for the admittivity:

$$y'_{\omega_1}(r) = \frac{a_1 + a_2 T(r) + a_3 T^2(r)}{A}. \quad (2.9)$$

Substituting (2.9) into (2.6), replacing A with $\pi(r_{out}^2 - r_{in}^2)$, and rearranging, gives an expression relating the measured admittance to the temperature distribution:

$$Y'_{\omega_1} = \frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r \left(a_1 + a_2 T(r) + a_3 T^2(r) \right) dr. \quad (2.10)$$

The term on the left hand side of this equation is our chosen EIS-metric: the real part of the admittance of the entire cell at the selected frequency, ω_1 .

Comment 1: It should be noted that Y'_{ω_1} is a scalar function of the internal temperature distribution but does not uniquely identify the temperature distribution. Therefore, additional information and/or assumptions are required, and these are the basis of the approaches described in the following chapters. In the ITD/T approach (Chapter 3), additional information is obtained from a surface temperature measurement and an assumption on the form of the temperature distribution. In the ITD/TM approach (Chapter 4), the use of a low-order thermal model is sufficient to ensure a unique solution.

Comment 2: Although it is not required in the later analysis, it is worth noting that an explicit expression for $\bar{T}_{EIS}$ can be found by equating the R.H.S. of Eq. (2.8) and (2.10), and solving the resulting quadratic equation (noting that the a_1 terms on each side cancel):

$$\bar{T}_{EIS} = -\frac{a_2}{2a_3} \pm \sqrt{\frac{a_2^2 (r_o^2 - r_i^2) + 8a_3 \left(a_2 \int_{r_i}^{r_o} r T(r) dr + a_3 \int_{r_i}^{r_o} r T(r)^2 dr \right)}{r_o^2 - r_i^2}} \quad (2.11)$$

Since the impedance temperature relationship is non-linear, the above expression is not necessarily equal to the standard volume average temperature, which in the 1-D case is given by

$$\bar{T} = \frac{2}{r_o^2 - r_i^2} \int_{r_i}^{r_o} r T(r) dr. \quad (2.12)$$

However, it should be noted that the two are typically close in value, particularly if the temperature variation within the cell is small (in the 2-D cases considered in Part II of this thesis, we do in fact make the assumption that $\bar{T}_{EIS}$ can be approximated by $\bar{T}$ in order to simplify the analysis).

2.2 Calibration experiments

2.2.1 Setup

In order to demonstrate the techniques on a real cell, experiments were carried out with a 2.3 Ah cylindrical cell (A123 Model ANR26650 m1-A) with LiFePO_4 positive electrode and a graphite negative electrode. The properties of the cell are given in Table 2.1. The cell was fitted with two thermocouples, one on the surface and another inserted into the core via a hole which was drilled in the positive electrode end. Cell cycling and impedance measurements were carried out using a Biologic HCP-1005 potentiostat/booster. The impedance was measured using Galvanostatic Impedance Spectroscopy (GEIS) with a 200 mA peak-to-peak perturbation current. The environmental temperature was controlled with a Vötsch VT4002 thermal chamber. The chamber includes a fan which operates continuously at a fixed speed during operation. Photos of the test equipment and a schematic of the experimental setup are shown in Fig. 2.2. The above description applies to the calibration experiments described in the following subsection (2.2.2), and to the validation experiments described in Chapters 3 and 4.

Table 2.1 Properties of the lithium-ion cell used for validation.

Model	A123 ANR-26650 m1-A	Nominal voltage	3.3 V
		Nominal capacity	2.3 Ah
Anode material	Graphite	Cell housing length	65 mm
Cathode material	LiFePO_4	Cell outer diameter	26 mm

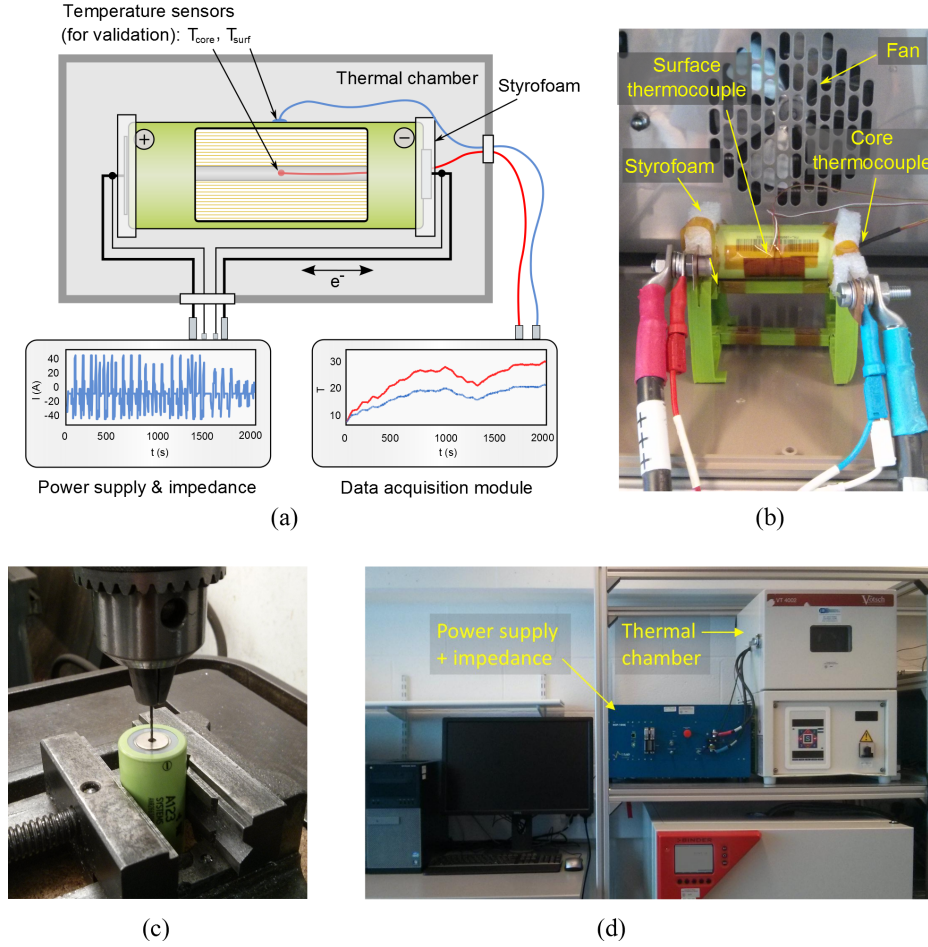


Fig. 2.2 Experimental setup for calibration experiments (and for validation experiments described in later chapters). (a) Schematic diagram with cutaway view showing cell core and jelly roll, (b) cell drilling procedure, (c) prepared cell inside thermal chamber, (d) power supply & thermal chamber.

2.2.2 Procedure

In order to calibrate the impedance against temperature, EIS measurements were conducted on the cell in thermal equilibrium conditions over a temperature range of -20°C to $+45^{\circ}\text{C}$ in intervals of 5°C , and over a range of 10-90% SoC in intervals of 20%. The EIS frequency range spanned 1 kHz to 1 Hz with 10 frequencies per decade and 3x averaging. The cell capacities at each temperature were first determined with a constant current constant voltage (CCCV) charge/discharge, with upper and lower cutoff voltages of 2.0 and 3.6 V respectively. The SoC was then adjusted to the required values by drawing a 0.9 C current. At each SoC, the cell was allowed to rest to ensure its temperature had equilibrated, which typically occurred in less than 2 hrs. This was

verified when the temperatures registered by the internal and surface thermocouples were within 0.2 °C and repeated impedance measurements over a 20 minute period yielded identical results.

2.2.3 Results

Fig. 2.3 shows an example impedance spectrum at a uniform cell temperature of 10°C, and various states of charge, over the frequency range 1 Hz to 1 kHz. It can be seen from this figure that the impedance at $f > 100$ Hz is approximately independent of SoC at this temperature. This is due to the fact that the impedance in this range is located on the high frequency semicircle of the Nyquist plot for this particular battery chemistry. As discussed in Section 1.2, the high frequency semicircle is primarily due to the SEI layer resistance, which is known to be independent of SoC [21], and is independent of the charge transfer and double layer capacitor resistances, which do depend on SoC. The frequency for temperature evaluation was hence chosen to be 215 Hz, since this was high enough to ensure negligible variation with SoC, while at higher frequencies the variation of impedance with temperature decreases (see Figs. 2.4 and 2.5). Similar behaviour is exhibited at the other investigated temperatures, such that the uncertainty in temperature predicted due to variation in SoC is never greater than 2°C. Therefore subsequent results focus on the 50% SoC behaviour only.

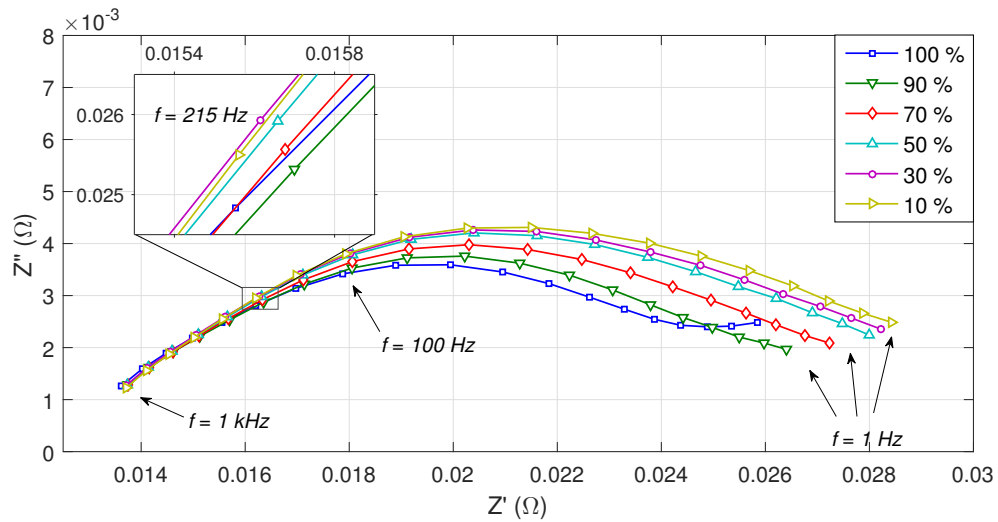


Fig. 2.3 Impedance at 10°C and various states of charge over the frequency range 1 kHz to 1 Hz. Note that the x and y axis scales are equal in this plot. Inset: Impedance at $f = 215$ Hz. Above this frequency the real part of the impedance is approximately independent of SoC.

Fig. 2.4 shows the full impedance spectrum at 50% SoC over the temperature range -20 to 45°C . Both the real and imaginary impedance vary by an order of magnitude over this temperature range, demonstrating the high sensitivity of impedance to temperature in this range. Fig. 2.5 shows a Bode plot of the impedance at 50% SoC. It is evident that both the real and imaginary impedance decrease consistently as temperature is increased at all frequencies, including at $f = 215$ Hz. It is also evident that toward the high end of the temperature range, the variation of impedance with temperature decreases. However, up to temperatures of 45°C the impedance monotonically increases with temperature.

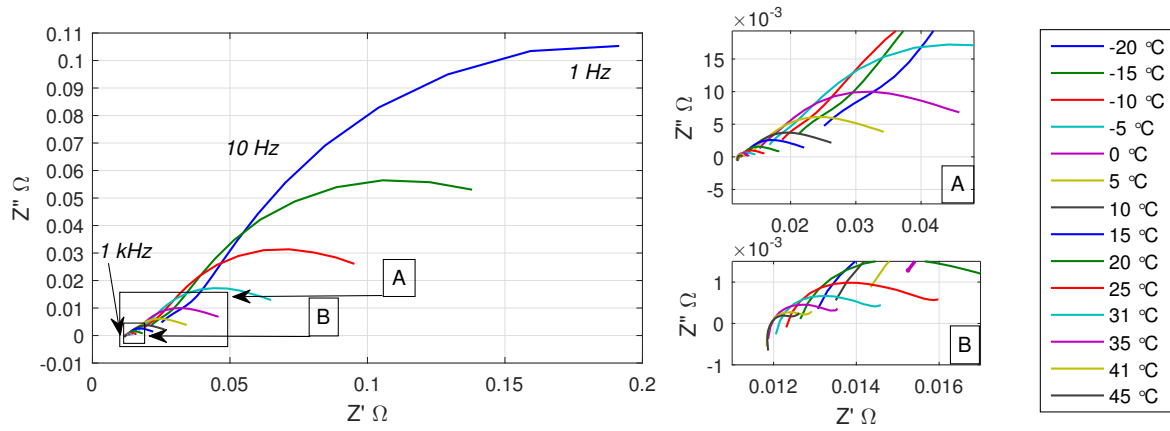


Fig. 2.4 Nyquist plots of impedance at 50% SoC at various temperatures over the range $f = 1$ Hz – 1 kHz. Note that the x and y axis scales are equal in these plots.

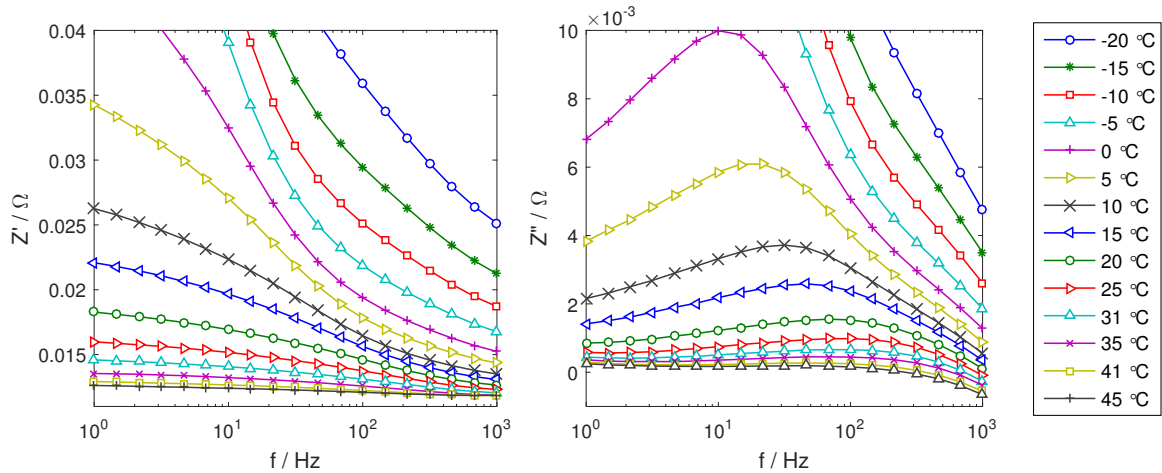


Fig. 2.5 Bode plots of Z' (left) and Z'' (right) at 50% SoC at various temperatures over the frequency range 1 Hz - 2 kHz.

The real impedance is expected to have an Arrhenius dependence on temperature, of the form

$$Z'(T) = k \cdot \exp\left(\frac{E_a}{RT}\right), \quad (2.13)$$

where k is a constant, E_a is the activation energy and R is the universal gas constant. Similar to [44], the electrical conductivity of the current collector was considered as constant over the investigated temperature range and so a constant resistance R_{col} was subtracted from the measured real impedance Z'_{meas} in order to obtain the active material impedance Z' :

$$Z'(T) = Z'_{meas}(T) - R_{col}. \quad (2.14)$$

The resulting cell impedance and Arrhenius fit are shown in the plot on the left in Fig. 2.6 (*left*), whilst the plot on the right shows the real admittance against temperature. In addition to an Arrhenius fit, this plot includes a quadratic polynomial fit directly to the admittance of the active material, $Y'(T) = 1/Z'(T)$. Both fits show good agreement with the experimental data ($R^2 > 0.99$ in each case), however the polynomial fit was used in the present model as previously discussed. The coefficients of the fitted polynomial are the values of a_1 , a_2 and a_3 used in Eq. (2.7), to relate admittance to temperature.

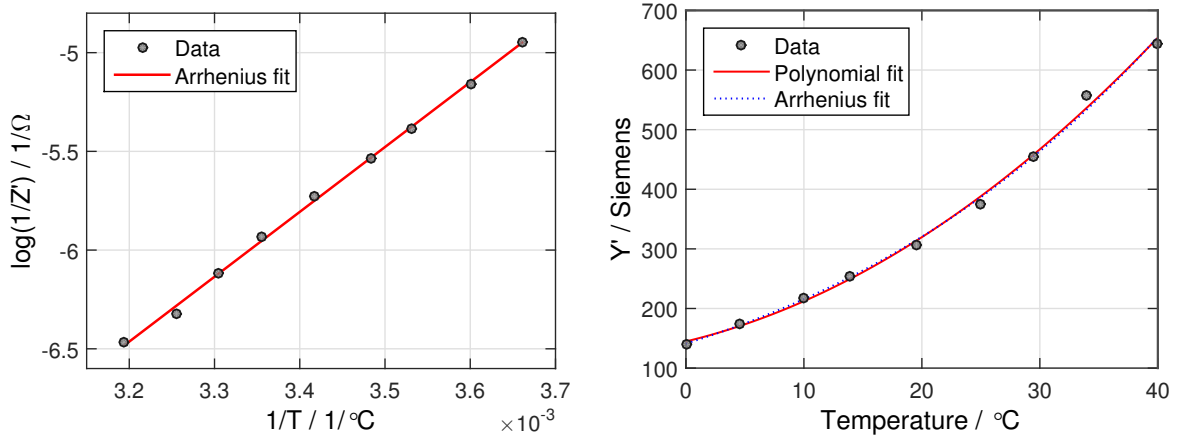


Fig. 2.6 *Left*: Arrhenius fit to the measured impedance (at $f = 215$ Hz and SoC = 50%), accounting for the constant resistance of the current collector. *Right*: Comparison of different fits to the experimental admittance vs. temperature data. Directly fitting a 2nd order polynomial to the admittance (blue line) gives approximately equivalent results to the Arrhenius fit.

Chapter 3

Hybrid Method I: ITD/T

This chapter presents the first of two hybrid methods for estimating non-uniform temperature in a cell under 1-D conditions: Impedance Temperature Detection with a surface temperature measurement (ITD/T). Section 3.1 provides a description of the method, in which a unique solution for the temperature distribution is obtained using two inputs - the real part of the impedance and the surface temperature - combined with an assumption on the

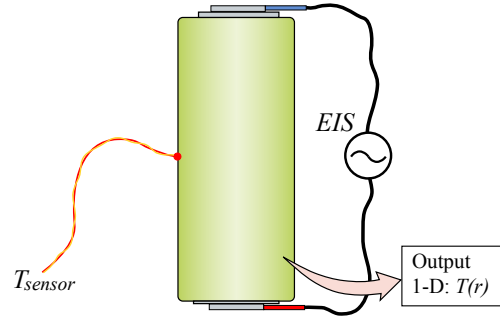


Fig. 3.1 ITD/T

form of the temperature distribution, identified by the solution of the steady state heat equation. This method does not require knowledge of cell thermal properties, heat generation or thermal boundary conditions. In Section 3.2, the validity of the assumed form is verified by comparison with an exact analytical solution of the transient heat equation in the frequency domain. Finally, in Section 3.3, the method is validated experimentally using the setup described in the previous chapter. The cell is heated by applying (1) current pulses of up to ± 20 A and (2) a 3500 s HEV drive cycle current profile, whilst monitoring the surface and core temperatures and measuring impedance at 215 Hz. During the drive cycle test, the battery core temperature increases by 20°C and the surface temperature increases by 14°C . The mean absolute error in the predicted maximum temperature throughout the cycle is 0.6°C (3% of the total core temperature increase), in contrast to a mean absolute error of 2.6°C if the temperature is assumed to be uniform (13% of the total core temperature increase).

This chapter is primarily based on our work published in [56], which was the first time ITD had been used to estimate non-uniform temperatures and the first time an ITD method had been validated experimentally.

3.1 Description of method

The method uses two measurement inputs - the real part of the impedance and the surface temperature - combined with an assumption on the form of the distribution to obtain a unique solution for the temperature distribution. The assumption is based on an analytical solution of the 1-D steady state cylindrical heat equation with uniform heat generation throughout the active material.¹ As shown in the following section, this equation can be solved offline using only knowledge of the cell dimensions, resulting in an expression for the temperature distribution as a function of the two measurement inputs, T_{surf} and Z' . The online measurements are then substituted into the expression and the temperature at the core (or any other desired radial location) is evaluated. This offline/online strategy was chosen as it results in an efficient numerical model which could be solved in real time in an online BMS. Since the cell does not actually operate at steady-state, the temperature profile will vary dynamically according to the heat generation history. However, since the steady-state solution only affects the "shape" of the temperature profile, whereas the absolute value is determined by the measurement inputs, the accuracy of the solution remains acceptable even for transient problems. Hence I denote this as a Pseudo Steady-State (PSS) approximation. Indeed, as the results in Section 3.3.2 show, the error introduced by the PSS approximation is relatively small for inputs based on a typical HEV drive cycle. An overview of the process is shown in Figure 3.2, and described below.

Offline: The calibration experiments (Section 2.2) provide values of Z'_{exp} at a range of temperatures (T_{exp}). From these, the coefficients of the polynomial (a_1 , a_2 and a_3) are obtained by least-squares fit (LSq Fit). These values, and the cell dimensions (r_{in} and r_{out}) are entered into the PSS algorithm (Section 3.1.1 - 3.1.2) to produce an analytical expression for the core temperature (or temperature at any radial location) as a function of T_{surf} and Z' (Eq. 3.4).

Online: The surface temperature is monitored whilst the voltage and current measurements are used to calculate Z' (using an online impedance technique such as [64]).

¹ It is clear that by reducing the model to a 1-D heat equation, several physical features are neglected, in particular the aluminium case and tabs. As discussed in Section 1.5, such simplifying assumptions are often necessary to achieve the desired computational efficiency for online modelling. Appendix C provides an analysis justifying these assumptions in the present case.

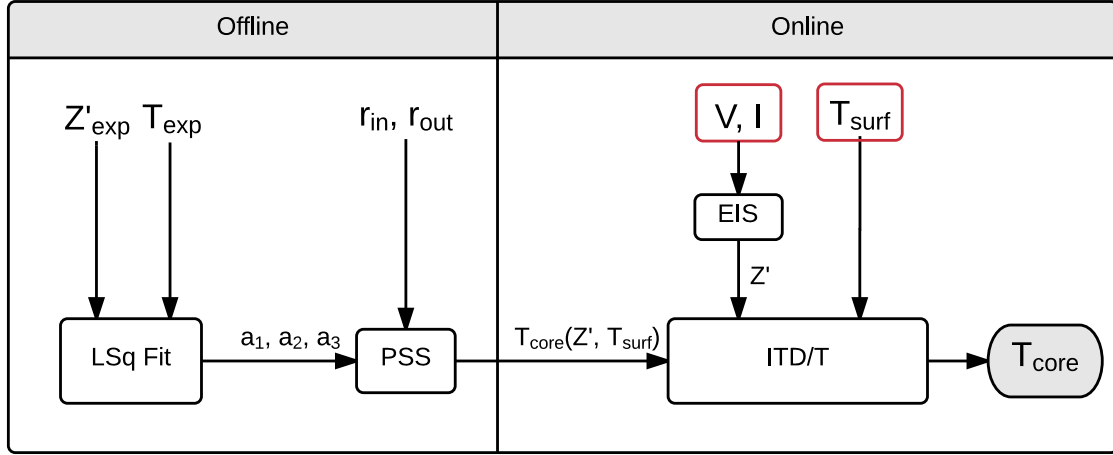


Fig. 3.2 ITD/T process flowchart.

Finally, these values are substituted into the stored analytical expression to give the desired output (T_{core}).

3.1.1 Steady-state thermal model

The one-dimensional steady-state solution to the heat equation for an annulus with uniform heat generation is [114]:

$$T(r) = T_{surf} + \zeta - \frac{\ln(r_{out}/r)}{\ln(r_{out}/r_{in})} (\zeta + T_{surf} - T_{core}), \quad (3.1)$$

where

$$\zeta = \frac{\dot{q} r_{out}^2}{4k} \left(1 - \frac{r^2}{r_{out}^2} \right). \quad (3.2)$$

At the inner surface of the active material, the rate of heat flow will be zero at steady-state, since the central mandrel does not generate heat. The temperature distribution can therefore be obtained as a function of r and the parameters r_{in} , r_{out} , T_{core} and T_{surf} only (i.e. it is independent of $\dot{q}$ and k). By differentiating Eq. (3.1) with respect to r , to obtain dT/dr , and setting the heat flux, q_i'' , to zero at $r = r_{in}$, the following boundary condition for the heat flux at the inner surface is obtained:

$$q_i'' = \frac{\dot{q} r_{in}}{2} - \frac{k(\zeta + T_{surf} - T_{core})}{r_{in} \ln(r_{out}/r_{in})} = 0. \quad (3.3)$$

By solving both equations (3.1) and (3.3) for $\dot{q}/k$, and equating the results, an expression for the temperature distribution, $T(r)$, which is independent of $\dot{q}$ and k , is obtained:

$$T(r) = T_{surf} + \frac{\eta r_{out}^2}{4} \left(1 - \frac{r^2}{r_{out}^2}\right) - \left[\frac{\eta r_{out}^2}{4} \left(1 - \frac{r^2}{r_{out}^2}\right) + T_{surf} - T_{core} \right] \frac{\ln(r_{out}/r)}{\ln(r_{out}/r_{in})}, \quad (3.4)$$

where

$$\eta = \frac{4(T_{surf} - T_{core})}{r_{out}^2 - r_{in}^2 (2 \ln(r_{out}/r_{in})) + 1}. \quad (3.5)$$

3.1.2 Constrained impedance model

Recall from Chapter 2 that the measured admittance is related to the temperature distribution by:

$$Y'_{\omega_1} = \frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r (a_1 + a_2 T(r) + a_3 T^2(r)) dr. \quad (2.10)$$

Substituting the solution for $T(r)$ (Eq. 3.4) into the above equation (Eq. 2.10), and integrating with respect to r over the interval r_{in} to r_{out} , gives an equation which relates measured cell admittance, Y_{ω_1} , to the parameters r_{in} , r_{out} , T_{core} and T_{surf} . The only unknown in this equation is T_{core} , the maximum temperature at the inner surface of the jelly roll. This simplifies to a quadratic equation of the form

$$T_{core}^2 + \alpha T_{core} + \beta = 0, \quad (3.6)$$

where α and β are terms containing r_{in} and r_{out} (which are known a priori), and T_{surf} and Y'_{ω_1} (which are measured in real time).

3.2 Frequency analysis

In this section the validity of the PSS approximation is investigated numerically. Specifically, its frequency response is compared with that of an exact analytical solution of the *transient* heat equation. For simplicity, it is assumed to be a solid cylinder (i.e. the inner radius is zero). In Sections 3.2.1 and 3.2.2 the analysis for the exact transient solution and the PSS approximation are presented and in Section 3.2.3 the corresponding results are presented and discussed.

3.2.1 Exact transient solution

The heat equation for 1D transient heat conduction in a cylinder is given by the following Boundary Value Problem (BVP) [71]:

$$\rho c_p \frac{\partial T(r, t)}{\partial t} = k \frac{\partial^2 T(r, t)}{\partial r^2} + \frac{k}{r} \frac{\partial T(r, t)}{\partial r} + \frac{Q(t)}{V_b}, \quad (3.7a)$$

where ρ , c_p and k are the density, specific heat capacity and thermal conductivity respectively, V_b is the cell volume, and Q is the heat generation rate. The boundary conditions are given by:

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=r_{out}} = -\frac{h}{k}(T(r_{out}, t) - T_{\infty}(t)), \quad (3.7b)$$

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=0} = 0, \quad (3.7c)$$

where T_{∞} is the temperature of the heat transfer fluid, and h is the convection coefficient.

Muratori et al. showed that the above problem can be solved analytically using a Laplace transform method [71]. First, the time domain PDE of (Eq. 3.7a) is transformed into an equivalent ODE problem in the frequency domain. The Laplace transform of Eq. (3.7) is given by

$$a^2 T(r, s) = \frac{\partial^2 T(r, s)}{\partial r^2} + \frac{1}{r} \frac{\partial T(r, s)}{\partial r} + \frac{Q(s)}{k V_b}, \quad (3.8a)$$

with boundary conditions:

$$\left. \frac{\partial T(r, s)}{\partial r} \right|_{r=r_{out}} = -\frac{h}{k}(T(r_{out}, s) - T_{\infty}(s)), \quad (3.8b)$$

$$\left. \frac{\partial T(r, s)}{\partial r} \right|_{r=0} = 0, \quad (3.8c)$$

where $a = \sqrt{\frac{\rho c_p s}{k}}$. The solution to Eq. (3.8) is of the form:

$$T(r, s) = \frac{1}{k a^2} Q(s) + C_1(s) J_0(ar) + C_2(s) Y_0(ar), \quad (3.9)$$

where $Q(s)$ is the transform of $Q(t)$, and J_i and Y_i are the i^{th} -order Bessel functions of the first kind [115]. The constants C_1 and C_2 are found by substituting Eq. (3.9) into

the expressions for the boundary conditions, Eqs. (3.8b)-(3.8c), and evaluating:

$$C_1 = \frac{\frac{h}{k_t}(T_\infty(s) - \frac{1}{ka^2}Q(s))}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}, \quad (3.10)$$

$$C_2 = 0. \quad (3.11)$$

The temperatures at the core and surface of the cell are then found by evaluating Eq. (3.9) at $r = 0$ and $r = r_{out}$, respectively:

$$T_{core}(s) = \frac{1}{k_t a^2}Q(s) + \frac{\frac{h}{k_t}(T_\infty(s) - \frac{1}{ka^2}Q(s))}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}, \quad (3.12)$$

$$T_{surf}(s) = \frac{1}{k_t a^2}Q(s) + \frac{\frac{h}{k_t}(T_\infty(s) - \frac{1}{ka^2}Q(s))}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}J_0(ar_{out}), \quad (3.13)$$

Eqs. (3.12) and (3.13) can be interpreted as the outputs of a continuous time dynamic system [71], where $\mathbf{u}(t) = [Q(t), T_\infty(t)]^T$ and $\mathbf{y}(t) = [T_{core}(t), T_{surf}(t)]^T$, such that the solution of the BVP is equivalent to the impulse response of the system:

$$\begin{bmatrix} T_{core}(s) \\ T_{surf}(s) \end{bmatrix} = \begin{bmatrix} H_{11}(s) & H_{12}(s) \\ H_{21}(s) & H_{22}(s) \end{bmatrix} \begin{bmatrix} Q(s) \\ T_\infty(s) \end{bmatrix} \quad (3.14)$$

where the $\mathbf{H}$ matrix is formed by the transfer functions:

$$H_{11}(s) = \frac{1}{k_t a^2} \frac{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out}) - \frac{h}{k_t}}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}, \quad (3.15)$$

$$H_{12}(s) = \frac{\frac{h}{k_t}}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}, \quad (3.16)$$

$$H_{21}(s) = \frac{1}{k_t a^2} \frac{-aJ_1(ar_{out})}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}, \quad (3.17)$$

$$H_{22}(s) = \frac{\frac{h}{k_t}J_0(ar_{out})}{\frac{h}{k_t}J_0(ar_{out}) - aJ_1(ar_{out})}. \quad (3.18)$$

Note that the Laplace variable, $s = j\omega$, is contained within the a term, as defined previously ($a = \sqrt{\rho c_p s / k}$). The above system of transfer functions gives frequency responses for the exact transient solution results plotted in Fig. 3.3.

3.2.2 Pseudo steady-state approximation

Using a similar approach, we can develop an analytical solution for the PSS approximation, where we denote the new transfer function $\mathbf{H}_{PSS}(s)$. In this case, both the volume-averaged cell temperature (identified via the impedance²) and the surface temperature are measured directly, and it is assumed that no other information is available (as discussed in the previous section).

Setting the inner radius to zero, the approximate temperature profile (Eq. (3.4)) simplifies to

$$T(r) = T_{surf} + (T_{core} - T_{surf}) \left(1 - \frac{r^2}{r_{out}^2}\right). \quad (3.19)$$

The volume average of the temperature distribution is then given by

$$\bar{T} = \frac{2}{r_{out}^2} \int_0^{r_{out}} r T_{PSS}(r) dr. \quad (3.20)$$

Substituting Eq. (3.19) into Eq. (3.20) and integrating, the core temperature is found to be

$$T_{core} = 2\bar{T} - T_{surf}. \quad (3.21)$$

Thus, an estimate for the core temperature is obtained directly from the surface and volume averaged temperature measurements. Since the surface temperature is measured, the values of $H_{PSS,21}(s)$ and $H_{PSS,22}(s)$ are identical to the corresponding values of the transient thermal model. The values of $H_{PSS,11}(s)$ and $H_{PSS,12}(s)$ can be obtained as follows: Substituting $\bar{T}$ from Eq. (3.20) into Eq. (3.21), the core temperature can be expressed as a function of the temperature distribution:

$$T_{core} = \frac{4}{r_{out}^2} \int_0^{r_{out}} (rT(r)dr - T_{surf}) dr. \quad (3.22)$$

Substituting Eqs. (3.12) and (3.13), for $T(r)$ and T_{surf} , respectively, and integrating (noting that $\int_0^{r_{out}} r J_0(ar) dr = r_{out} J_1(ar_{out})/a$), we obtain:

$$T_{core} = \frac{Q(s)}{k_t a^2} + \frac{\frac{h}{k_t}(T_\infty(s) - \frac{1}{k_t a^2} Q(s))}{\frac{h}{k_t} J_0(ar_{out}) - a J_1(ar_{out})} \left[\frac{4J_1(ar_{out})}{ar_{out}} - J_0(ar_{out}) \right]. \quad (3.23)$$

²As discussed in Section 2.1, the impedance actually identifies $\bar{T}_{EIS}$, which is not necessarily equal to $\bar{T}$. However, the assumption that $\bar{T}_{EIS} = \bar{T}$ is satisfactory for the purpose of identifying the frequencies at which errors relative to the analytical solution become significant, and is only used for this purpose in this thesis.

Thus, the PSS system model is given by:

$$\begin{bmatrix} T_{core}(s) \\ T_{surf}(s) \end{bmatrix} = \begin{bmatrix} H_{PSS,11}(s) & H_{PSS,12}(s) \\ H_{PSS,21}(s) & H_{PSS,22}(s) \end{bmatrix} \begin{bmatrix} Q(s) \\ T_{\infty}(s) \end{bmatrix} \quad (3.24)$$

where the $\mathbf{H}$ matrix is formed by the functions:

$$H_{PSS,11}(s) = -\frac{k_t a^2 r_{out} J_1(ar_{out}) - 2hr_{out} a J_0(ar_{out}) + 4hJ_1(ar_{out})}{k_t r_{out} a^3 (hJ_0(ar_{out}) - k_t a J_1(ar_{out}))}, \quad (3.25)$$

$$H_{PSS,21}(s) = \frac{-hk_t a^3 J_0 ar_{out} + 4hk_t a^2 J_1 ar_{out}}{k_t r_{out} a^3 (hJ_0 ar_{out} - k_t a J_1(ar_{out}))}, \quad (3.26)$$

$$H_{PSS,12}(s) = H_{12}(s), \quad (3.27)$$

$$H_{PSS,22}(s) = H_{22}(s). \quad (3.28)$$

3.2.3 Results

In this section the numerical results obtained from the foregoing analysis are analysed. Note that the transient model requires values of thermal properties for the cylindrical cell, which were based on the values given in Table 4.1; the identification of these values is presented in detail in Chapter 4.

Fig. 3.3 shows the impact of changes in heat generation on T_{core} and T_{surf} (H_{11} and H_{21} respectively), and the impact of changes in cooling fluid temperature T_{∞} on T_{core} and T_{surf} (H_{12} and H_{22} respectively), for the exact transient solution and the PSS model. The subplot below each main plot shows the difference between the two solutions (i.e. the error in the PSS solution). The response of H_{11} and H_{21} for the PSS model is in good agreement with the exact solution (note that the error in the response of H_{21} and H_{22} is 0 since the PSS model takes the measured surface temperature as one of its inputs). However, the response to changes in T_{∞} is less satisfactory. In particular, H_{12} shows a rapid increase in error relative to the analytical solution at frequencies above $\sim 10^{-3}$ Hz. On the one hand, the cooling fluid temperature in a typical BTMS changes much more slowly than the heat generation input to the cell, and so the requirement on the response to changes in T_{∞} is less stringent. However, in practice, this condition is still likely to be violated, and hence models which are more robust to higher frequencies (such as those to be discussed in Chapter 4) are preferable. In the subsequent section, the method is validated experimentally under steady external temperature conditions.

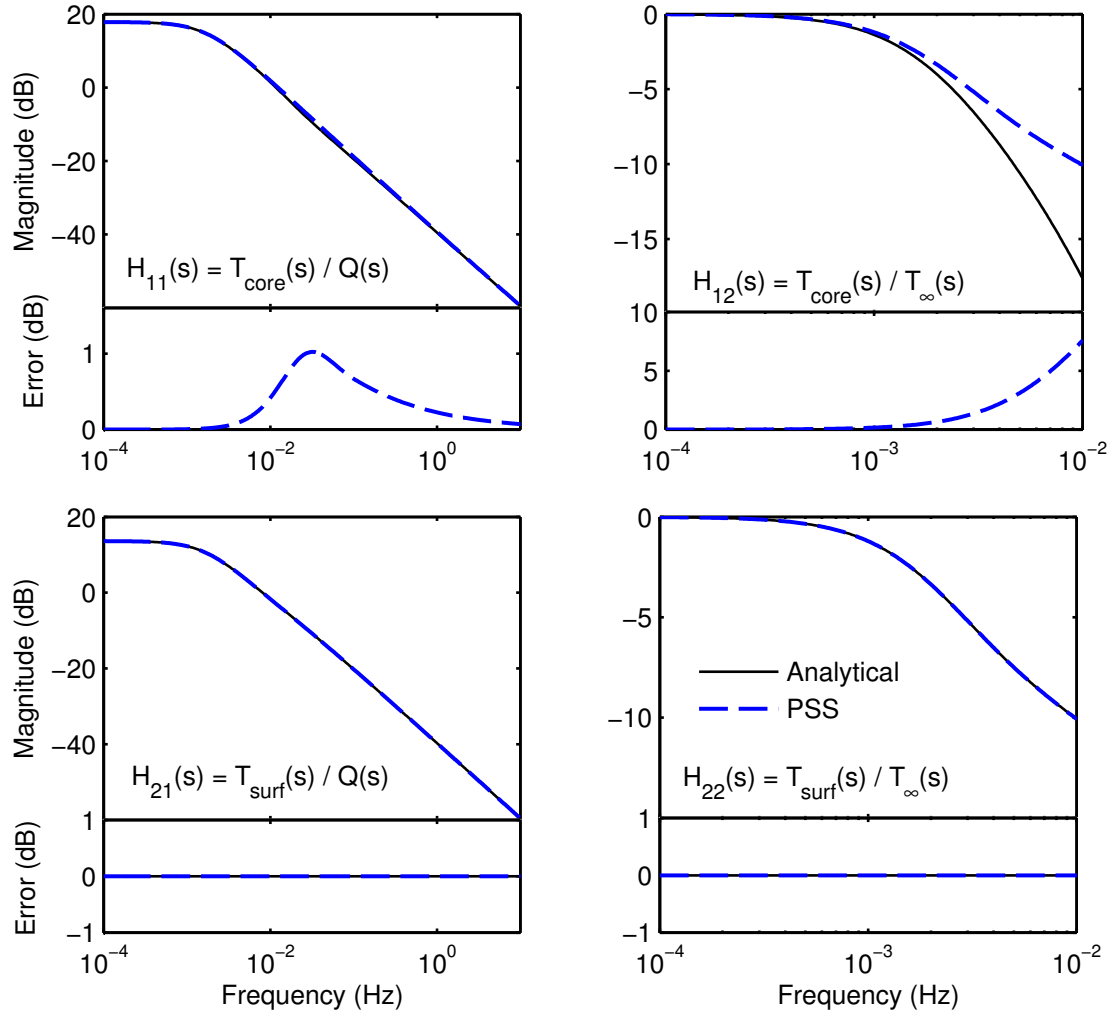


Fig. 3.3 Comparison of frequency responses of (i) the exact solution to the transient heat equation, (ii) the PSS model.

3.3 Experimental validation

3.3.1 Procedure

The method was validated experimentally using the setup described in the previous chapter (Section 2.2.1). The experiments consisted of applying (1) symmetrical current pulses and (2) a HEV drive cycle to the cell whilst single frequency (215 Hz) impedance measurements were carried out periodically and the surface and internal temperatures were monitored. This frequency was selected based on the analysis of the full spectrum impedance results as discussed in Section 2.2.3. Before each experiment, the SoC was

adjusted to 50 % by drawing a 0.9 C current. The temperature of the thermal chamber was set to 8°C and the cell was allowed to rest until its temperature equilibrated.

Besides being a function of temperature and SoC, the impedance is also a function of DC current, mainly due to the charge transfer polarization decreasing with increasing current [116]. Preliminary results confirmed that when the EIS perturbation current is superposed over an applied current load (e.g. the current pulses or drive cycle), the impedance measurement is altered. To overcome this, the cell was allowed to rest for 4 seconds before each EIS measurement was taken. The duration of this rest period was kept as short as possible to ensure that the thermal response of the cell to the applied cycle was not significantly altered, and it was found that the core cell temperature dropped by at most 0.25°C during any one of these rest periods. In practice, it may be possible to carry out impedance measurements during natural rest periods in a drive cycle, although ultimately it would be preferable to be able to handle impedance measurements under load. As discussed in Section 1.3.3, this issue is the focus of recent investigations by other researchers [54, 117, 118].

In the current pulse experiments, symmetric and periodic current pulses with 0.03 Hz frequency and magnitudes of ± 10 A and ± 20 A were applied. The single frequency impedance measurements were taken between each current pulse. The current pulses were maintained until the battery internal temperature reached an approximate steady state. After this time, the current was switched off to allow for temperature relaxation, and the impedance measurements continued to be taken every 60 seconds, until the temperature of the cell had equilibrated with the temperature of the chamber. In the HEV drive cycle experiment, a 3500 second portion of a HEV drive cycle was applied to the cell and the EIS measurements were taken every 24 seconds, i.e. 20 s periods of the drive cycle followed by 4 s rests. This drive cycle profile is referred to as HEV-I in this thesis (since other HEV drive cycles are also used in later chapters). The profile was generated by looping over different portions of an Artemis HEV drive cycle [119]; this approach was adopted (rather than using just a full drive cycle) due to memory limitations of the experimental equipment. The current profile was obtained from the velocity traces by assuming that the current was proportional to the vehicle acceleration and that 50% of the energy from deceleration was recovered to charge the battery. The scaling factor was selected to ensure that the applied currents were in the range -23 A to $+30$ A, in order to generate the desired temperature differences between surface and core.

3.3.2 Results and discussion

Fig. 3.4 displays the results of the current pulse validation experiments, including (1) the surface and core temperature measurements $T_{surf,exp}$ and $T_{core,exp}$, (2) the impedance-based volume average temperature $\bar{T}_{EIS}$, and (3) the predicted core temperature $T_{core,est.}$, identified by combining the impedance and surface temperature measurements using the hybrid method. Under 10 A pulses the difference between estimated and measured core temperature lies within 0.4°C at all times, and under 20 A pulses the difference lies within 0.9°C. The performance of the model for a HEV drive cycle is investigated in a similar manner (Fig. 3.5). The predicted maximum temperature shows good agreement with the measured core temperature, with a mean absolute error, $|\epsilon|_{mean}$, of 0.6°C (3% of the total core temperature increase from 8°C to 28°C). In contrast, if the temperature of the cell is assumed uniform (as in previous studies [42, 43]), and $\bar{T}_{EIS}$ equated to a uniform jelly roll temperature, then the maximum temperature of the cell is consistently underestimated and $|\epsilon|_{mean}$ is 2.6°C (13% of the total core temperature increase from 8 °C to 28 °C). Fig. 3.6 shows the absolute error distributions for the each of these two cases, along with the mean and maximum errors and standard deviation in each case. These results reinforce the earlier assertion that failing to account for temperature non-uniformity results in consistent underestimation of the core temperature.

It should be noted that since the uncertainty of the impedance measurement typically increases as impedance decreases, the temperature estimates could be more uncertain at higher temperatures. Hence, the implementation of this technique could be more challenging at higher ambient temperature conditions than those studied here. This issue was addressed by Spinner et al. [3], who applied a secondary, empirical fit for the upper temperature range to improve accuracy, as discussed in Section 1.3.3. A similar approach could be applied using the hybrid method presented here, for applications involving higher temperature.

Lastly, it should be noted that the method should only necessarily perform as described above (i.e. identifying the temperature distribution and hence maximum temperature), under *normal operating conditions* and when the assumptions on the sources of heat generation and dissipation etc. are correct. For instance, it would be less accurate under conditions whereby a hotspot (i.e. a localised portion³ of the cell which is hotter than the surrounding regions) has arisen due to anomalous heat generation. Since the

³The portion is actually a small volume element of the cell, and if this volume is considered infinitesimal it would be treated as a point. However, if a 2-D or 1-D model is assumed then the point would really represent a line or surface respectively.

impedance identifies a type of volume average temperature, the effect on the impedance would depend on both the localised temperature rise and on the volume of space it occupied by this localised portion of cell. Hence, the impedance would certainly respond to such changes but further assumptions or measurements would be necessary to elucidate details of localised hotspots. This is also true of the methods presented in subsequent chapters, as discussed later.

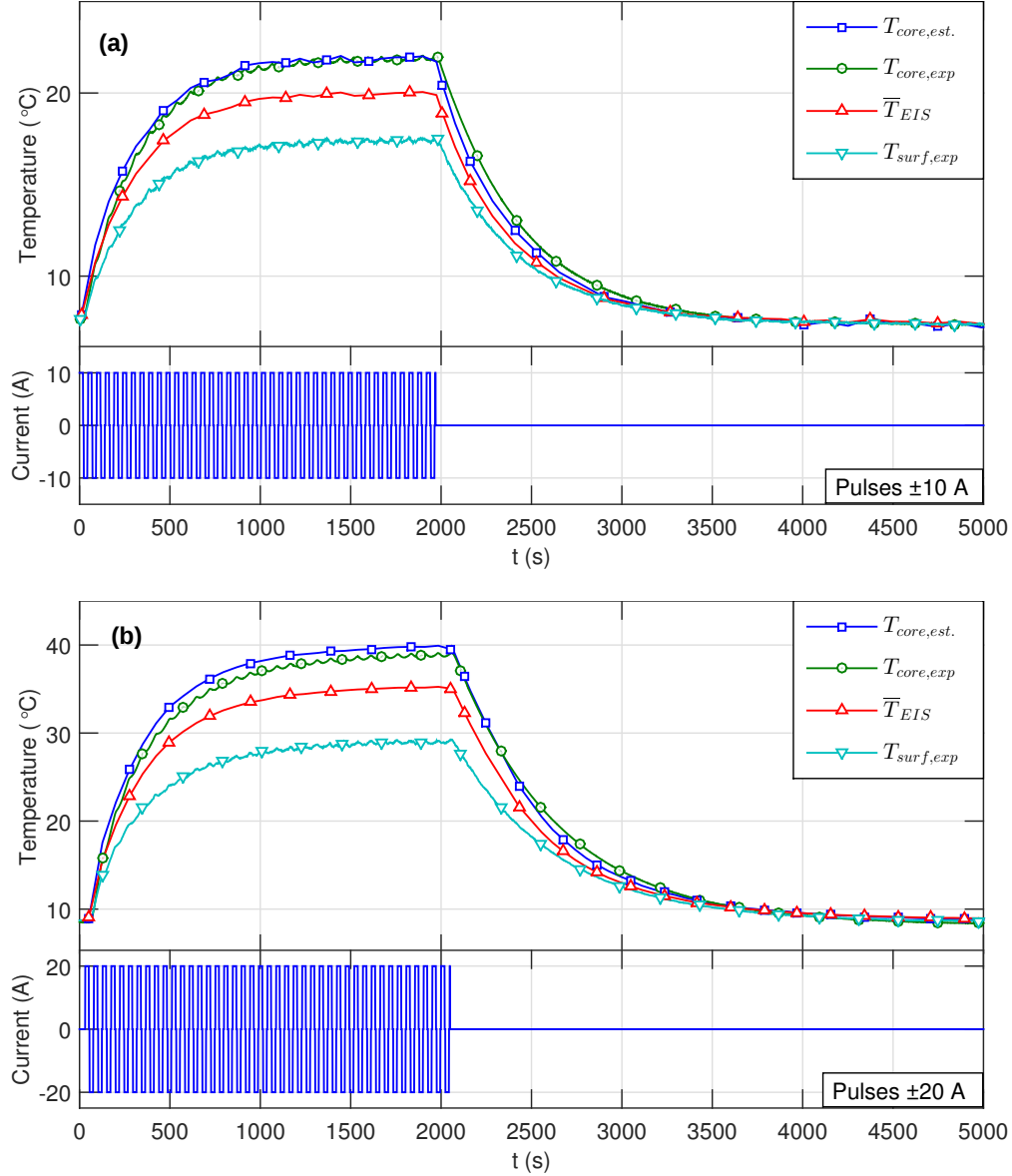


Fig. 3.4 Current pulse experiment results: (a) ± 10 A and (b) ± 20 A.

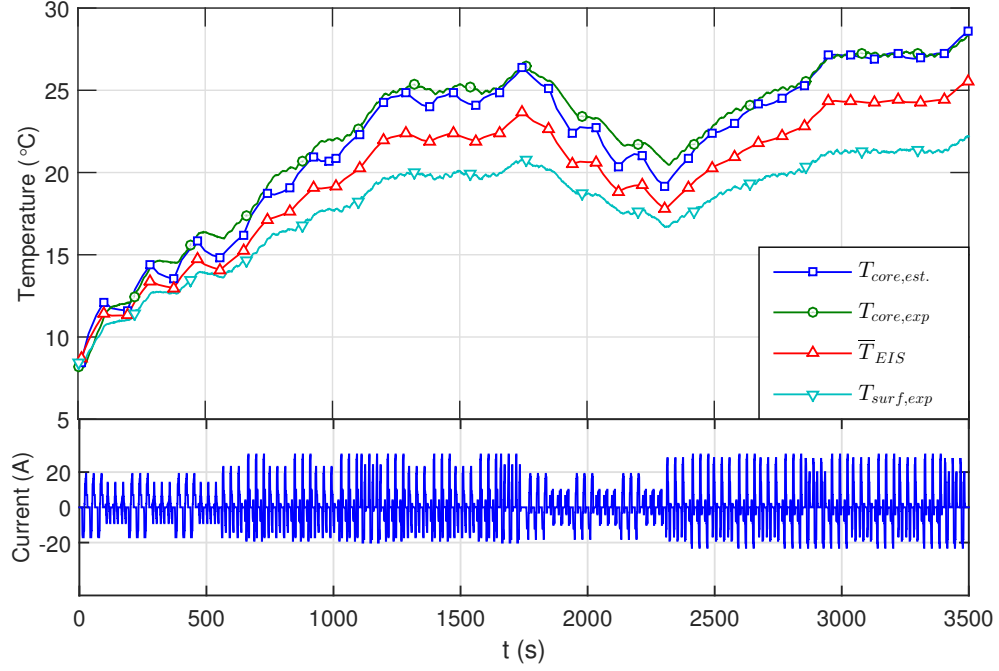


Fig. 3.5 Experimental results: HEV drive cycle.

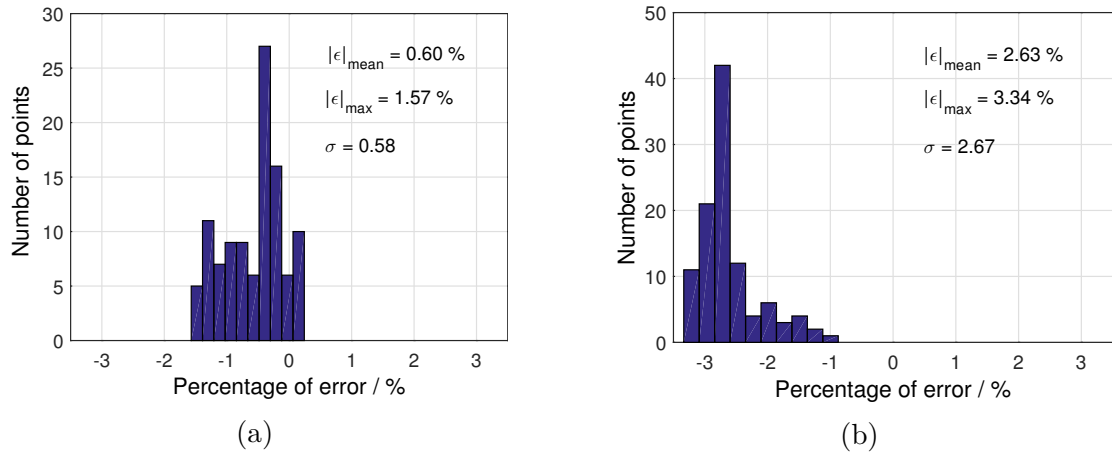


Fig. 3.6 Artemis drive cycle error analysis. (a) $\epsilon = T_{core,exp} - T_{core,est.}$; (b) $\epsilon = T_{core,exp} - \bar{T}_{EIS}$

Chapter 4

Hybrid Method II: ITD/TM

This chapter presents the second hybrid method for estimating non-uniform temperature in a cell under 1-D conditions - Impedance Temperature Detection with a Thermal Model (ITD/TM) - and is primarily based on our work published in [57]. Matlab code to run the state-estimation algorithm presented in this chapter is available online¹. Section 4.1 provides a description of the method, in which a unique solution for the temperature distribution is obtained using a single measurement

input - the real part of the impedance - combined with a dynamic thermal model. Unlike the method in the previous chapter, the model requires knowledge of the cell thermal properties, heat generation rates and boundary conditions. In Section 4.2, the performance of the thermal model is validated by comparison with the exact analytical solution of the transient heat equation in the frequency domain. Next, the performance of the method is demonstrated experimentally using the setup described in Chapter 2. The experimental procedure is described in Section 4.3, whilst the parameterisation and validation of the thermal model is described in Section 4.4. Sections 4.5 and 4.6 present analysis and results of the online state/parameter estimation procedure. The results show that an extended Kalman filter, consisting of a reduced order thermal model coupled with current, voltage and impedance measurements, is capable of accurately predicting the core and surface

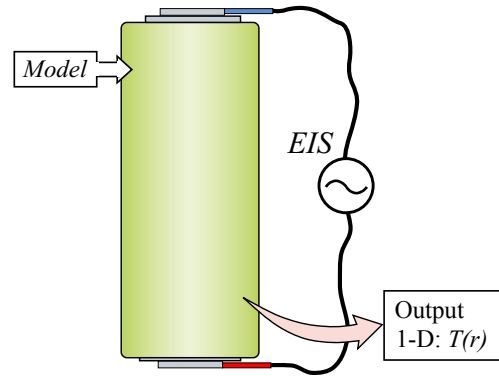


Fig. 4.1 ITD/TM

¹www.github.com/robert-richardson/EKF-Battery-Impedance-Temperature

temperatures for a current excitation profile based on a vehicle drive cycle. A dual extended Kalman filter (DEKF) based on the same thermal model and impedance measurement input is capable of estimating the convection coefficient at the cell surface when the latter is unknown. The performance of the DEKF using impedance as the measurement input is comparable to an equivalent dual Kalman filter using a conventional surface temperature sensor as measurement input.

4.1 Description of method

The method uses a single measurement input - the real impedance at 215 Hz - combined with a dynamic thermal model to obtain a unique solution for the temperature distribution. The thermal model is a low-order (2-state) model assuming only radial heat transfer, based on the Polynomial Approximation (PA) approach. An overview of the process is shown in Fig. 4.2 and described below, and a detailed description of the model is given in Sections 4.1.1 - 4.1.3.

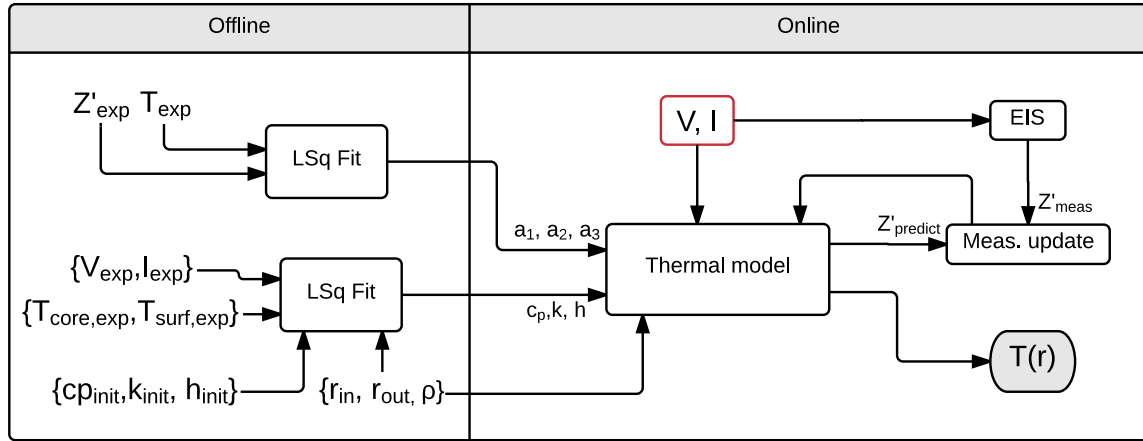


Fig. 4.2 ITD/TM process flowchart.

Offline: The calibration experiments (Section 2.2) provide values of Z'_{exp} at a range of temperatures (T_{exp}). From these, the coefficients of the polynomial (a_1 , a_2 and a_3) are obtained by least-squares fit (LSq Fit). Meanwhile, the unknown thermal properties of the cell (c_p , k and h) are identified using a least squares fit to experimental data (V_{exp} , I_{exp} , $T_{core,exp}$, $T_{surf,exp}$) from a parameterisation drive cycle (the dimensions of the cell and the density are considered known a priori) (Section 4.4). The identified thermal properties, along with the aforementioned polynomial coefficients are then available to the online thermal model.

Online: The thermal model (Sections 4.1.1 - 4.1.3) uses online measurements of the voltage and current (V , I) to predict the heat generation, temperature distribution, and cell real impedance at each time step. This is compared to the measured real impedance which is then used to update the state estimate of the model via an Extended Kalman Filter algorithm (EKF) (Section 4.5). This scheme can also be extended to include parameter estimation via a Dual Extended Kalman Filter (DEKF) as discussed later.

4.1.1 Thermal model

The cell thermal model consists of the heat equation for 1D transient heat conduction in a cylinder, as presented in the previous chapter (Section 3.2.1):

$$\rho c_p \frac{\partial T(r, t)}{\partial t} = k \frac{\partial^2 T(r, t)}{\partial r^2} + \frac{k}{r} \frac{\partial T(r, t)}{\partial r} + \frac{Q(t)}{V_b} \quad (3.7a)$$

where ρ , c_p and k are the density, specific heat capacity and thermal conductivity respectively, V_b is the cell volume, and Q is the heat generation rate. The boundary conditions are given by:

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=r_{out}} = -\frac{h}{k}(T(r_{out}, t) - T_{\infty}(t)), \quad (3.7b)$$

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=0} = 0, \quad (3.7c)$$

where T_{∞} is the temperature of the heat transfer fluid, and h is the convection coefficient. A commonly employed expression for the heat source in a lithium-ion battery is

$$Q = I(V - U_{OCV}) + IT \frac{\partial U_{OCV}}{\partial T}, \quad (4.2)$$

which is a simplified version of the expression first proposed by Bernardi et al [120]. The first term is the heat generation due to ohmic losses in the cell, charge transfer overpotential and mass transfer limitations. The current I and voltage V for this expression are measured online. The open circuit voltage U_{OCV} is a function of SoC but is approximated here as a constant value measured at 50 % SoC, since the HEV drive cycles employed in this study operate the cell within a small range of SoC (47 – 63 %) and therefore OCV variation. If necessary, an estimator of U_{OCV} could also be constructed (for example using a dynamic electrical model [121]), but for simplicity this is neglected here. The second term, the entropic heat, is neglected in this study because (i) the term $\partial U_{avg}/\partial T$ is small ($0 < \partial U_{avg}/\partial T < 0.1 \text{ mVK}^{-1}$) within

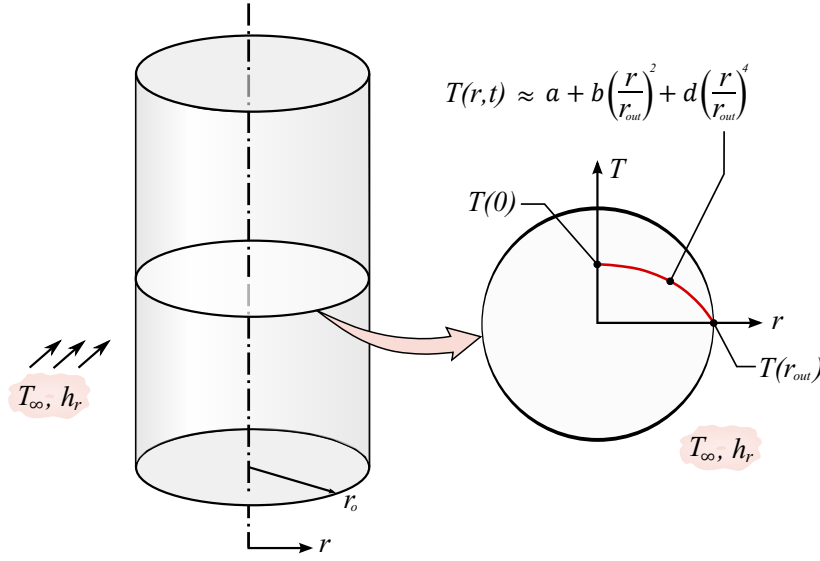


Fig. 4.3 Schematic diagram of the 1D cylinder model.

the operated range of SoC [23], and (ii) the net reversible heat would be close to zero when the cell is operating in HEV mode. A schematic of the model is shown in Fig. 4.3.

4.1.2 Polynomial Approximation

Recall from Section 1.5 that the Polynomial Approximation (PA) approach consists of integrating the governing equation over a domain, and assuming a polynomial form of the temperature profile applies over this domain. Here, a PA model is used to approximate the solution of Eq. (3.7a). The approximation was first introduced in [24] and [25] and is described in detail in those articles, although I present it in full here for clarity and completeness².

The model assumes a temperature distribution of the form

$$T(r, t) = a(t) + b(t) \left(\frac{r}{r_{out}} \right)^2 + d(t) \left(\frac{r}{r_{out}} \right)^4, \quad (4.3)$$

which satisfies the requirement of zero heat flux at the core, as required by symmetry considerations. Note that the choice of polynomial is not unique - other forms of polynomial may achieve similar accuracy [92] - however, the above form was found to

²In Appendix A, I derive and validate two additional PA models: 1-D Cartesian coordinates (suitable for simulating prismatic cells) and a 1-D annulus (an extension of the solid cylinder model to cases where the inner radial dimension is non-zero). In each case, the PA model derivation is presented and the model is validated by comparison in the frequency domain with the corresponding analytical solution of the 1D heat equation. These models are suitable for ITD/TM in their respective geometries.

be satisfactory for the present purpose. It follows from Eq. (4.3) that the core and surface temperatures are:

$$T_{core} = a(t), \quad T_{surf} = a(t) + b(t) + d(t). \quad (4.4)$$

The two states of the model are the volume averaged temperature $\bar{T}$ and temperature gradient $\bar{\gamma}$:

$$\bar{T} = \frac{2}{r_{out}^2} \int_0^{r_{out}} rT dr, \quad \bar{\gamma} = \frac{2}{r_{out}^2} \int_0^{r_{out}} r \left(\frac{\partial T}{\partial r} \right) dr. \quad (4.5)$$

Substituting (4.3) into (4.5), and integrating, yields³:

$$\bar{T} = a(t) + \frac{b(t)}{2} + \frac{d(t)}{3}, \quad \bar{\gamma} = \frac{4b(t)}{3r_{out}} + \frac{8d(t)}{5r_{out}}. \quad (4.6)$$

Rearranging (4.4) and (4.6), the time-varying constants are found to be:

$$\begin{aligned} a(t) &= 4T_{surf} - 3\bar{T} - \frac{15r_{out}}{8}\bar{\gamma}, \\ b(t) &= -18T_{surf} + 18\bar{T} + \frac{15r_{out}}{2}\bar{\gamma}, \\ d(t) &= 15T_{surf} - 15\bar{T} - \frac{45r_{out}}{8}\bar{\gamma}. \end{aligned} \quad (4.7)$$

Substituting (4.7) into (4.3), the temperature distribution can be expressed as a function of $\bar{T}$, $\bar{\gamma}$, and the cell surface temperature, T_{surf} :

$$\begin{aligned} T(r, t) &= 4T_{surf} - 3\bar{T} - \frac{15r_{out}}{8}\bar{\gamma} + \left[-18T_{surf} + 18\bar{T} + \frac{15r_{out}}{2}\bar{\gamma} \right] \left(\frac{r}{r_{out}} \right)^2 \\ &\quad + \left[15T_{surf} - 15\bar{T} - \frac{45r_{out}}{8}\bar{\gamma} \right] \left(\frac{r}{r_{out}} \right)^4. \end{aligned} \quad (4.8)$$

By obtaining the volume-average of Eq. (3.7a) and of its partial derivative with respect to r ,

$$\frac{2}{r_{out}^2} \int_0^{r_{out}} r \left(\rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial r^2} - \frac{k}{r} \frac{\partial T}{\partial r} - \frac{Q}{V_b} \right) dr = 0, \quad (4.9)$$

³Note that Eq. (4.6) was presented with an error when published in [25]. The equation as shown here gives the correct result.

$$\frac{2}{r_{out}^2} \int_0^{r_{out}} r \frac{\partial}{\partial r} \left(\rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial r^2} - \frac{k}{r} \frac{\partial T}{\partial r} - \frac{Q}{V_b} \right) dr = 0, \quad (4.10)$$

the PDE is reduced to two ODEs:

$$\frac{d\bar{T}}{dt} + \frac{48\alpha}{r_{out}^2} \bar{T} - \frac{48\alpha}{r_{out}^2} T_{surf} + \frac{15\alpha}{r_{out}} \bar{\gamma} - \frac{\alpha}{kV_b} Q = 0, \quad (4.11a)$$

$$\frac{d\bar{\gamma}}{dt} + \frac{320\alpha}{r_{out}^3} \bar{T} - \frac{320\alpha}{r_{out}^3} T_{surf} + \frac{120\alpha}{r_{out}^2} \bar{\gamma} = 0. \quad (4.11b)$$

Using 3.7b, the surface temperature can be expressed as

$$T_{surf} = \frac{24k}{24k + r_{out}h} \bar{T} + \frac{15kr_{out}}{48k + 2r_{out}h} \bar{\gamma} + \frac{r_{out}h}{24k + r_{out}h} T_{\infty}. \quad (4.12)$$

Thus, a two-state thermal model consisting of two ODEs is given by:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \\ \mathbf{y} &= \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \end{aligned} \quad (4.13)$$

where $\mathbf{x} = [\bar{T} \ \bar{\gamma}]^T$, $\mathbf{u} = [Q \ T_{\infty}]^T$ and $\mathbf{y} = [T_{core} \ T_{surf}]^T$ are state, inputs and outputs respectively. The system matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ are defined as:

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} \frac{-48\alpha h}{r_{out}(24k+r_{out}h)} & \frac{-15\alpha h}{24k+r_{out}h} \\ \frac{-320\alpha h}{r_{out}^2(24k+r_{out}h)} & \frac{-120\alpha(4k+r_{out}h)}{r_{out}^2(24k+r_{out}h)} \end{bmatrix} \\ \mathbf{B} &= \begin{bmatrix} \frac{\alpha}{kV_b} & \frac{48\alpha h}{r_{out}(24k+r_{out}h)} \\ 0 & \frac{320\alpha h}{r_{out}^2(24k+r_{out}h)} \end{bmatrix} \\ \mathbf{C} &= \begin{bmatrix} \frac{24k-3r_{out}h}{24k+r_{out}h} & -\frac{120r_{out}k+15r_{out}^2h}{8(24k+r_{out}h)} \\ \frac{24k}{24k+r_{out}h} & \frac{15r_{out}k}{48k+2r_{out}h} \end{bmatrix} \\ \mathbf{D} &= \begin{bmatrix} 0 & \frac{4r_{out}h}{24k+r_{out}h} \\ 0 & \frac{r_{out}h}{24k+r_{out}h} \end{bmatrix} \end{aligned} \quad (4.14)$$

where $\alpha = k/\rho c_p$ is the cell thermal diffusivity.

4.1.3 Impedance measurement

Recall from Chapter 2 that the measured admittance is related to the temperature distribution by:

$$Y'_{\omega_1} = \frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r \left(a_1 + a_2 T(r) + a_3 T^2(r) \right) dr. \quad (2.10)$$

This equation applies to an annulus with inner radius r_{in} and outer radius r_{out} . If the inner radius is sufficiently small, the cell may be treated as a solid cylinder, and Eq. (2.10) becomes

$$Y' = \frac{2}{r_{out}^2} \int_0^{r_{out}} r \left(a_1 + a_2 T(r) + a_3 T^2(r) \right) dr. \quad (4.15)$$

Substituting Eq. (4.8) in Eq. (4.15), the real admittance can be expressed as a function of T_{surf} , $\bar{T}$, and $\bar{\gamma}$:

$$Y' = \frac{a_1 + a_2 \bar{T} + 3a_3 \bar{T}^2 + 2a_3 T_{surf}^2 - 4a_3 \bar{T} T_{surf}}{r_{out}^2} + \frac{15a_3 r_{out}^2 \bar{\gamma}^2}{32} + \frac{15a_3 r_{out} \bar{T} \bar{\gamma}}{8} - \frac{15a_3 r_{out} T_{surf} \bar{\gamma}}{8}. \quad (4.16)$$

Noting from Eq. (4.12) that T_{surf} is itself a function of $\bar{T}$, $\bar{\gamma}$ and T_∞ and the cell parameters, admittance is ultimately a function of $\bar{T}$ and $\bar{\gamma}$, along with the known thermal parameters and environmental temperature. In other words, for known values of r_{out} , k , c_p , ρ , and h , the impedance is a function of the cell state and T_∞ , thus:

$$Z' = f(\bar{T}, \bar{\gamma}, T_\infty). \quad (4.17)$$

4.2 Frequency analysis

In this section the error associated with the PA model is analysed by comparing it's frequency response against that of the exact analytical solution of the transient heat equation. The frequency response function of the PA thermal system, $\mathbf{H}(s)$, is calculated by

$$\mathbf{H}(s) = \mathbf{D} + \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}, \quad (4.18)$$

where $s = j\omega$ and $\mathbf{I}$ is the identity matrix. The analysis for the frequency response of the analytical model was presented in the Section 3.2.1. As in the previous chapter, the thermal properties of the studied cell from Table 4.1 are used.

Fig. 4.4 shows the impact of changes in heat generation on T_{core} and T_{surf} ($\mathbf{H}_{11}$ and $\mathbf{H}_{21}$ respectively), and the impact of changes in cooling fluid temperature T_{∞} on T_{core} and T_{surf} ($\mathbf{H}_{12}$ and $\mathbf{H}_{22}$ respectively), for the exact transient solution and the PA model. The subplot below each main plot shows the difference between the two solutions (i.e. the error in the PA model solution).

The response for all four cases ($\mathbf{H}_{11}$, $\mathbf{H}_{21}$, $\mathbf{H}_{12}$ and $\mathbf{H}_{21}$) of the PA model are in good agreement with the exact analytical solution, over the frequency ranges of interest in EV/HEV applications (1×10^{-4} to 1×10^1 for the heat generation input, 1×10^{-4} to 1×10^{-2} for the cooling fluid temperature). It should be noted that in general the error in the PA model is slightly less than that of the PSS model from the previous chapter (Fig. 3.3). In particular, the response to changes in T_{∞} are acceptable up to higher frequencies than the PSS model ($\sim 10^{-2}$ Hz compared to $\sim 10^{-3}$ Hz). Although 10^{-2} Hz is still quite a low frequency, it is feasible that such inaccuracies could be acceptable in certain scenarios, given the slow rate at which the cooling fluid temperature fluctuates in a typical battery thermal management system. However, if such conditions were not met, then models with better performance at these frequencies would be necessary.

4.3 Validation experiments: procedure

Dynamic experiments were then conducted using the experimental setup described in Chapter 2 (Section 2.2.1). Two 3500 s current excitation profiles were used: HEV-I and HEV-II (note that HEV-I was also used in Chapter 3). Both cycles were generated by looping over different portions of a HEV drive cycle, and scaling the applied currents to the range -23 A to $+30$ A. HEV-I was used to parameterise the thermal model, and HEV-II to validate the identified parameters and to demonstrate the temperature estimation technique. The current, voltage and calculated heat generation for HEV-I are shown in Fig. 4.5.

The procedure for the experiment was similar to that of the validation experiments in the previous chapter (Section 3.3): single frequency (215 Hz) impedance measurements were carried out every 24 s with 4 sec pauses before each impedance measurement, and the surface and internal temperatures were also monitored. Before each experiment, the SoC was adjusted to 50% by drawing a 0.9 C current. The temperature of the thermal chamber was set to 8 °C and the cell was allowed to rest until its temperature equilibrated before experiments began.

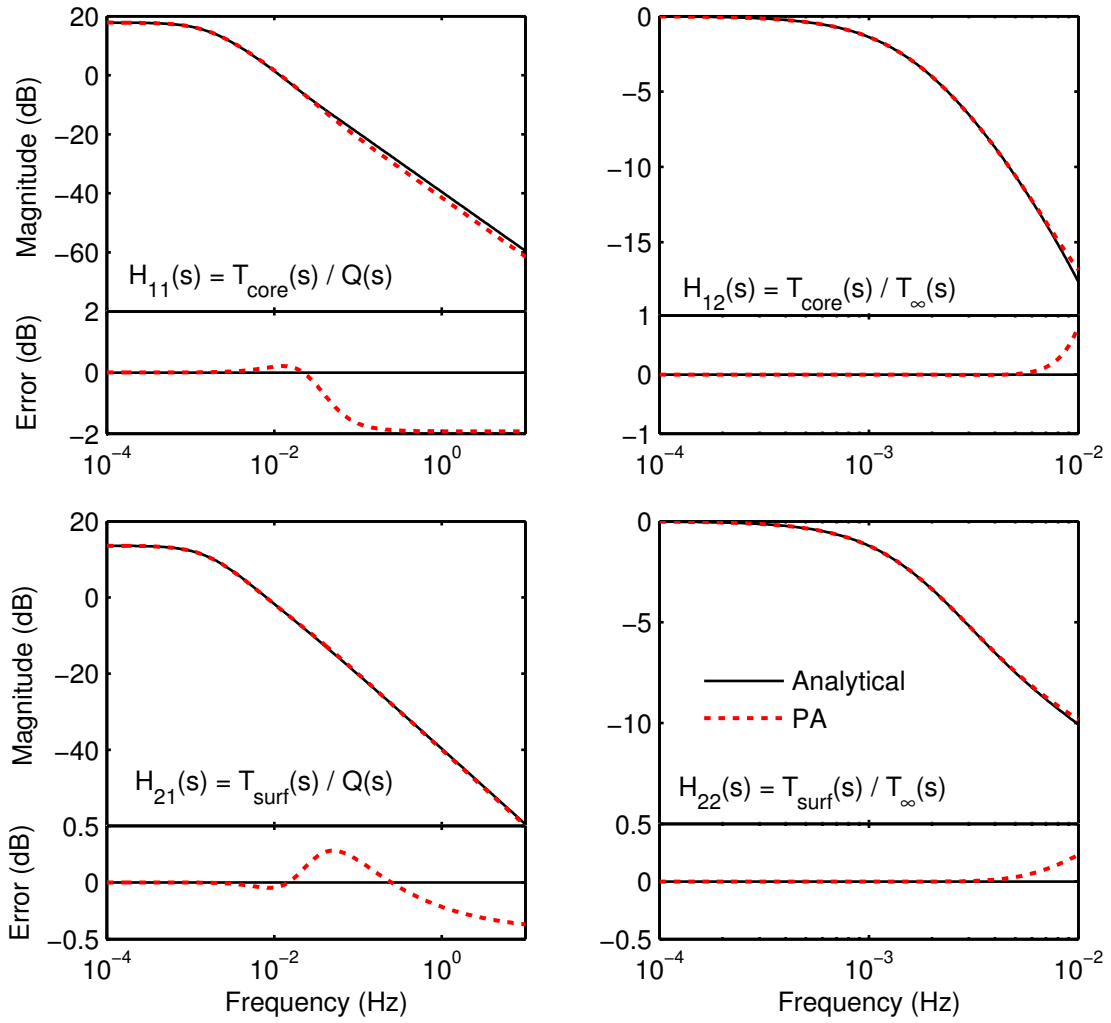


Fig. 4.4 Comparison of frequency responses of (i) the exact analytical solution to the transient heat equation, and (ii) the PA model.

4.4 Model parameterisation & validation

Parameterisation was performed to estimate the values of k , c_p , and h . The density ρ was identified in advance by measuring the cell mass and dividing by its volume. The values from HEV-I (comprising cell current, voltage, and surface and core temperatures, and the chamber temperature) were used for the estimation.

The parameterisation was carried out offline using *fminsearch* in Matlab to minimise the magnitude of the Euclidean distance between the measured and estimated core and surface temperatures, as in [25]. Table 4.1 compares the identified parameters with the initial guesses and parameters for the same cell from the literature. The estimated parameters are close to those reported in the literature. The deviations may

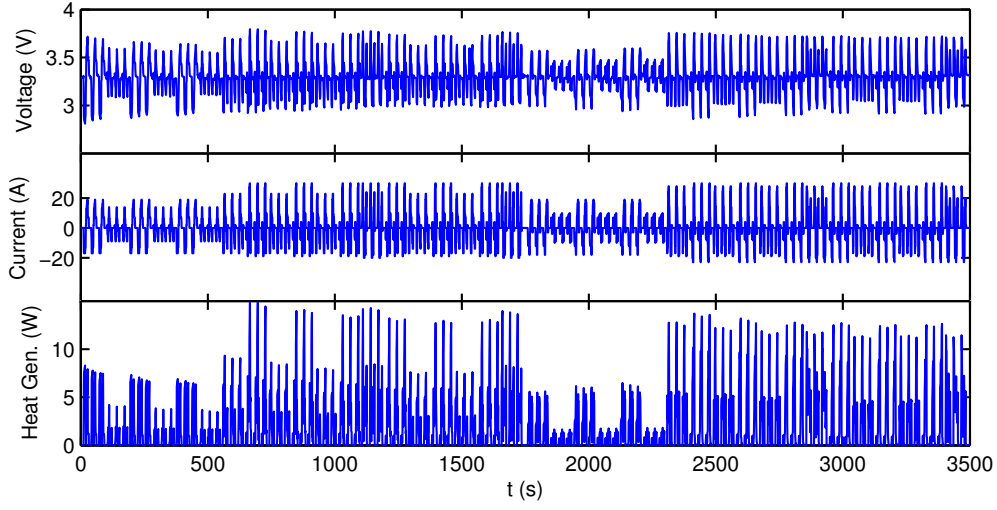


Fig. 4.5 HEV-I drive cycle data: current, voltage and heat generation.

be attributed to manufacturing variability, error in the heat generation calculation (due to the omission of entropic heating in all of these studies), heat generation in the contact resistances between the cell and connecting wires and/or measurement uncertainty in the temperature. The convection coefficient is within the range expected of forced convection air cooling [114].

Table 4.1 Comparison of reference and estimated parameters

Parameter	Units	Reference	Initial	Identified
ρ	kg m^{-3}	2047-2118 [25, 122, 79]	-	2107
c_p	$\text{J kg}^{-1} \text{K}^{-1}$	1004.9-1109.2 [23, 27, 25]	1050	1171.6
k	$\text{W m}^{-1} \text{K}^{-1}$	0.488-0.690 [71, 122, 25]	0.55	0.404
h	W m^{-2}	-	20	39.3

The measured core and surface temperatures (subscript ‘exp’) and the corresponding model predictions (subscript ‘m’) for the parameterised model are shown in Fig. 4.6a. The root-mean-square errors (RMSE) in the surface and core temperatures are 0.19 °C and 0.18 °C respectively. The model with identified parameters was validated against the second current excitation profile, HEV-II (Fig. 4.6b). The RMSEs in the core and surface temperatures were 0.21 °C and 0.16 °C respectively in this case. These errors are only marginally greater than those in the parameterisation test, indicating that the estimation is satisfactory.

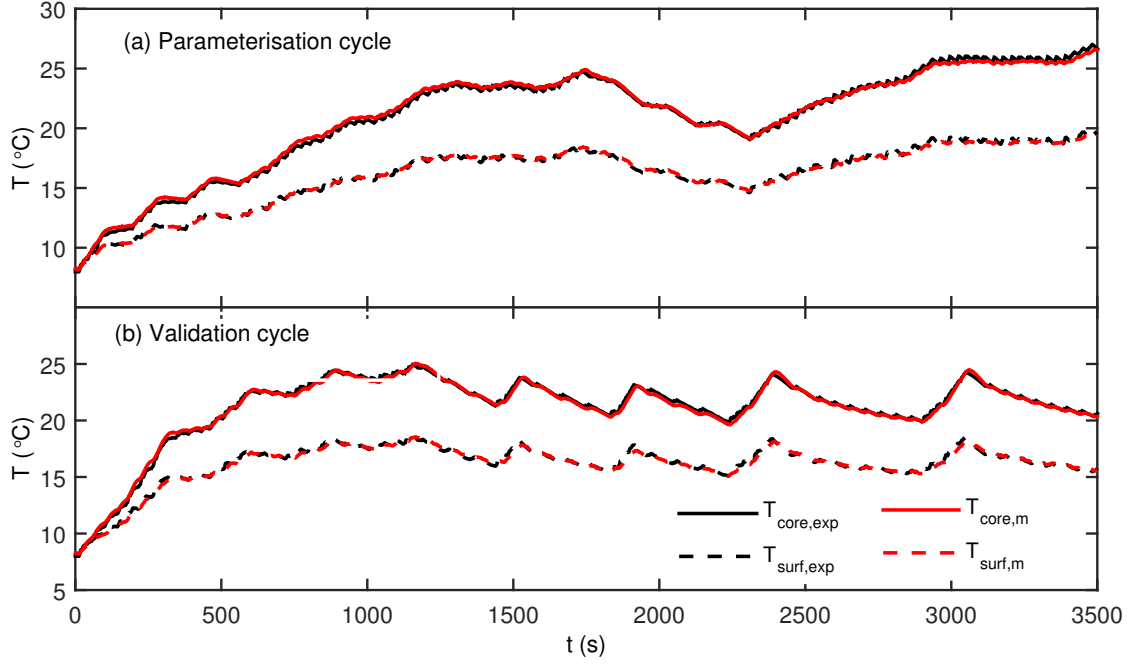


Fig. 4.6 Comparison between measured and predicted core and surface temperatures for (a) HEV-I, used to parameterise the drive cycle and (b) HEV-II, used to validate the parameterised cycle.

4.5 State estimation

Kim et al. [24] showed that the effect of changes to the value of h on the predicted surface and core temperatures is greater than the effect of changes to the other thermal parameters. Moreover, h depends strongly on the thermal management system settings and its calculation often relies on empirical correlations between coolant flow rates and heat transfer. Thus, it would be advantageous to identify the convection coefficient online during operation. This section outlines the use of a dual extended Kalman filter (DEKF) [123] for estimating the core and surface temperatures and the convection coefficient. The DEKF reduces to an EKF if the convection coefficient is assumed known and provided to the model in advance. Kalman filtering methods were chosen since, unlike conventional observers, they are capable of handling measurement noise (as discussed in Section 1.5.3). By combining noisy measurements with uncertain model inputs the KF produces a statistically optimal best estimate of the current state. This is clearly advantageous in the present case where we have an imperfect model with noisy impedance/temperature measurements.

We firstly modify Eq. (4.14) by rewriting it as a discrete time model, setting the impedance as the model output, and explicitly including the dependency on the

parameter, h_k :

$$\mathbf{x}_{k+1} = \bar{\mathbf{A}}(h_k)\mathbf{x}_k + \bar{\mathbf{B}}(h_k)\mathbf{u}_k + \mathbf{v}_k, \quad (4.19)$$

$$y_k = f(\mathbf{x}_k, h_k) + n_k, \quad (4.20)$$

$$h_{k+1} = h_k + e_k, \quad (4.21)$$

where $y_k = Z'$ and $f(\mathbf{x}_k, h_k)$ is the non-linear function relating the state vector to the measurement (i.e. Eq. (4.17)), and $\mathbf{v}_k$, n_k and e_k are the noise inputs of the covariance matrices $\mathbf{R}^v$, R^n and R^e . The states, inputs and measured outputs are thus $\mathbf{x} = [\bar{T} \ \bar{\gamma}]^T$, $\mathbf{u} = [Q \ T_\infty]^T$ and $y = Z'$. Note that, although the impedance is now the model output, the core and surface temperatures are also computed from the identified states and parameter at each time step using Eq. (4.13), for validation against the thermocouple measurements. $\bar{\mathbf{A}}$ and $\bar{\mathbf{B}}$ are system matrices in the discrete-time domain, given by

$$\bar{\mathbf{A}} = e^{(\mathbf{A}\Delta t)}, \quad \bar{\mathbf{B}} = \mathbf{A}^{-1}(\bar{\mathbf{A}} - \mathbf{I})\mathbf{B}, \quad (4.22)$$

where Δt is the sampling time of 1 s. The update processes are then given as follows. The time update processes for the parameter filter are:

$$\hat{h}_k^- = \hat{h}_{k-1}, \quad (4.23)$$

$$(P_k^h)^- = P_{k-1}^h + R^e, \quad (4.24)$$

where $\hat{h}_k^-$ and $\hat{h}_k$ are the *a priori* and *a posteriori* estimates of the parameter h , and $(P_k^h)^-$ and P_{k-1}^h are the corresponding error covariances. The time update processes for the state filter are:

$$\hat{\mathbf{x}}_k^- = \bar{\mathbf{A}}_{k-1}\hat{\mathbf{x}}_{k-1} + \bar{\mathbf{B}}_{k-1}\mathbf{u}_{k-1}, \quad (4.25)$$

$$(\mathbf{P}_k^{\mathbf{x}})^- = \bar{\mathbf{A}}_{k-1}\mathbf{P}_{k-1}^{\mathbf{x}}\bar{\mathbf{A}}_{k-1}^T + \mathbf{R}^v, \quad (4.26)$$

where $\hat{\mathbf{x}}_k^-$ and $\hat{\mathbf{x}}_k$ are the *a priori* and *a posteriori* estimates of the state, and $(\mathbf{P}_k^{\mathbf{x}})^-$ and $\mathbf{P}_{k-1}^{\mathbf{x}}$ are the corresponding error covariances. The matrices $\bar{\mathbf{A}}_{k-1}$ and $\bar{\mathbf{B}}_{k-1}$ are calculated by:

$$\bar{\mathbf{A}}_{k-1} = \bar{\mathbf{A}}(h) \Big|_{h=\hat{h}_k^-}, \quad \bar{\mathbf{B}}_{k-1} = \bar{\mathbf{B}}(h) \Big|_{h=\hat{h}_k^-}. \quad (4.27)$$

Since the relationship between impedance and the cell state is non-linear, the measurement model must be linearised about the predicted observation at each measurement.

The measurement update equations for the state filter are:

$$\mathbf{K}_k^{\mathbf{x}} = (\mathbf{P}_k^{\mathbf{x}})^- (\mathbf{H}_k^{\mathbf{x}})^T \left(\mathbf{H}_k^{\mathbf{x}} (\mathbf{P}_k^{\mathbf{x}})^- (\mathbf{H}_k^{\mathbf{x}})^T + R^n \right)^{-1}, \quad (4.28)$$

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_k^- + \mathbf{K}_k^{\mathbf{x}} \left(z_k - f(\hat{\mathbf{x}}_k^-, \hat{h}_k^-) \right), \quad (4.29)$$

$$\mathbf{P}_k^{\mathbf{x}} = (\mathbf{I} - \mathbf{K}_k^{\mathbf{x}} \mathbf{H}_k^{\mathbf{x}}) (\mathbf{P}_k^{\mathbf{x}})^-, \quad (4.30)$$

where $\mathbf{K}_k^{\mathbf{x}}$ is the Kalman gain for the state, and $\mathbf{H}_k^{\mathbf{x}}$ is the Jacobian matrix of partial derivatives of f with respect to $\mathbf{x}$:

$$\mathbf{H}_k^{\mathbf{x}} = \left. \frac{\partial f(\mathbf{x}_k, h_k)}{\partial \mathbf{x}_k} \right|_{\mathbf{x}_k = \hat{\mathbf{x}}_k^-}. \quad (4.31)$$

The measurement update processes for the parameter filter are:

$$K_k^h = (P_k^h)^- (H_k^h)^T \left(H_k^h (P_k^h)^- (H_k^h)^T + R^n \right)^{-1}, \quad (4.32)$$

$$\hat{h}_k = \hat{h}_k^- + K_k^h \left(z_k - f(\hat{\mathbf{x}}_k, \hat{h}_k^-) \right), \quad (4.33)$$

$$P_k^h = (I - K_k^h H_k^h) (P_k^h)^-, \quad (4.34)$$

where H_k^h is the Jacobian matrix of partial derivatives of f with respect to h :

$$H_k^h = \left. \frac{\partial f(\mathbf{x}_k, h_k)}{\partial h_k} \right|_{h_k = \hat{h}_k^-}. \quad (4.35)$$

The above algorithm can be simplified to a standard EKF by omitting the parameter update processes (Eqs. (4.21), (4.23)-(4.24) and (4.32)-(4.35)) and assuming the convection coefficient is fixed. In the following section the performance of both the baseline EKF and the full DEKF algorithm are investigated.

4.6 Results and discussion

This section first investigates the performance of an EKF estimator whereby the convection coefficient is provided and assumed fixed. The performance of the DEKF algorithm is then compared with that of the baseline EKF when an incorrect initial estimate of the convection coefficient is provided. Lastly, the performance of the DEKF is compared with that of a dual Kalman filter (DKF) based on the same thermal model but with T_{surf} as the measurement input rather than Z' .

4.6.1 Convection coefficient known

The initial state estimate provided to the battery is $\hat{\mathbf{x}}_0 = [25, 0]$, i.e. the battery has a uniform temperature distribution at 25 °C. The true initial battery state is a uniform temperature distribution at 8 °C. The covariance matrices are calculated as $R^n = \sigma_n^2$ and $\mathbf{R}^v = \beta_v^2 \text{diag}(2, 2)$. The first tuning parameter is chosen as $\sigma_n = 1 \times 10^{-4} \Omega$, which is a rough estimate of the standard deviation of the impedance measurement. The second tuning parameter was chosen as $\beta_v = 0.1$, by trial and error. Fig. 4.7 shows that, using the EKF, the core and surface temperatures quickly converge to the correct values and are accurately estimated throughout the entire excitation profile. The RMSEs of core and surface temperature are 1.35 °C and 1.34 °C respectively. In contrast, the RMSEs for the open loop model (subscript ‘m’) with no measurement feedback are 6.66 °C and 4.42 °C respectively. As discussed in the previous chapter, the implementation of this technique could be more challenging at higher ambient temperature conditions than those studied here.

It should be noted that similar performance was also achieved using a simpler EKF based on Z' with the assumption that the impedance is related directly to $\bar{T}$ rather than to $\bar{T}_{EIS}$. However, this assumption may lead to unsatisfactory results for cells with a larger radius or when larger temperature gradients exist within the cell.

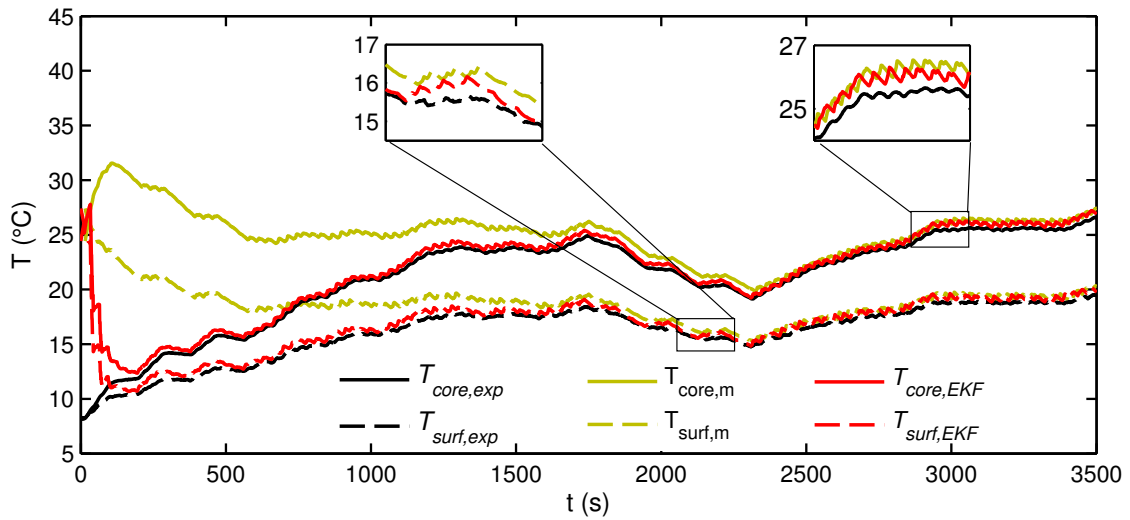


Fig. 4.7 Temperature results for EKF using Z' as measurement input.

4.6.2 Convection coefficient unknown

Next, the performance of the DEKF is investigated. The same incorrect initial state estimate is provided to the battery, $\hat{\mathbf{x}}_0 = [25, 0]$. Moreover, an incorrect initial estimate for the convection coefficient is provided, $\hat{h}_0 = 2 \times h_{true}$. This value of h is also provided to the EKF. The error covariance matrix for the parameter estimator is $R^e = \beta_e^2$ where the tuning parameter is chosen as $\beta_e = 2.5$. Fig. 4.8 compares the results of both of these cases against the thermocouple measurements. The EKF is shown to overestimate the core temperature and underestimate the surface temperature for the duration of the experiments. This is expected, since the impedance measurement ensures the accuracy of the volume averaged cell temperature but the model assumes that the convection coefficient is higher than in reality, and therefore the temperature difference across the cell is overestimated. In contrast, the DEKF corrects the convection coefficient, and thus improves the accuracy of the subsequent temperature predictions. This is evident

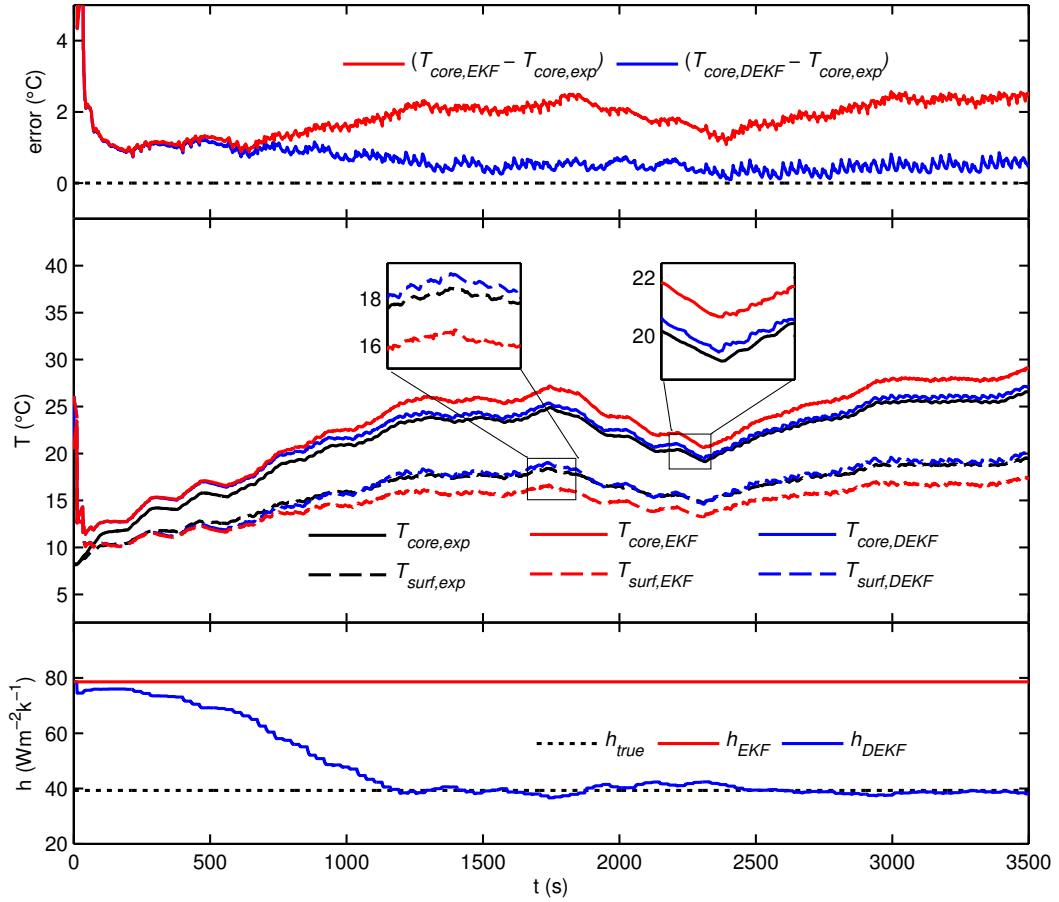


Fig. 4.8 Temperature results for DEKF using Z' as measurement input.

from the errors in the core temperature estimate (top plot of Fig. 4.8), which initially are similar in both cases but drop to much smaller values for the DEKF once the correct convection coefficient is identified. The RMSEs of core and surface temperature in each case are shown in Table 4.2, along with the values for the time period, $1200 < t < 3500$ s (i.e. after the convection coefficient value has converged).

Finally, we consider the case where T_{surf} is used as the measurement ($y = T_{surf}$) to the estimator rather than Z' . This results in a linear KF and DKF exactly equivalent to that studied in [25]. The tuning parameters for the covariance matrices are also chosen to be the same as those employed in [25]. The same initial state and parameter estimates are provided as for the DEKF. Fig. 4.9 shows that the standard EKF in this case overpredicts the core temperature by a greater margin than the EKF based on Z' , although the surface temperature estimate is much more accurate. This is because the surface thermocouple ensures an accurate surface temperature estimate and to reconcile this with the overestimated convection coefficient, the core temperature estimate is forced to be much greater. The DKF correctly identifies the correct convection coefficient, in the same way as the DEKF. Since the thermocouple measurement exhibits less noise than the impedance measurement, the model converges to the correct estimate for h more quickly than in the DEKF case, as shown by the RMSE values in Table 4.2.

In conclusion, the temperature and convection coefficient estimators using Z' as measurement input are capable of accurately estimating the core and surface temperatures and the convection coefficient. The performance is comparable to that of an estimator using the same thermal model coupled with surface temperature measurements.

Table 4.2 Comparison of RMSEs for core and surface temperatures ($^{\circ}\text{C}$) with unknown convection coefficient.

Method	$0 < t < 3500$ s		$1200 < t < 3500$ s	
	T_{core}	T_{surf}	T_{core}	T_{surf}
EKF + Z'	2.04	2.06	1.79	1.98
KF + T_{surf}	2.49	1.44	2.90	1.58
DEKF + Z'	1.43	1.24	0.47	0.42
DKF + T_{surf}	0.36	0.33	0.16	0.14

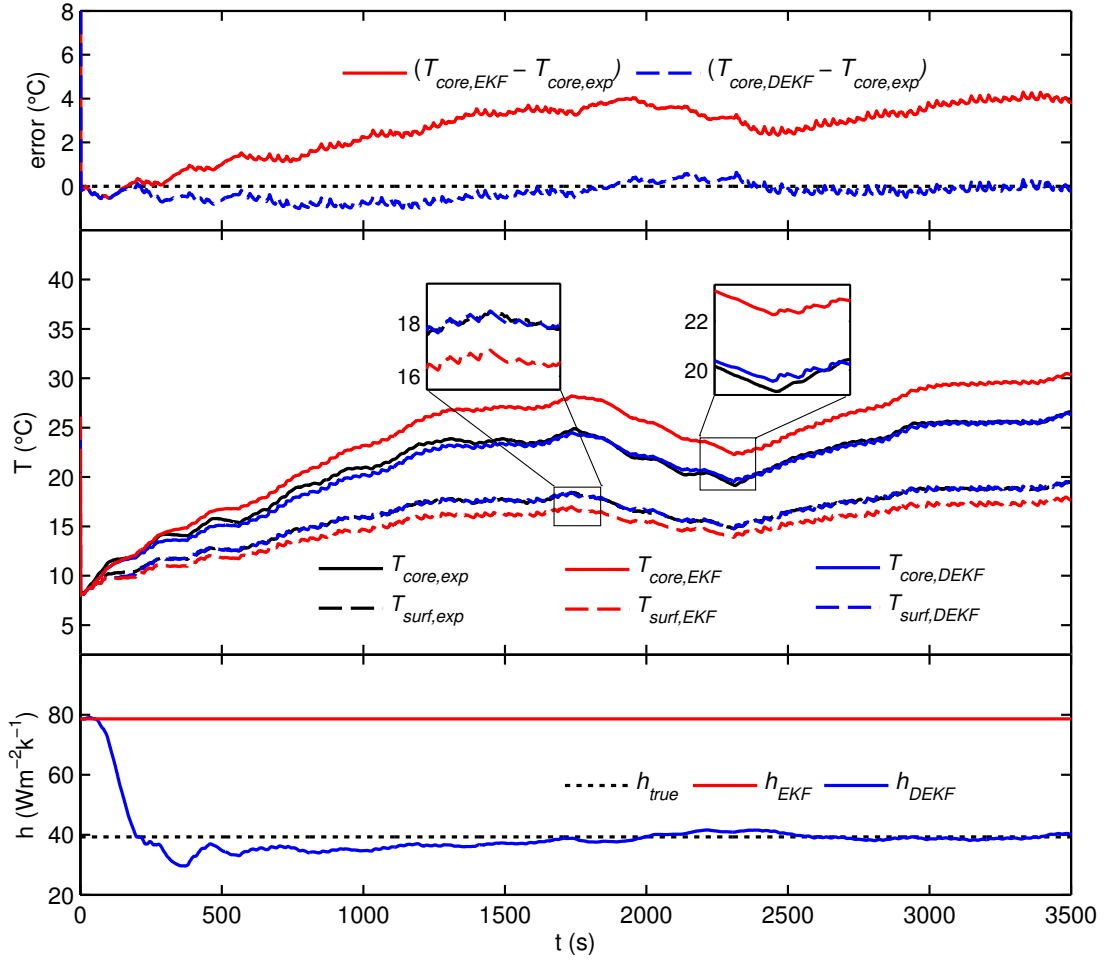


Fig. 4.9 Temperature results for DKF using T_{surf} as measurement input.

4.7 Conclusions

This chapter introduced the second hybrid method, which uses ITD as the measurement input to a thermal model, enabling robust estimation of the core and surface temperatures without any temperature sensors. An EKF using a parameterised PA thermal model with ITD measurement input was shown to accurately predict core and surface temperatures for a current excitation profile based on an Artemis HEV drive cycle. A DEKF based on the same thermal model and measurement input is capable of accurately identifying the convection coefficient when the latter is not provided to the model in advance. The performance of the DEKF using impedance as measurement input is comparable to an equivalent DKF estimator using surface temperature as measurement input, although the latter is slightly superior due to the higher accuracy

of the thermocouple. In Part II of this thesis, this method will be extended to apply to problems with 2-D thermal dynamics, enabling it to be applied to more general scenarios such as end cooling via liquid-coolant plates.

Part II

Temperature Monitoring in 2-D

Chapter 5

Spectral-Galerkin model

The second part of this thesis focuses on battery temperature monitoring under conditions involving 2-D thermal dynamics. This chapter presents and validates a suitable 2-D model (see Fig. 5.1); the subsequent chapter uses this model in a 2-D temperature monitoring scheme (Hybrid Method II: ITD/TM). The present chapter is primarily based on our work published in [101]. Matlab code to simulate the model presented in this chapter is available online¹.

Spectral-Galerkin (SG) methods are introduced in Section 5.1 by means of a toy example. A mathematical description of the 2-D model is then presented in Section 5.2. The model is based on a Chebyshev SG method, and is capable of predicting the full temperature distribution with a similar efficiency to a Thermal Equivalent Circuit (TEC). For consistency, only a cylindrical geometry is studied here, although the model could easily be applied to prismatic cells by a suitable change of coordinates. The model accounts for transient heat generation, anisotropic heat conduction, and non-homogeneous convection boundary conditions with different convection coefficients and external temperatures at each surface. As discussed in Section 1.5, this generality makes it suitable for simulating various battery cooling configurations, such as side or end cooling, or scenarios with different cooling fluids at each surface. The model is validated in Section 5.3. The results are firstly compared with finite element simulations, which show that the 2-D temperature field of a large format (64 mm diameter) cell can be accurately modelled with as few as 4 states. Secondly, the performance of the model for a range of Biot numbers is investigated via frequency analysis. For larger cells or highly transient thermal dynamics, the model order can be increased for improved accuracy.

¹www.github.com/robert-richardson/Spectral-Thermal-Model-2D

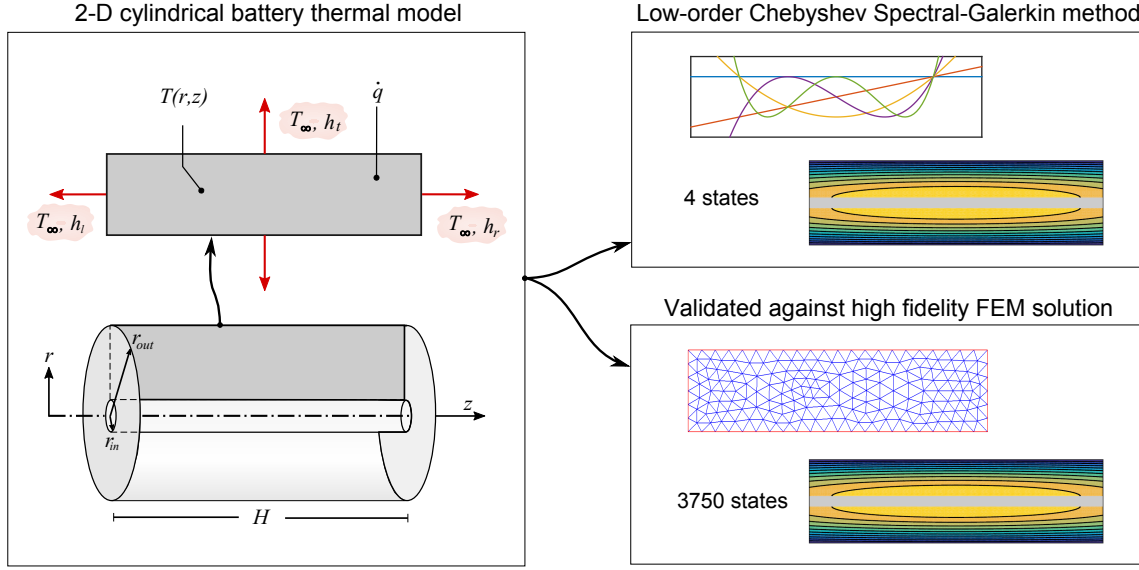


Fig. 5.1 Spectral-Galerkin model. This chapter presents a 2-D spectral-Galerkin thermal model of a cylindrical cell and validates it against a high order finite element solution.

5.1 Toy problem

As discussed in Section 1.5.2, SG methods are a type of weighted residual method whereby the solution is obtained by forcing the residual of an integral multiplied by a test function to zero. In this section, SG methods are introduced by means of a simple example - a 1-D heat equation in Cartesian coordinates on the domain $\hat{x} \in [-1, 1]$, with non-homogeneous boundary conditions.

Governing equation

The governing equation is given by:

$$\rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial \hat{x}^2} - q = 0, \quad (5.1)$$

where t is time, $\hat{x} \in [-1, 1]$ is the position coordinate and ρ , c_p and k are the density, specific heat capacity, and thermal conductivity respectively. The convection boundary conditions are given by

$$a_+ T + b_+ \frac{\partial T}{\partial \hat{x}} = e_r \quad \text{at } \hat{x} = 1 \quad (5.2)$$

$$a_- T + b_- \frac{\partial T}{\partial \hat{x}} = e_l \quad \text{at } \hat{x} = -1 \quad (5.3)$$

where

$$a_+ = h/k, \quad b_+ = 1, \quad (5.4)$$

$$a_- = -h/k, \quad b_- = 1, \quad (5.5)$$

$$e_r = a_+ T_\infty, \quad e_l = a_- T_\infty, \quad (5.6)$$

where h is the convection coefficient and T_∞ is the external temperature. For simplicity the convection coefficient and external temperature at each boundary are assumed to be the same.

Finite sum approximation

The starting point of the SG method is to approximate the solution T of Eq. (5.1) by a finite sum

$$T = \sum_{n=0}^N a_n \phi_n(\hat{x}) + T_\infty, \quad (5.7)$$

where a_n are unknown solution coefficients, and ϕ_n are the *trial (or basis) functions* which must satisfy the Robin boundary conditions (Eqs. (5.2) and (5.3)).

Basis functions

In principle any Jacobi polynomial may be used for the basis functions, however, for this example, Chebyshev functions were used since they can be conveniently defined such that they adhere to any of a broad class of boundary conditions [95] We denote by C_n the n th degree Chebyshev polynomial of the first kind and then let $\{\phi_n(\hat{x})\}_{n=0}^N$ be a basis function such that

$$\phi_n = C_n(\hat{x}) + \zeta_n C_{n+1}(\hat{x}) + \eta_n C_{n+2}(\hat{x}), \quad (5.8)$$

where ζ_n and η_n are defined according to the formula in Lemma 4.3 of [95] such that they adhere to the boundary conditions,

$$\zeta_n = \{4(n+1)(a_+ b_- + a_- b_+)\}/\text{DET}_n, \quad (5.9)$$

and

$$\begin{aligned} \eta_n = \{ & -2a_- a_+ + (n^2 + (n+1)^2)(a_+ b_- - a_- b_+) \\ & + 2b_- b_+ n^2(n+1)^2 \}/\text{DET}_n, \end{aligned} \quad (5.10)$$

where

$$\begin{aligned} \text{DET}_n &= 2a_+a_- + \left((n+1)^2 + (n+2)^2\right) \\ &\quad (a_-b_+ - a_+b_-) - 2b_-b_+(n+1)^2(n+2)^2. \end{aligned} \quad (5.11)$$

From this point on, ϕ_n are considered known functions.

Schematic diagrams visualising the composition of the basis functions using this approach (i.e. Eqs. (5.8)-(5.11)) are presented in Figs. 5.2 and 5.3. Fig. 5.3 applies to Robin boundaries (as in this example), whilst Fig. 5.2 shows a similar problem with Dirichlet BCs.

The values of ζ_n and η_n from Lemma 4.3 of [95] ensure that each basis function adheres to the specified boundary conditions (and hence any weighted sum of these functions will also adhere to the BCs). This is most apparent from plot (a), whereby the Dirichlet boundary conditions ensure that each basis function is fixed to a specific value (in this case, 0) at the boundaries. The temperature is then given by a sum of basis functions weighted by the (time varying) coefficients a as defined by Eq. (5.7). Note that these plots are for schematic purposes only; the values of the parameters used to generate them are arbitrary.

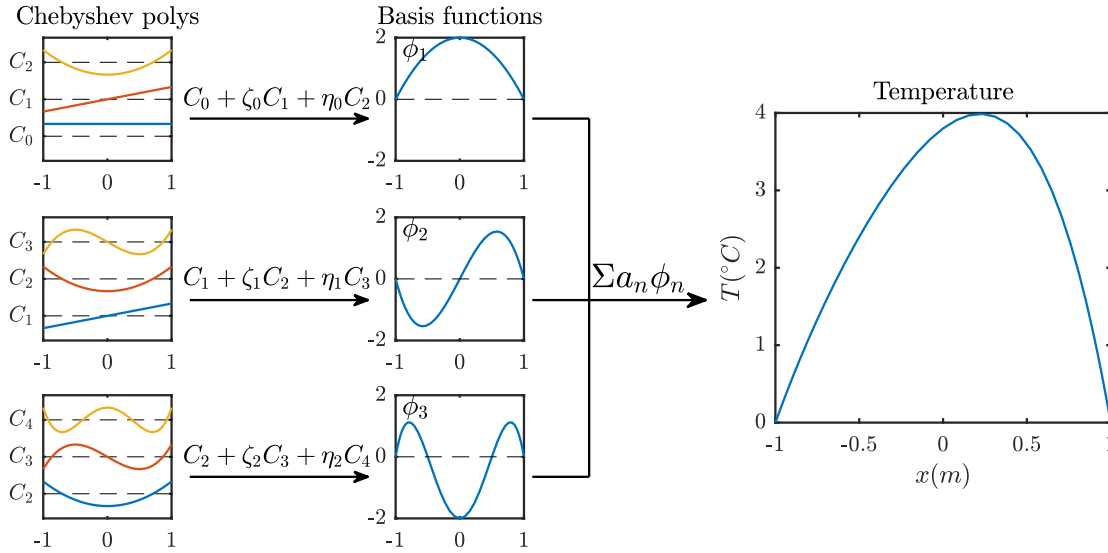


Fig. 5.2 Construction of basis functions as weighted sums of Chebyshev polynomials for Dirichlet boundary conditions.

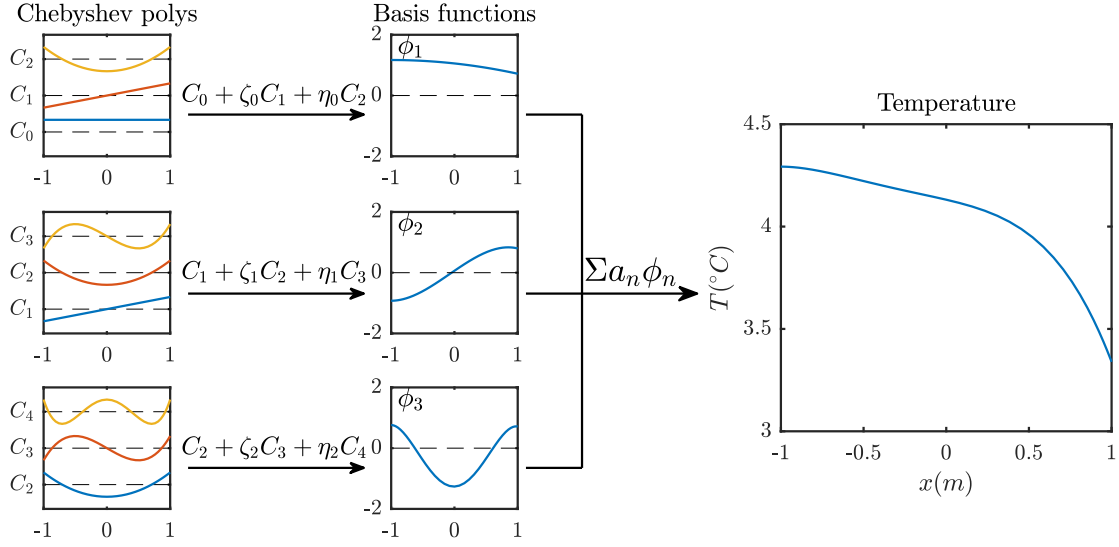


Fig. 5.3 Construction of basis functions as weighted sums of Chebyshev polynomials for Robin boundary conditions.

Residual equation

Substituting Eq. (5.7) for T into Eq. (5.1) leads to the *residual*:

$$R := \rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial x^2} - q \neq 0. \quad (5.12)$$

The principle of the SG method is to force an integral of the residual to zero by requiring

$$(R, \nu) := \int_{-1}^1 R(\hat{x}) \nu(\hat{x}) d\hat{x} = 0 \quad (5.13)$$

where ν_n are *test functions*. By definition, for a Galerkin method, the test functions, ν_n , are set equal to the trial functions, ϕ_n , and hence this is the approach we adopt here². Substituting Eq. (5.12) for R into Eq. (5.13) gives

$$\int_{-1}^1 \left(\rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial x^2} - q \right) \nu d\hat{x} = 0. \quad (5.14)$$

Substituting Eq. (5.7) for T and ϕ_n for ν into Eq. (5.14), we have

²For certain problems, such as for PDEs involving odd-order terms, it can be useful to have test functions which are different to the trial functions; in such cases the method is referred to as a Petrov-Galerkin method [95].

$$\rho c_p \begin{bmatrix} \int_{-1}^1 \phi_0 \phi_n d\hat{x}, \dots, \int_{-1}^1 \phi_N \phi_n d\hat{x} \end{bmatrix} \begin{bmatrix} \dot{a}_0 \\ \vdots \\ \dot{a}_N \end{bmatrix} - k \begin{bmatrix} \int_{-1}^1 \frac{\partial^2 \phi_0}{\partial \hat{x}^2} \phi_n d\hat{x}, \dots, \int_{-1}^1 \frac{\partial^2 \phi_N}{\partial \hat{x}^2} \phi_n d\hat{x} \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_N \end{bmatrix} - q \int_{-1}^1 \phi_n d\hat{x} = 0. \quad (5.15)$$

State space equation

With $n = 0, 1, \dots, N$, the above $N + 1$ equations representing the spatial discretisation can be written in compact form as

$$\mathbf{E}\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}, \quad (5.16)$$

where

$$\mathbf{x} = [a_0, \dots, a_N], \quad (5.17)$$

$$\mathbf{u} = [q, T_\infty], \quad (5.18)$$

and

$$\mathbf{E}(i, j) = \rho c_p \int_{-1}^1 \phi_i \phi_j d\hat{x}, \quad (5.19)$$

$$\mathbf{A}(i, j) = k \int_{-1}^1 \frac{\partial^2 \phi_j}{\partial \hat{x}^2} \phi_i d\hat{x}, \quad (5.20)$$

$$\mathbf{B}(i, 1) = \int_{-1}^1 \phi_i d\hat{x}, \quad (5.21)$$

$$\mathbf{B}(i, 2) = 0. \quad (5.22)$$

Letting the outputs of the system be the temperature at the left and right boundaries, $T(\hat{x} = -1)$ and $T(\hat{x} = 1)$, we have

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u}, \quad (5.23)$$

where

$$\mathbf{y} = [T_{\hat{x}=-1}, T_{\hat{x}=1}]^T, \quad (5.24)$$

$$\mathbf{C}_{1,j} = [\phi_0(\hat{x} = -1), \dots, \phi_N(\hat{x} = -1)], \quad (5.25)$$

$$C_{2,j} = [\phi_0(\hat{x} = 1), \dots, \phi_N(\hat{x} = 1)], \quad (5.26)$$

$$\mathbf{D} = \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}. \quad (5.27)$$

As we shall see, the actual 2-D problem of interest presented in the following section is more complex than the above problem, for the following reasons: (i) it involves cylindrical rather than Cartesian coordinates, (ii) the physical domain is not necessarily in the range $[-1, 1]$ and must be scaled accordingly, and (iii) it is 2-D, which renders the homogenisation step of the non-homogeneous boundary conditions non-trivial. However, the solution process in both cases are equivalent.

5.2 Thermal model

5.2.1 Overview

This section now describes the full 2-D SG model. As discussed in Section 1.5, the most difficult aspect of the 2-D SG model is accounting for non-homogeneous boundary conditions. Here, the treatment of the non-homogeneous boundary conditions is achieved by an efficient boundary lifting algorithm, a modification of a recently developed boundary lifting algorithm for elliptic problems [124]. Since the underlying basis functions implicitly satisfy the boundary conditions, there is no need for additional equations to impose the boundary conditions. As a result accurate models can be generated using as few as two basis functions in each direction, and thus $2^2 \equiv 4$ states. The accuracy can be improved arbitrarily by increasing the number of basis functions in either dimension.

A step-by-step procedure of the model is given as follows. In Section 5.2.2, the 2-D thermal problem is defined. In Section 5.2.3, the model is scaled from the physical coordinates to a coordinate system suitable for implementation of the SG algorithm. In Section 5.2.4, the scaled model is decomposed into a homogeneous problem and a (time-invariant) boundary lifting function. Section 5.2.5 presents the solution to the homogeneous problem using the SG method and Section 5.2.6 presents the calculation of the boundary lifting function. Finally, Section 5.2.7 presents the overall solution to the original problem which combines the solutions obtained from Sections 5.2.5 and 5.2.6. The overall procedure ultimately generates a state-space model; the resulting model can then be solved efficiently online.

5.2.2 Model definition

The model consists of the transient energy conservation equation in cylindrical coordinates. Heat generation is assumed to be uniform in space but time-dependant. As in the 1-D case, the multi-layer structure of the battery is treated as a homogeneous solid with anisotropic thermal conductivity in the radial and axial directions. The temperature variation in the azimuthal (φ) direction is neglected. Convective heat transfer is assumed to occur at the outside surfaces, and the properties of the heat transfer fluid (i.e. the heat transfer coefficient and the fluid free-stream temperature) may be different for each surface (see Fig. 5.4).

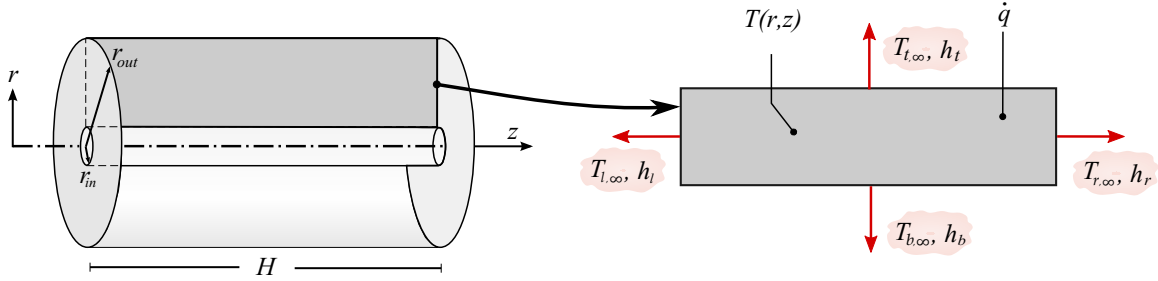


Fig. 5.4 Schematic of cylindrical cell geometry for the thermal model, showing different convection coefficients and/or external temperatures at each surface.

The resulting model is governed by the following 2-D boundary value problem [92]:

$$\rho c_p \frac{\partial T}{\partial t} - k_r \frac{\partial^2 T}{\partial r^2} - \frac{k_r}{r} \frac{\partial T}{\partial r} - k_z \frac{\partial^2 T}{\partial z^2} = q \quad (5.28)$$

where t is time and r and z are the position coordinates in the radial and axial directions respectively. The functions $T(r, z, t)$ and $q(t)$ are the temperature distribution and volumetric heat generation rate, respectively. The parameters ρ and c_p are the density and specific heat capacity respectively, and k_r and k_z are the anisotropic thermal conductivities in the r and z directions. The boundary conditions are given by:

$$\frac{\partial T}{\partial r} = -\frac{h_r}{k_r}(T - T_{r,\infty}) \quad \text{at } r = r_{out} \quad (5.29a)$$

$$\frac{\partial T}{\partial r} = \frac{h_l}{k_r}(T - T_{l,\infty}) \quad \text{at } r = r_{in} \quad (5.29b)$$

$$\frac{\partial T}{\partial z} = -\frac{h_t}{k_z}(T - T_{t,\infty}) \quad \text{at } z = H \quad (5.29c)$$

$$\frac{\partial T}{\partial z} = \frac{h_b}{k_z}(T - T_{b,\infty}) \quad \text{at } z = 0 \quad (5.29d)$$

where $\{T_{\sigma,\infty}; \sigma = t, b, r \text{ and } l\}$ are the free-stream temperatures of the heat transfer fluid at the top, bottom, right and left surfaces³, and $\{h_\sigma; \sigma = t, b, r \text{ and } l\}$ are the corresponding convection coefficients.

5.2.3 Change of scale

In order to exploit the orthogonality properties of the polynomial basis functions it is necessary to scale from the original (physical) domain, (r, z) where $r \in [r_{in}, r_{out}]$, $z \in [0, H]$, to the spectral domain, $(\hat{r}, \hat{z})$ where $\hat{r} \in [-1, 1]$, $\hat{z} \in [-1, 1]$. We define the spectral coordinates by

$$\hat{r} = 2 \frac{r - r_{in}}{r_{out} - r_{in}} - 1 \quad \text{s.t.} \quad \begin{cases} \hat{r}(r = r_{in}) &= -1 \\ \hat{r}(r = r_{out}) &= 1 \end{cases} \quad (5.30a)$$

$$\hat{z} = \frac{2z}{H} - 1 \quad \text{s.t.} \quad \begin{cases} \hat{z}(z = 0) &= -1 \\ \hat{z}(z = H) &= 1 \end{cases}. \quad (5.30b)$$

Rearranging (5.30a) and (5.30b), the original coordinates are given by

$$r = \frac{1 + \hat{r} + \alpha r_{in}}{\alpha}, \quad (5.31a)$$

$$z = \frac{\hat{z} + 1}{\beta}. \quad (5.31b)$$

where α and β are scaling factors defined by $\alpha = 2/(r_{out} - r_{in})$ and $\beta = 2/H$.

Substituting (5.31a) and (5.31b) into the original equation (5.28), we obtain the governing equation in the spectral domain:

$$\rho c_p \frac{\partial T}{\partial t} - \alpha^2 k_r \frac{\partial^2 T}{\partial \hat{r}^2} - \frac{\alpha^2 k_r}{1 + \alpha r_{in} + \hat{r}} \frac{\partial T}{\partial \hat{r}} - \beta^2 k_z \frac{\partial^2 T}{\partial \hat{z}^2} = q \quad (5.32)$$

with the boundary conditions:

$$a_+ T + b_+ \frac{\partial}{\partial \hat{r}} T = e_t \quad \text{at } \hat{r} = 1 \quad (5.33a)$$

$$a_- T + b_- \frac{\partial}{\partial \hat{r}} T = e_b \quad \text{at } \hat{r} = -1 \quad (5.33b)$$

³Note that although we have prescribed constant (w.r.t the spatial variable) external temperatures at each side, the model is also capable of handling spatially dependant temperatures (e.g. $T_{r,\infty}(z)$ or $T_{t,\infty}(r)$). However, since the external temperatures would rarely be known with such a high fidelity in a real application, we chose constant values for the sake of simplicity.

$$c_+T + d_+\frac{\partial}{\partial\hat{z}}T = e_r \quad \text{at } \hat{z} = 1 \quad (5.33c)$$

$$c_-T + d_-\frac{\partial}{\partial\hat{z}}T = e_l \quad \text{at } \hat{z} = -1, \quad (5.33d)$$

where,

$$\begin{aligned} a_+ &= h_r/k_r, & b_+ &= \alpha, \\ a_- &= -h_l/k_r, & b_- &= \alpha, \\ c_+ &= h_t/k_z, & d_+ &= \beta, \\ c_- &= -h_b/k_z, & d_- &= \beta, \\ e_t &= a_+T_{t,\infty}, & e_b &= a_-T_{b,\infty}, \\ e_r &= c_+T_{r,\infty}, & e_l &= c_-T_{l,\infty}. \end{aligned} \quad (5.34)$$

5.2.4 Homogenization of the boundary conditions

Next, the problem with non-homogeneous boundary conditions is transformed into a problem with homogeneous boundary conditions using a boundary lifting algorithm, as follows: We set

$$T = \tilde{T} + T_e, \quad (5.35)$$

where $T_e(\hat{r}, \hat{z})$ is an arbitrary function satisfying the original boundary conditions (Eqs. (5.33a) - (5.33d)) (see later), and $\tilde{T}(\hat{r}, \hat{z}, t)$ is an auxiliary function satisfying the modified problem

$$\rho c_p \frac{\partial \tilde{T}}{\partial t} - \alpha^2 k_r \frac{\partial^2 \tilde{T}}{\partial \hat{r}^2} - \frac{\alpha^2 k_r}{1 + \alpha r_{in} + \hat{r}} \frac{\partial \tilde{T}}{\partial \hat{r}} - \beta^2 k_z \frac{\partial^2 \tilde{T}}{\partial \hat{z}^2} = q^*, \quad (5.36)$$

subject to the homogeneous boundary conditions

$$a_{\pm} \tilde{T} + b_{\pm} \tilde{T} \frac{\partial}{\partial \hat{r}} \tilde{T} = 0, \quad (5.37a)$$

$$c_{\pm} \tilde{T} + d_{\pm} \tilde{T} \frac{\partial}{\partial \hat{z}} \tilde{T} = 0, \quad (5.37b)$$

where

$$q^* = q - \left(-\alpha k_r \frac{\partial^2 T_e}{\partial \hat{r}^2} - \frac{\alpha^2 k_r}{1 + r_{in} + \hat{r}} \frac{\partial T_e}{\partial \hat{r}} - \beta k_z \frac{\partial^2 T_e}{\partial \hat{z}^2} \right). \quad (5.38)$$

The boundary lifting is similar to that in [124], except that here we apply it to cylindrical coordinates and neglect the corner component of the lifting (since we are assuming constant external temperatures).

5.2.5 Chebyshev-Galerkin approximation

Now we would like to solve the modified problem (5.36) using the Galerkin method. The first step is to multiply the equation by a test function, ν , and integrate over the entire domain,

$$\left(\frac{1 + \alpha r_{in} + \hat{r}}{\alpha} \left[\rho c_p \frac{\partial \tilde{T}}{\partial t} - \alpha^2 k_r \frac{\partial^2 \tilde{T}}{\partial \hat{r}^2} - \frac{\alpha^2 k_r}{1 + \alpha r_{in} + \hat{r}} \frac{\partial \tilde{T}}{\partial \hat{r}} - \beta^2 k_z \frac{\partial^2 \tilde{T}}{\partial \hat{z}^2} \right], \nu \right) = \left(\frac{1 + \alpha r_{in} + \hat{r}}{\alpha} q^*, \nu \right) \quad (5.39)$$

where (f, ν) denotes the integral of f weighted by ν , throughout the domain $\hat{r}, \hat{z}$,

$$(f, \nu) = \int_{-1}^1 \int_{-1}^1 f(\hat{r}, \hat{z}) \nu(\hat{r}, \hat{z}) d\hat{r} d\hat{z}. \quad (5.40)$$

Note the inclusion of the r terms as defined in (5.31a) on each side of equation (5.39) to account for cylindrical coordinates.

The second step is to approximate the solution $\tilde{T}(\hat{r}, \hat{z}, t)$ with a finite number of functions

$$\tilde{T} = \sum_{k=0}^N \sum_{j=0}^N x_{kj} \phi_k^{\hat{r}}(\hat{r}, a_{\pm}, b_{\pm}) \phi_j^{\hat{z}}(\hat{z}, c_{\pm}, d_{\pm}) \quad (5.41)$$

where x_{kj} are unknown solution coefficients, and $\phi_k^{\hat{r}}$ and $\phi_j^{\hat{z}}$ are the basis functions which must satisfy the homogeneous boundary conditions (5.37a) and (5.37b) respectively. For simplicity, the same number of basis functions, N , are chosen for the radial and axial directions but it should be noted that different values could be chosen if one dimension required greater resolution than the other.

Suitable 2-D basis functions are obtained by first finding basis functions in the radial and axial directions separately. Each of these is obtained in a similar manner to that of the toy problem (Eqs. (5.8) - (5.11)): we denote by C_k the k th degree Chebyshev polynomial of the first kind and then let $\{\phi_k^{\hat{r}}(\hat{r}, a_{\pm}, b_{\pm})\}_{k=0}^N$ be a basis in the radial direction such that

$$\phi_k^{\hat{r}} = C_k(\hat{r}) + \zeta_k^{\hat{r}} C_{k+1}(\hat{r}) + \eta_k^{\hat{r}} C_{k+2}(\hat{r}), \quad (5.42)$$

where $\zeta_k^{\hat{r}}(a_{\pm}, b_{\pm})$ and $\eta_k^{\hat{r}}(a_{\pm}, b_{\pm})$ are defined according to the formula in Lemma 4.3 of [95] such that they adhere to the boundary conditions in the radial direction,

$$\zeta_k^{\hat{r}} = \{4(k+1)(a_+ b_- + a_- b_+)\} / \text{DET}_k^{\hat{r}}, \quad (5.43)$$

and

$$\eta_k^{\hat{r}} = \{-2a_-a_+ + (k^2 + (k+1)^2)(a_+b_- - a_-b_+) + 2b_-b_+k^2(k+1)^2\}/\text{DET}_k^{\hat{r}}, \quad (5.44)$$

where

$$\begin{aligned} \text{DET}_k^{\hat{r}} &= 2a_+a_- + ((k+1)^2 + (k+2)^2) \\ &(a_-b_+ - a_+b_-) - 2b_-b_+(k+1)^2(k+2)^2. \end{aligned} \quad (5.45)$$

Similarly, we let $\{\phi_j^{\hat{z}}(\hat{z}, c_{\pm}, d_{\pm})\}_{j=0}^N$ be a basis in the axial direction such that

$$\phi_j^{\hat{z}} = C_j(\hat{z}) + \zeta_j^{\hat{z}}C_{j+1}(\hat{z}) + \eta_j^{\hat{z}}C_{j+2}(\hat{z}), \quad (5.46)$$

where $\zeta_j^{\hat{z}}(c_{\pm}, d_{\pm})$ and $\eta_j^{\hat{z}}(c_{\pm}, d_{\pm})$ adhere to the boundary conditions in the axial direction,

$$\zeta_j^{\hat{z}} = \{4(j+1)(c_+d_- + c_-d_+)\}/\text{DET}_j^{\hat{z}}, \quad (5.47)$$

and

$$\begin{aligned} \eta_j^{\hat{z}} &= \{-2c_-c_+ + (j^2 + (j+1)^2)(c_+d_- - c_-d_+) \\ &+ 2d_-d_+j^2(j+1)^2\}/\text{DET}_j^{\hat{z}}, \end{aligned} \quad (5.48)$$

where

$$\begin{aligned} \text{DET}_j^{\hat{z}} &= 2c_+c_- + ((j+1)^2 + (j+2)^2) \\ &(c_-d_+ - c_+d_-) - 2d_-d_+(j+1)^2(j+2)^2. \end{aligned} \quad (5.49)$$

It should be noted that the choice of basis function is not limited to Chebyshev polynomials. In general, various Jacobi polynomials may work equally well. In particular, we verified that almost identical results were obtained using Legendre polynomials.

5.2.6 Boundary lifting function

We now wish to determine the boundary lifting function, $T_e(\hat{r}, \hat{z})$. Recall that $T_e(\hat{r}, \hat{z})$ must satisfy the original (non-homogeneous) boundary conditions (5.33a-5.33d), such that when subtracted from the actual temperature, T , (Eq. (5.35)) the resulting auxiliary function, $\tilde{T}$, satisfies the homogeneous boundary conditions. Hence, the aim

of this section is to derive a function which is constant with respect to time and satisfies the non-homogeneous boundary conditions. Since this cannot be achieved exactly, the boundary conditions must instead be satisfied in a weak sense (i.e. the solution converges as more basis functions are included). To begin, we adopt a similar approach to [124] by assuming a form of the solution as follows:

$$T_e = \left[\sum_{k=0}^N \left(d_k^I \hat{z} + d_k^{II} \hat{z}^2 \right) \phi_k^{\hat{r}} \right] + \left[\sum_{j=0}^N \left(d_j^{III} \hat{r} + d_j^{IV} \hat{r}^2 \right) \phi_j^{\hat{z}} \right]. \quad (5.50)$$

The conditions at the vertical and horizontal sides are defined as follows. For the right side, we have

$$c_+ T_e + d_+ \frac{\partial T_e}{\partial \hat{z}} \approx e_r \quad \text{at } \hat{z} = +1 \quad (5.51)$$

where $\approx$ denotes weakly satisfying conditions. Substituting 5.50 in 5.51 gives

$$\begin{aligned} & \sum_{k=0}^N \left(d_k^I (c_+ \hat{z} + d_+) + d_k^{II} (c_+ \hat{z}^2 + 2d_+ \hat{z}) \right) \phi_k^{\hat{r}} \\ & + \sum_{j=0}^N \left(\hat{r} d_j^{III} + \hat{r}^2 d_j^{IV} \right) \left(c_+ \phi_j^{\hat{z}} + d_+ \frac{\partial \phi_j^{\hat{z}}}{\partial \hat{z}} \right) \approx e_r. \end{aligned} \quad (5.52)$$

Substituting for $\hat{z} = 1$ and noting that the term $\left(c_+ \phi_j^{\hat{z}} + d_+ \frac{\partial \phi_j^{\hat{z}}}{\partial \hat{z}} \right)$ is equal to zero (since the basis functions by definition satisfy the homogeneous boundary conditions), equation (5.52) simplifies to

$$\sum_{k=0}^N \left(d_k^I (c_+ + d_+) + d_k^{II} (c_+ + 2d_+) \right) \phi_k^{\hat{r}} \approx e_r. \quad (5.53)$$

The weak boundary condition can now be replaced by the appropriate integral equation,

$$\sum_{k=0}^N \left(d_k^I (c_+ + d_+) + d_k^{II} (c_+ + 2d_+) \right) \langle \phi_k^{\hat{r}}, \phi_i^{\hat{r}} \rangle_{\hat{r}} = \langle e_r, \phi_i^{\hat{r}} \rangle_{\hat{r}}, \quad (5.54)$$

where $\langle f, g \rangle_{\hat{r}}$ denotes the integral,

$$\langle f, g \rangle_{\hat{r}} = \int_{-1}^1 \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha} \right) f(\hat{r}) g(\hat{r}) d\hat{r}. \quad (5.55)$$

Through a similar process for the left, top and bottom sides, we find that

$$\sum_{k=0}^N \left(d_k^{\text{I}}(-c_- + d_-) + d_k^{\text{II}}(c_- - 2d_-) \right) \langle \phi_k^{\hat{r}}, \phi_i^{\hat{r}} \rangle_{\hat{r}} = \langle e_l, \phi_i^{\hat{r}} \rangle_{\hat{r}}, \quad (5.56)$$

$$\sum_{j=0}^N \left(d_j^{\text{III}}(a_+ + b_+) + d_j^{\text{IV}}(a_+ + 2b_+) \right) \langle \phi_j^{\hat{z}}, \phi_i^{\hat{z}} \rangle_{\hat{z}} = \langle e_t, \phi_i^{\hat{z}} \rangle_{\hat{z}}, \quad (5.57)$$

$$\sum_{j=0}^N \left(d_j^{\text{III}}(-a_- + b_-) + d_j^{\text{IV}}(a_- - 2b_-) \right) \langle \phi_j^{\hat{z}}, \phi_i^{\hat{z}} \rangle_{\hat{z}} = \langle e_b, \phi_i^{\hat{z}} \rangle_{\hat{z}}, \quad (5.58)$$

where $\langle f, g \rangle_{\hat{z}}$ denotes the integral,

$$\langle f, g \rangle_{\hat{z}} = \int_{-1}^1 f(\hat{z})g(\hat{z})d\hat{z}. \quad (5.59)$$

Equations (5.54) and (5.56) and equations (5.57) and (5.58) form two linear systems which can be each solved for the corresponding $\mathbf{d}^\sigma$ vectors:

$$\mathbf{d}^{\text{I}} = \frac{k_4 e_r - k_2 e_l}{k_1 k_4 - k_2 k_3} (\mathbf{P}^{rl})^{-1} \mathbf{s}^{rl}, \quad (5.60a)$$

$$\mathbf{d}^{\text{II}} = \frac{k_1 e_l - k_3 e_r}{k_1 k_4 - k_2 k_3} (\mathbf{P}^{rl})^{-1} \mathbf{s}^{rl}, \quad (5.60b)$$

$$\mathbf{d}^{\text{III}} = \frac{j_4 e_t - j_2 e_b}{j_1 j_4 - j_2 j_3} (\mathbf{P}^{tb})^{-1} \mathbf{s}^{tb}, \quad (5.60c)$$

$$\mathbf{d}^{\text{IV}} = \frac{j_1 e_b - j_3 e_t}{j_1 j_4 - j_2 j_3} (\mathbf{P}^{tb})^{-1} \mathbf{s}^{tb}, \quad (5.60d)$$

where $\{\mathbf{d}^\sigma = (d_0^\sigma, d_1^\sigma, \dots, d_N^\sigma)^T; \sigma = \text{I, II, III and IV}\}$ are vectors of unknown expansion coefficient, $\{\mathbf{s}^\sigma = (s_0^\sigma, s_1^\sigma, \dots, s_N^\sigma)^T; \sigma = rl \text{ and } tb\}$ are vectors of known source terms, and

$$\begin{aligned} k_1 &= c_+ + d_+, & j_1 &= a_+ + b_+, \\ k_2 &= c_+ + 2d_+, & j_2 &= a_+ + 2b_+, \\ k_3 &= d_- - c_-, & j_3 &= b_- - a_-, \\ k_4 &= c_- - 2d_-, & j_4 &= a_- - 2b_-. \end{aligned} \quad (5.61)$$

The $\mathbf{P}$ matrix for the right and left edges is defined as $\{\mathbf{P}^{rl} = p_{i,k}^{rl}; i, k = 0, 1, \dots, N\}$, where

$$p_{i,k}^{rl} = \int_{-1}^1 \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha} \right) \phi_i^{\hat{r}} \phi_k^{\hat{r}} d\hat{r}, \quad (5.62a)$$

and that for the top and bottom sides as $\{\mathbf{P}^{tb} = p_{i,j}^{tb}; i, j = 0, 1, \dots, N\}$, where

$$p_{i,j}^{tb} = \int_{-1}^1 \phi_i^{\hat{z}} \phi_j^{\hat{z}} d\hat{z}. \quad (5.62b)$$

Lastly, the source terms are defined as $\{\mathbf{s}^\sigma = s_i^\sigma; i = 0, 1, \dots, N; \sigma = rl \text{ and } tb\}$, where

$$s_i^{rl} = \int_{-1}^1 \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha} \right) \phi_i^{\hat{r}} d\hat{r}, \quad (5.63a)$$

$$s_i^{tb} = \int_{-1}^1 \phi_i^{\hat{z}} d\hat{z}. \quad (5.63b)$$

Thus, an explicit expression for the unknown expansion coefficients, $\mathbf{d}^\sigma$ is obtained, and so the boundary lifting function, T_e , can be considered known at this stage.

5.2.7 Solution algorithm

Finally, we present the solution algorithm to the modified problem. Equation (5.36) can be expressed in state space form, as follows:

$$\mathbf{E}\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \quad (5.64)$$

where

$$\mathbf{x} = (x_{00}, x_{10}, \dots, x_{N0}, x_{01}, x_{11}, \dots, x_{N1}, \dots, x_{0N}, \dots, x_{NN})^T, \quad (5.65)$$

and $\mathbf{u} = [q(t), 1]^T$. The system matrices are defined as follows. First, let us denote the column vector

$$\Psi = (\phi_0^{\hat{r}} \phi_0^{\hat{z}}, \phi_1^{\hat{r}} \phi_0^{\hat{z}}, \dots, \phi_N^{\hat{r}} \phi_0^{\hat{z}}, \phi_0^{\hat{r}} \phi_1^{\hat{z}}, \phi_1^{\hat{r}} \phi_1^{\hat{z}}, \dots, \phi_N^{\hat{r}} \phi_1^{\hat{z}}, \dots, \phi_0^{\hat{r}} \phi_N^{\hat{z}}, \dots, \phi_N^{\hat{r}} \phi_N^{\hat{z}})^T \quad (5.66)$$

and take $\nu = \psi_i$; then:

$$\mathbf{E} = [e_{ij}], \quad e_{ij} = \rho c_p \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha} \psi_j, \psi_i \right), \quad (5.67)$$

where $[e_{ij}]$ denotes the i th row and j th column of the matrix $\mathbf{E}$.

$$\begin{aligned} \mathbf{A} &= [a_{ij}], \\ a_{ij} &= \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha} \left[\alpha^2 k_r \frac{\partial^2 \psi_j}{\partial \hat{r}^2} + \beta^2 k_z \frac{\partial^2 \psi_j}{\partial \hat{z}^2} \right] + \alpha k_r \frac{\partial \psi_j}{\partial \hat{r}}, \psi_i \right) \end{aligned} \quad (5.68)$$

for $i, j = 0, 1, \dots, N$, and,

$$\begin{aligned} \mathbf{B} &= [b_{i1}, b_{i2}], \\ b_{i1} &= \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha}, \psi_i \right), \\ b_{i2} &= \left(\frac{1 + \hat{r} + \alpha r_{in}}{\alpha} \left[\alpha^2 k_r \frac{\partial^2 T_e}{\partial \hat{r}^2} + \beta^2 k_z \frac{\partial^2 T_e}{\partial \hat{z}^2} \right] + \alpha k_r \frac{\partial T_e}{\partial \hat{r}}, \psi_i \right) \end{aligned} \quad (5.69)$$

for $i = 0, 1, \dots, N$.

The complete solution to the original non-homogeneous problem is then given by:

$$T(\hat{r}, \hat{z}, t) = \tilde{T}(\hat{r}, \hat{z}, t) + T_e(\hat{r}, \hat{z}) \quad (5.70)$$

We choose as outputs the temperatures at the bottom-centre, left-centre, top-centre and right-centre locations, i.e. $T_1 = T(\hat{r} = -1, \hat{z} = 0)$, $T_2 = T(\hat{r} = 0, \hat{z} = -1)$, $T_3 = T(\hat{r} = 1, \hat{z} = 0)$ and $T_4 = T(\hat{r} = 0, \hat{z} = 1)$ (see Fig. 5.5). Thus, the outputs are given by:

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \quad (5.71)$$

where $\mathbf{y} = (T_1, T_2, T_3, T_4)^T$, $\mathbf{D} = (0, 0, 0, 0; T_{e,1}, T_{e,2}, T_{e,3}, T_{e,4})^T$, and,

$$\mathbf{C} = (c_{i,j}), \quad \begin{cases} c_{1,j}, &= \psi_j(\hat{r} = -1, \hat{z} = 0), \\ c_{2,j}, &= \psi_j(\hat{r} = 0, \hat{z} = -1), \\ c_{3,j}, &= \psi_j(\hat{r} = 1, \hat{z} = 0), \\ c_{4,j}, &= \psi_j(\hat{r} = 0, \hat{z} = 1) \end{cases} \quad (5.72)$$

for $j = 0, 1, \dots, N$.

The frequency domain response of the above linear system, $H(s)$, is calculated by

$$\mathbf{H}(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} \quad (5.73)$$

where $s = j\omega$ is the Laplace variable and $\mathbf{I}$ is the identity matrix.

The above algorithm was implemented both numerically (using Clanshaw-Curtis quadrature) and analytically using the Matlab Symbolic Maths Toolbox. The numerical implementation allows the state matrices to be generated more efficiently than the symbolic approach, although the resulting state space model is identical (and therefore equally efficient) in each case.

Lastly, it should be noted that since the method ultimately results in a state space model, with state matrices which can be evaluated offline, the online implementation merely requires matrix-vector multiplication and vector-vector addition operations (i.e. $\mathbf{Ax} + \mathbf{By}$). These scale as $\mathcal{O}(n^2)$ and $\mathcal{O}(n)$ respectively, where n is the side length of the matrix (i.e. the number of states in the state vector). Hence the lower the number of states, the lower the computational requirement.

5.3 Results and discussion

To validate the SG model, the results were compared with high fidelity FEM simulations, implemented using the Matlab Partial Differential Equation Toolbox. To ensure the accuracy of the FEM solution, a fine mesh consisting of 3,760 elements⁴ was used. The time step for both the SG and FEM models was set at 1 s.

The thermo-physical parameters chosen for the model validation are shown in Table 5.1. The dimensions were chosen to match those of the large format lithium-ion cell employed in [73], and the remaining thermal parameters were chosen based on typical properties of lithium iron phosphate cells ([71, 28, 25]).

5.3.1 Time domain

Time domain simulations were carried out using two different cooling scenarios, as shown in Table 5.2. Case 1 represents forced convection air cooling, with equal temperatures and convection coefficients at each of the external sides. Case 2 represents forced

⁴The number of elements (3,760) was chosen as an arbitrary, large number as a conservative means of ensuring high fidelity simulations. The comparison between the number of states or elements in the FE model and that of the SG model should not be taken as a direct comparison of computational requirements, since finite element models often involve sparse matrices, which can be operated on using efficient computational methods.

Table 5.1 Thermophysical properties for model validation.

Parameter	Symbol	Value
Inner radius	r_{in}	4 mm
Outer radius	r_{out}	32 mm
Height	H	198 mm
Density	ρ	2,118 kg m ⁻³
Specific heat capacity	c_p	765 J kg ⁻¹ K ⁻¹
Radial thermal conductivity	k_r	0.66 W mK ⁻¹
Axial thermal conductivity	k_z	66 W mK ⁻¹

convection liquid cooling at the left end of the cell (for instance, via a cooling plate [125]), and natural convection to the ambient air at the remaining faces. Thus, the temperature at the left face is set to 3°C and a large convection coefficient typical of forced cooling via water or glycol is applied, whereas the remaining faces are exposed to a small convection coefficient at 18°C. This case was chosen to highlight the ability of the model to account for different external temperatures and/or convection coefficients at each side. Note that the convection coefficient at the bottom side (the inner radius of the jelly roll) was set to zero in both cases since negligible cooling occurs here in a typical thermal management system; however a non-zero value could easily be applied if it were required.

Table 5.2 Convection coefficients for the two cooling scenarios.

	Case 1		Case 2	
	h (W m ⁻²)	T_∞ (°C)	h (W m ⁻²)	T_∞ (°C)
Left	100	18	400	3
Right	100	18	30	18
Top	100	18	30	18
Bottom	0	18	0	18

To ensure highly transient conditions with large internal temperature gradients, pulsed power load profiles with large heat generation rates but relatively short durations were applied. The load profiles and resulting temperature distributions for the two cases are compared against the corresponding FEM solutions in Figs. 5.6 and 5.7. The locations of the model outputs are shown in Fig. 5.5.

The results show that the SG method with $N_s = 4$ states (i.e. 2 basis functions in each of the radial and axial directions) is capable of accurately capturing the temperatures in both cases. Slightly greater accuracy is achieved using $N_s = 25$ states (5 basis

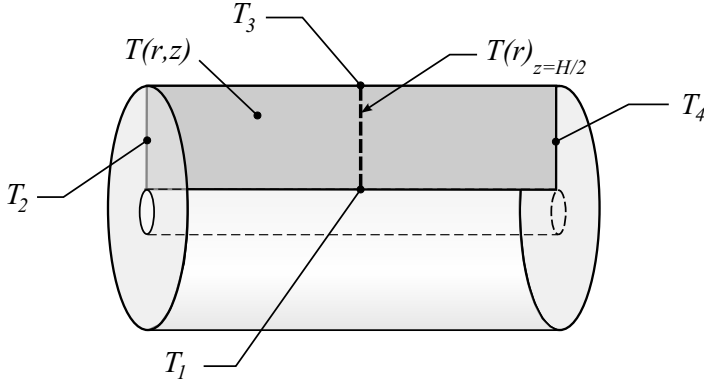


Fig. 5.5 Schematic of cell showing the model outputs displayed in Figs. 5.6 and 5.7.

functions in each direction). In Case 1, the temperatures, T_1 and T_3 (i.e. the first and third model outputs from equation 5.71) are plotted (see Fig. 5.6a) since the temperature gradient is primarily in the radial direction in this case. In Case 2, the temperatures T_2 and T_4 were plotted since a large gradient occurs in the axial direction in this case. Plots of $T(r)_{z=H/2}$ are shown in part (b) of these figures. In each case, the first two sub-plots show the distribution at instances of highly transient dynamics (i.e. just after a load is applied or removed), which is more difficult to capture accurately for a low-order thermal model, although the results are still in good agreement in both cases. The third sub-plot in each case shows the solution at a later time - when the problem is dominated by slow thermal dynamics - and the SG and FEM solutions are in nearly perfect agreement at these times. The full 2-D contour plots are shown in Figs. 5.8 and ???. Again, the solution is plotted at an instant with transient dynamics to demonstrate the ability of the low-order model to accurately simulate the temperature field under these conditions. The advantage of increasing the number of model states is apparent in Fig. ??, as the result using $N_s = 25$ states is in better agreement with that of the FEM solution than the result with $N_s = 4$ states. Although the absolute errors in each case are small.

Lastly, we note that the model with 4 states is of a similar order to an equivalent circuit thermal model and so could be applied with similar computational efficiency (since both can be expressed and solved using a state-space form). Moreover, a similar order model implemented using a spectral-collocation method would not give results as accurate as those presented in this section, since in the SG method the boundary conditions are implicitly satisfied by the basis functions, whereas additional equations are required to enforce the boundary conditions in the collocation case.

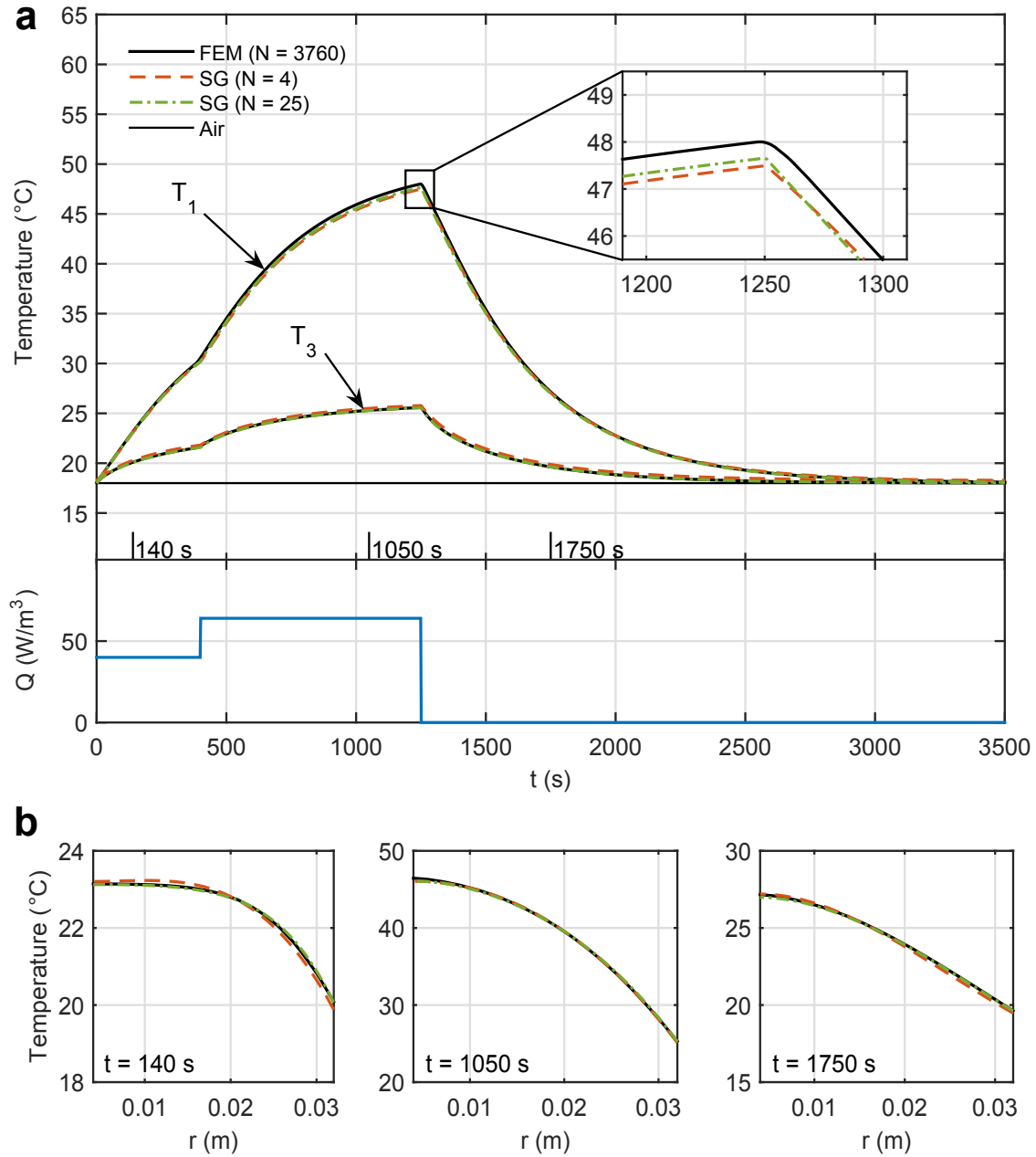


Fig. 5.6 Comparison of SG vs. FEM results for Case 1: forced air convection. (a) Evolution of temperatures, T_1 (core) and T_3 (outer surface), with pulsed load profile shown in subplot; (b) Temperature distribution along the centre-line ($z = H/2$) of the cell at denoted times.

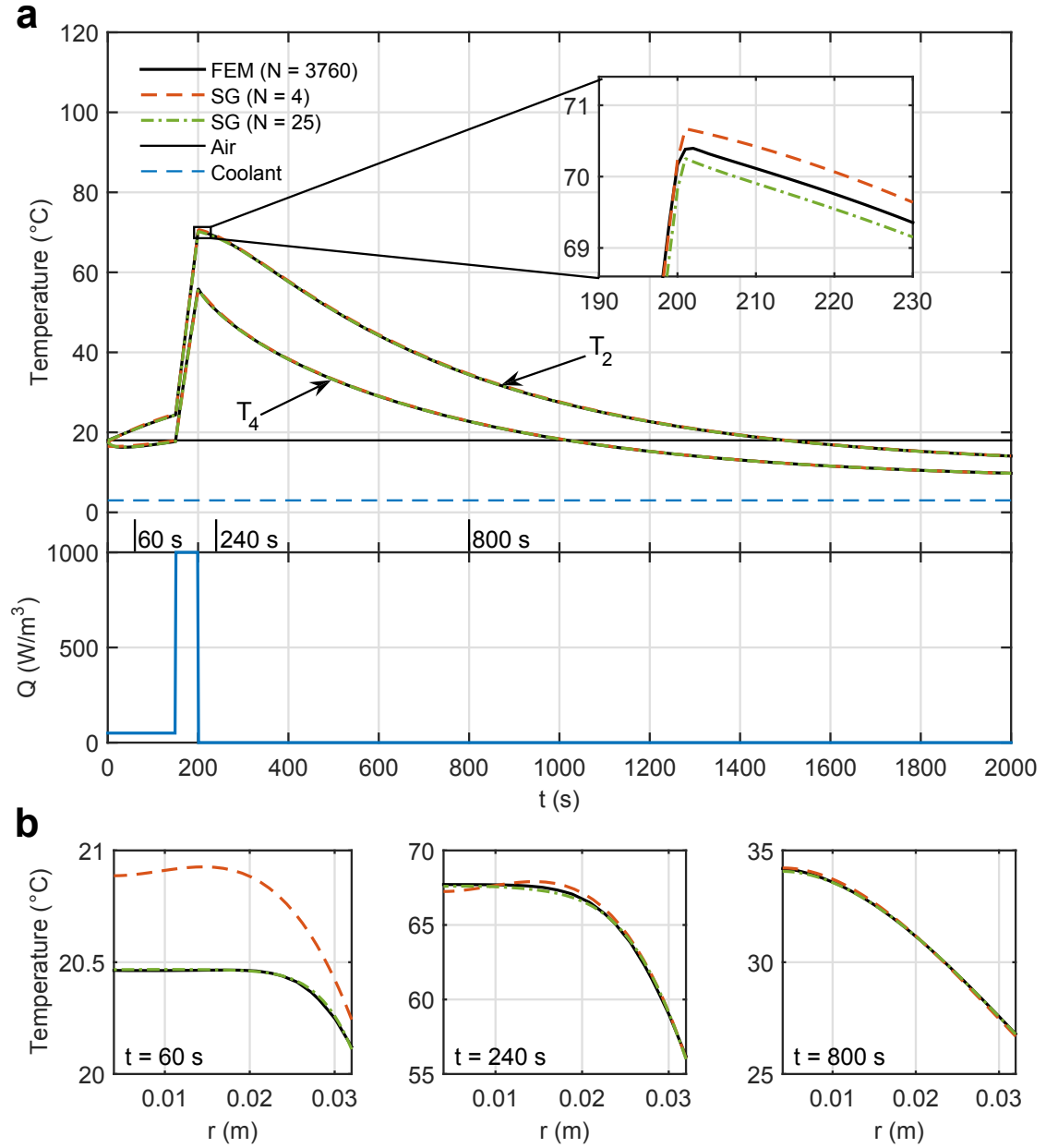


Fig. 5.7 Comparison of SG vs. FEM results for Case 2: end-plate liquid cooling. (a) Evolution of temperatures, T_2 and T_4 , with pulsed load profile shown in subplot; (b) Temperature distribution along the centre-line ($z = H/2$) of the cell at denoted times

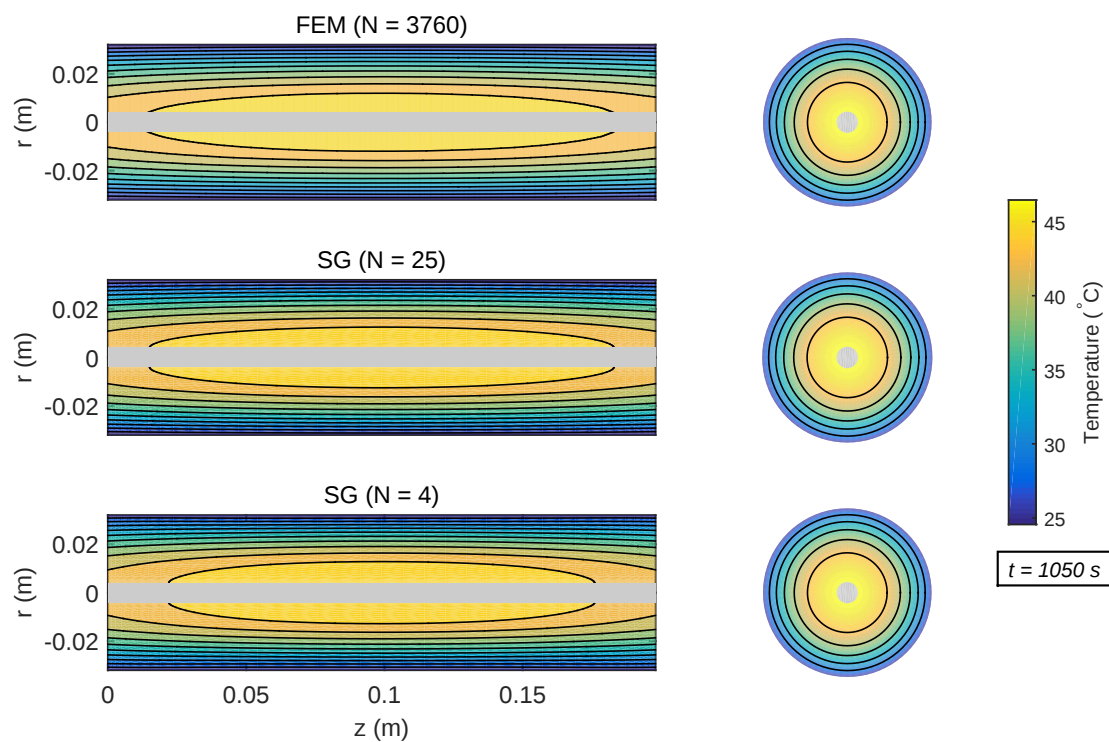


Fig. 5.8 Contour plots of SG and FEM methods for Case 1

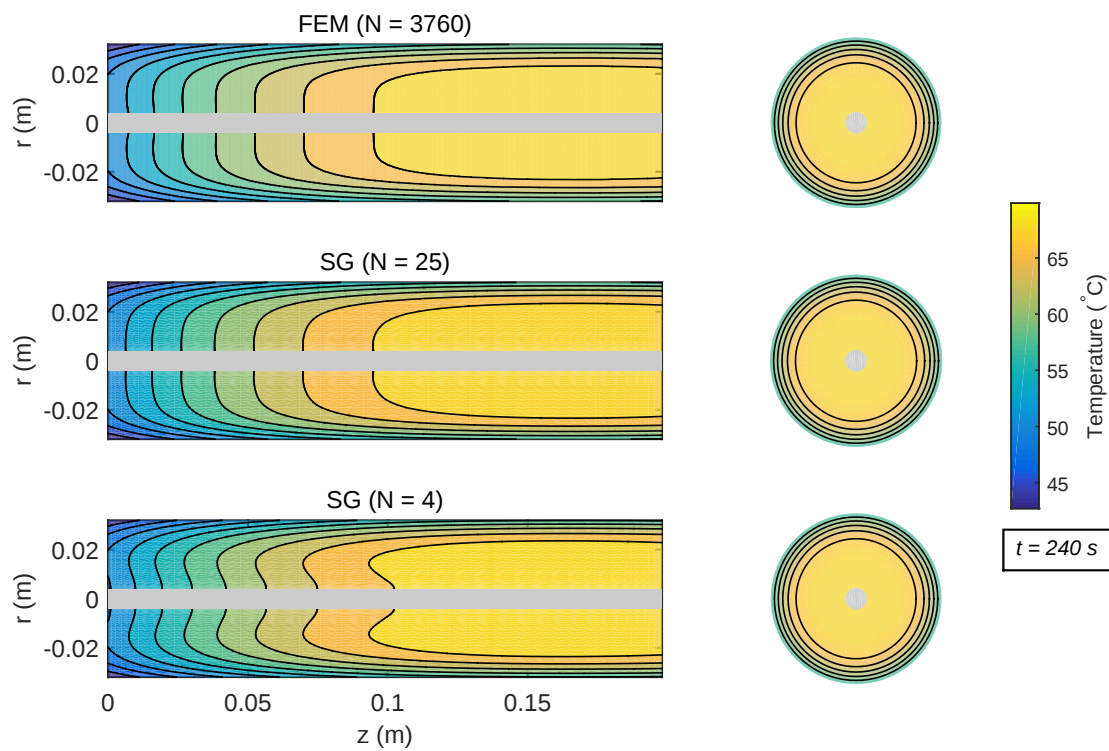


Fig. 5.9 Contour plots of SG and FEM methods for Case 2

5.3.2 Frequency domain

In this section we compare the frequency response of the low-order SG models against a baseline solution obtained by using an SG model with a large number of states ($N_s = 225$). Specifically, we examine the impact of changes in heat generation on the core temperature, T_1 , given by the transfer function $H(s) = T_1(s)/q(s)$. This is calculated using Eq. (5.71), using only the rows and columns of the $\mathbf{B}$ and $\mathbf{C}$ matrices corresponding to the heat generation input and T_1 output.

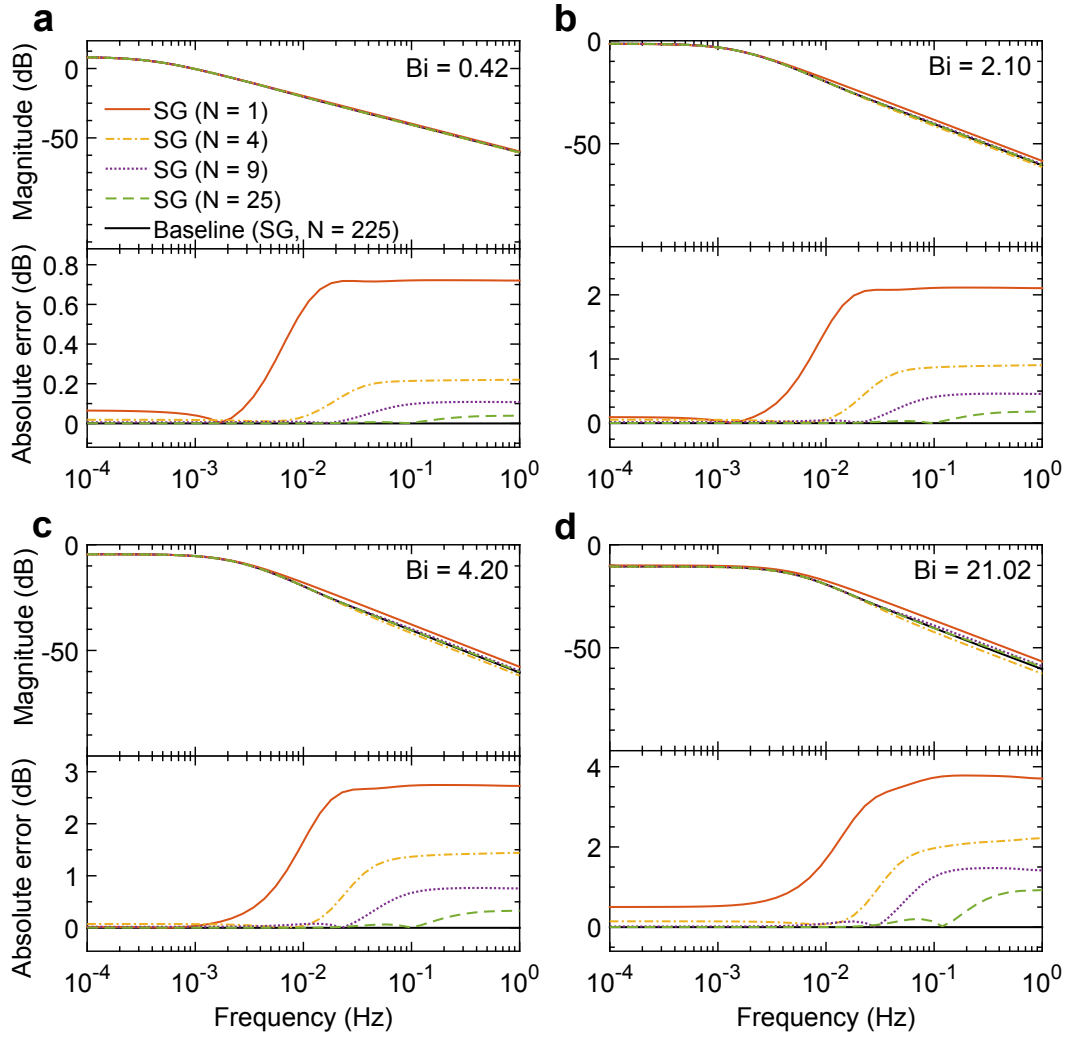


Fig. 5.10 Frequency response, $T_1(s)/q(s)$, of the SG method with different model orders for a range of Biot number conditions as indicated. A large order ($N_s = 225$) SG method is used as the baseline solution.

The parameters chosen are the same as those in Case 1 of the previous section. However, a variety of different Biot numbers ($Bi = h(r_{out} - r_{in})/k$) are obtained by varying

the magnitude of the convection coefficients on each side. Convection coefficients of $h = \{10, 50, 100, 500\} \text{ Wm}^{-2}$ are chosen, resulting in Biot numbers of $Bi = \{0.42, 2.10, 4.20 \text{ and } 21.02\}$, respectively. The size of the model is varied by increasing the number of basis functions in both the radial and axial directions. Models with 1, 2, 3 and 5 basis functions in each direction are chosen, resulting in $N_s = 1, 4, 9 \text{ and } 25$ states respectively.

Figs. 5.10(a)-(d) show the magnitude of the frequency response in the range $f = 1 \times 10^{-4}$ to 1×10^0 Hz for each of the four Biot numbers, along with the error of the low order models relative to the high fidelity solution. These plots show that as the model order (i.e. the number of states) is increased, the magnitude of the error is reduced. Moreover, for all cases, there is a critical frequency at which the error becomes non-negligible, and this critical frequency increases as the model order is increased. We also note that the error increases as (i) the Biot number increases, and (ii) the perturbation frequency increases. These trends are as expected. Thus, if a particular application involves larger Biot numbers or higher frequencies (for instance, due to larger cells, more aggressive drive cycles or higher performance cooling), the model order could be increased accordingly to achieve a required accuracy.

5.4 Conclusions

Computationally efficient thermal models are necessary for control-oriented applications. The model presented in this chapter is of a similar order to a thermal equivalent circuit (TEC) model - and so could be applied with similar computational efficiency - but has much greater spatial resolution. Moreover, although the model applies to a cylindrical cell, it can easily be modified to apply to 2-D simulation of prismatic cells.

Whilst implementing a single cell model involves almost negligible computational cost, the cost of implementation would become a relevant factor for large multi-cell systems (such as EV battery packs) containing hundreds or thousands of cells. Since matrix multiplications scale as $\mathcal{O}(n^2)$ (as discussed in Section 5.2.7), the computational requirement on the micro-controller will be $(n_c n_s)^2 \Delta t$ FLOPS, where n_c and n_s are the number of cells and the number of states per cell respectively, and Δt is the time step. Hence if we use a time step of 1 s and 1,000 cells, then the computational requirements will be $(1 \times 10^6) n_s$. If, for instance, the SG method requires 4 states per cell for a given accuracy, whereas a TEC method requires 8, then the requirements on the controller would be 4×10^6 for the SG compared to 8×10^6 for the TEC. This difference in FLOP requirements is on the same order as low-cost micro-controllers (clock speeds

are in the range of MHz) and, given that the thermal model is not the only model that would be required in most applications (SoC estimation, balancing etc.), this could mean the difference between requiring a particular micro-controller model or a higher performance (more expensive) one. Hence, the present approach clearly has the potential to be advantageous for practical implementation in an EV application. However, it is also worth reiterating that it is difficult to apply the SG method to more complex problems such as multi-cell systems, due to the intricacy of its derivation, and so this additional cost in terms of development time and expertise requirements must also be considered. Hence, for certain configurations involving several cells or non-uniform cooling, TECs may remain favourable due to their relative simplicity. In the following chapter, the model is incorporated into a state estimation scheme (Hybrid Method II: ITD/TM) and the predicted temperatures at four locations (one internal and three on the cell surface) are validated experimentally against thermocouple measurements.

Chapter 6

Hybrid Method II (2-D)

This chapter presents an application of Hybrid Method II to a 2-D problem. The method is conceptually similar to the 1-D method presented in Chapter 4, with a number of slight differences discussed below. As in the 1-D case, the method requires knowledge of the cell thermal properties, heat generation rates and boundary conditions, but does not rely on any online temperature measurements. This chapter is primarily based on our work published in [101]. Matlab code to run the state-estimation algorithm presented in this chapter is available online¹.

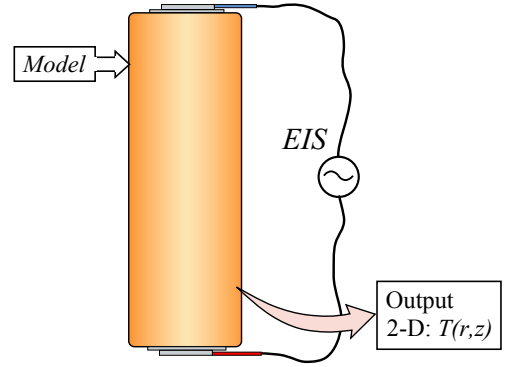


Fig. 6.1 ITD/TM (2-D)

The chapter is organised as follows. Section 6.1 provides an overview of the method. Section 6.2 presents the thermal model and state estimation algorithm. Section 6.3 describes the experimental setup and procedure; the setup is similar to that described in Chapter 2, but with asymmetric cooling to enforce 2-D thermal dynamics and including additional temperature sensors to capture the associated 2-D temperature gradients.

The remaining sections present experimental results. First, the full spectrum impedance measurements are presented (Section 6.4), verifying that the impedance at the selected frequency is independent of SoC. Section 6.5 then presents the parameterisation and validation of the thermal parameters. Lastly, results of the state estimation applied to two different sets of experiments are presented. The first (Section 6.6), uses HEV drive

¹www.github.com/robert-richardson/EKF-Impedance-2D-Temperature

cycle data as the input. As in previous chapters, the impedance is carried out during 4 s rests in the drive cycle. The results show that an extended Kalman filter, consisting of the 2-D thermal model coupled with current, voltage and impedance measurements, is capable of accurately predicting the core and multiple surface temperatures for each of the HEV drive cycles. As in the 1-D case, the performance of the EKF using impedance as the measurement input is comparable to - although slightly less accurate than - an equivalent Kalman filter using a conventional surface temperature sensor as measurement input. In certain practical applications (for instance, back-up energy storage systems), the applied load required from the battery may be constant. Hence, the second set of tests (Section 6.7) uses constant discharge currents. In this case, the impedance is carried out without any pause in the cycle (i.e. under the superposed DC current). To enable this, the impedance coefficients were also calibrated under the same DC-offset current. This example highlights a simple case in which the requirement for a pause in the applied current load is mitigated.

6.1 Overview of method

The method is conceptually very similar to the 1-D method presented in Chapter 4 with the exception of the following:

- In the present case the thermal model is the 2-D SG model presented in the previous chapter, rather than the 1-D PA model.
- The imaginary - rather than the real - impedance was used as the measurement input. As discussed in Chapter 1, the optimum impedance-metric is still an area of research; however in this case the imaginary impedance was used as it was found to be less susceptible to variation due to applied loads.
- The impedance is assumed to be directly related to the volume average temperature, $\bar{T}$, rather than the more exact impedance-based volume average temperature, $\bar{T}_{EIS}$. This was a necessary compromise since the calculation of the cell impedance with temperature gradients in both the r and z directions is more complex and computationally intensive than the 1-D case. As discussed in Chapter 2, this may introduce error into the method, in particular under very large temperature gradients or for highly non-linear impedance-temperature correlations. However, the results show that the method is acceptable for the present case.
- The impedance coefficients were calibrated using data from a single drive cycle, rather than by measurements at multiple uniform cell temperatures as in the

1-D case. This greatly reduces the time required for the calibration step, since it overcomes the need for cell thermal equalization at multiple steady-state temperatures.

An overview of the process is shown in Fig. 6.2 and described below. More detailed descriptions of each of the steps in the process are given in the subsequent sections of this chapter (Sections 6.2-6.6).

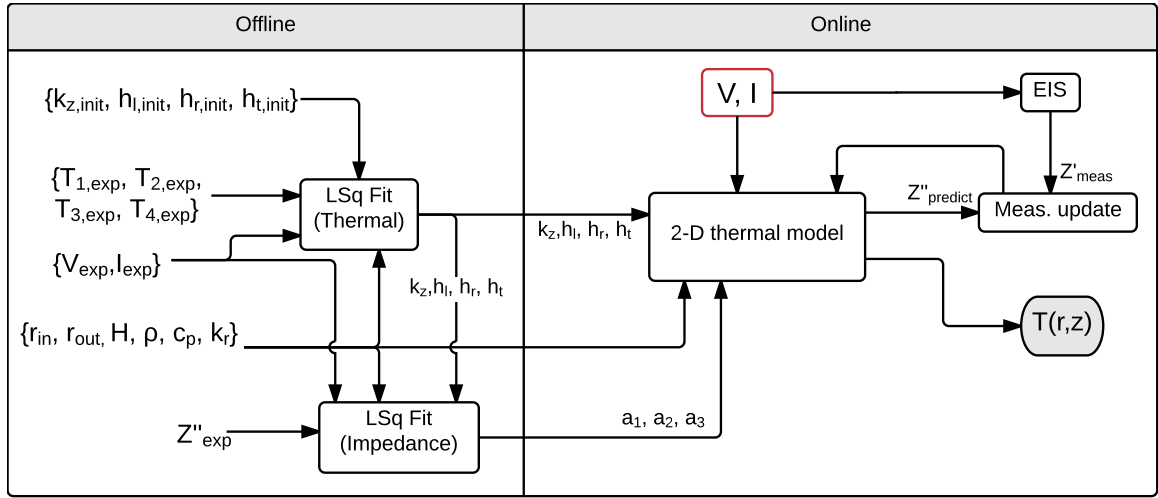


Fig. 6.2 ITD/TM process flowchart (2-D).

Offline: The cell dimensions (r_{in} , r_{out} , H) are measured and therefore known a-priori; the thermal properties (ρ , c_p , k_r) are available from the literature [28], and therefore also known a-priori. The remaining thermal parameters (k_z , h_l , h_r , and h_t) are then estimated using a recursive least squares estimation algorithm (Section 6.5). Specifically, the thermal model is simulated using experimental current and voltage data (V_{exp} , I_{exp}), from a parameterization drive cycle and the temperature outputs at four locations (T_1 , T_2 , T_3 , and T_4) are compared with their corresponding thermocouple measurements. The parameterised model is used to fit the impedance coefficients (Sections 6.6.1 and 6.7.1). Specifically, the predicted mean temperature ($\bar{T}$) from the model is paired with the corresponding measured impedance value (Z'') at each sample. A second order polynomial fit is then applied to the resulting impedance-temperature data, thus identifying coefficients (a_1 , a_2 , a_3). Finally, the known and identified thermal parameters and the identified impedance coefficients are provided to the online thermal model.

Online: The thermal model (Chapter 5) uses online measurements of the voltage and current (V , I) to predict the heat generation, 2-D temperature distribution, and cell

imaginary impedance at each time step. This is compared to the measured imaginary impedance which is then used to update the state estimate of the model via an Extended Kalman Filter algorithm (EKF) (Section 6.2.2).

6.2 Theory

6.2.1 2-D thermal model

The thermal model consists of the 2-D spectral-Galerkin model described in Chapter 5:

$$\mathbf{E}\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \quad (5.64)$$

where the model states are given by

$$\mathbf{x} = (x_{00}, x_{10}, \dots, x_{N0}, x_{01}, x_{11}, \dots, x_{N1}, \dots, x_{0N}, \dots, x_{NN})^T, \quad (5.65)$$

and the state matrices are as defined in equations 5.67 to 5.72. The model inputs are: $\mathbf{u} = [q(t), 1]^T$, where the heat generation is assumed to be uniformly distributed throughout the cell volume, in the same manner as the 1-D case (Eq. (4.2)):

$$q = \frac{1}{V_b} I(V - U_{OCV}), \quad (6.1)$$

where V_b is the cell volume, I and V are the measured current and voltage respectively, and U_{OCV} is the cell open circuit voltage.

The boundary conditions are given by 5.29a - 5.29d. The convection coefficient, h_b , is set to zero (since this corresponds to the inner radius of the cell jelly roll, which is not exposed to cooling). The convection coefficient, h_t , corresponds to the curved surface of the cell, whilst h_l and h_r correspond to left and right ends of the cell. Note that the placement of the heat sink results in an increased value of h_l .

Four temperature outputs are chosen corresponding to the positions $T_1 = T(r = r_{in}, z = H/2)$, $T_2 = T(r = r_{out}, z = 0)$, $T_3 = T(r = r_{out}, z = H/2)$ and $T_4 = T(r = r_{out}, z = H)$ (see Fig. 6.3). These outputs were chosen to match the thermocouple measurements in the experimental setup as described in the following section. Hence, the outputs (scaled to the domain $\hat{r} \in [-1, 1]$, $\hat{z} \in [-1, 1]$) are given by

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \quad (6.2)$$

where $\mathbf{y} = (T_1, T_2, T_3, T_4)^T$, $\mathbf{D} = (0, 0, 0, 0; T_{e,1}, T_{e,2}, T_{e,3}, T_{e,4})^T$, and,

$$\mathbf{C} = (c_{i,j}), \quad \begin{cases} c_{1,j}, &= \psi_j(\hat{r} = -1, \hat{z} = 0), \\ c_{2,j}, &= \psi_j(\hat{r} = 1, \hat{z} = -1), \\ c_{3,j}, &= \psi_j(\hat{r} = 1, \hat{z} = 0), \\ c_{4,j}, &= \psi_j(\hat{r} = 1, \hat{z} = 1) \end{cases} \quad (6.3)$$

for $j = 0, 1, \dots, N$.

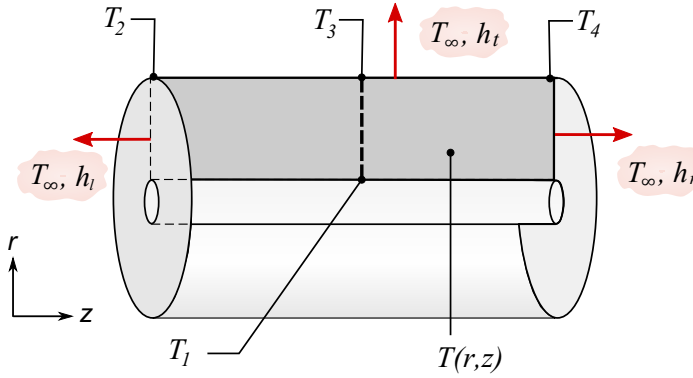


Fig. 6.3 Schematic of cylindrical cell geometry for the thermal model, showing convection coefficients and model outputs.

The mean temperature is also included as an output for the calibration cycle, since this is used for calibrating the impedance coefficients as described later. Hence, an additional row is appended to the C matrix,

$$c_{5,j} = \frac{1}{H} \frac{2}{r_{out}^2 - r_{in}^2} \int_0^H \int_{r_{in}}^{r_{out}} r \psi_j(r, z) dr dz, \quad (6.4)$$

for $j = 0, 1, \dots, N$, and an additional element is included in the boundary lifting function,

$$T_{e,5} = \frac{1}{H} \frac{2}{r_{out}^2 - r_{in}^2} \int_0^H \int_{r_{in}}^{r_{out}} r T_e(r, z) dr dz, \quad (6.5)$$

such that mean temperature is computed as an output.

Once the impedance coefficients are known, the cell impedance is computed for the validation cycles:

$$Z'' = a_1 + a_2 \bar{T} + a_3 \bar{T}^2 \quad (6.6)$$

The computed impedance is used as the measurement input in the state estimation algorithm described next.

6.2.2 State estimation

The state estimation consists of an extended Kalman filter (EKF), for estimating the temperatures at each of the four thermocouple locations, with the cell impedance as measurement input. The EKF is equivalent to that employed in Chapter 4 for the 1-D case, except that here it is applied to the 2-D SG model.

We firstly modify Eq. (5.64) by rewriting it as an explicit state-space model in discrete time:

$$\mathbf{x}_{k+1} = \bar{\mathbf{A}}\mathbf{x}_k + \bar{\mathbf{B}}\mathbf{u}_k + \mathbf{v}_k, \quad (6.7)$$

where $\bar{\mathbf{A}}$ and $\bar{\mathbf{B}}$ are system matrices in the discrete-time domain, given by

$$\bar{\mathbf{A}} = e^{(\mathbf{E}^{-1}\mathbf{A})\Delta t}, \quad (6.8)$$

$$\bar{\mathbf{B}} = (\mathbf{E}^{-1}\mathbf{A})^{-1}(\bar{\mathbf{A}} - \mathbf{I})(\mathbf{E}^{-1}\mathbf{B}), \quad (6.9)$$

where Δt is the sampling time of 1 s. We then set the impedance as the model output

$$y_k = f(\mathbf{x}_k) + n_k, \quad (6.10)$$

where $f(\mathbf{x}_k)$ is the non-linear function relating the state vector to the impedance measurement (i.e. Eq. (6.6)), and $\mathbf{v}_k$ and n_k are the noise inputs of the covariance matrices $\mathbf{R}^v$ and R^n . Note that, although the impedance is now the model output, the temperatures at each of the four thermocouple locations are also computed from the identified states at each time step, for validation against the thermocouple measurements.

The time update processes are then given by:

$$\hat{\mathbf{x}}_k^- = \bar{\mathbf{A}}\hat{\mathbf{x}}_{k-1} + \bar{\mathbf{B}}\mathbf{u}_{k-1}, \quad (6.11)$$

$$(\mathbf{P}_k^x)^- = \bar{\mathbf{A}}\mathbf{P}_{k-1}^x\bar{\mathbf{A}}^T + \mathbf{R}^v, \quad (6.12)$$

where $\hat{\mathbf{x}}_k^-$ and $\hat{\mathbf{x}}_k$ are the *a priori* and *a posteriori* estimates of the state, and $(\mathbf{P}_k^x)^-$ and $\mathbf{P}_{k-1}^x$ are the corresponding error covariances. Since the relationship between impedance and the cell state is non-linear, the measurement model must be linearised about the predicted observation at each measurement. The measurement update equations are:

$$\mathbf{K}_k^x = (\mathbf{P}_k^x)^-(\mathbf{H}_k^x)^T \left(\mathbf{H}_k^x(\mathbf{P}_k^x)^-(\mathbf{H}_k^x)^T + R^n \right)^{-1}, \quad (6.13)$$

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_k^- + \mathbf{K}_k^x \left(z_k - f(\hat{\mathbf{x}}_k^-) \right), \quad (6.14)$$

$$\mathbf{P}_k^{\mathbf{x}} = (\mathbf{I} - \mathbf{K}_k^{\mathbf{x}} \mathbf{H}_k^{\mathbf{x}}) (\mathbf{P}_k^{\mathbf{x}})^-, \quad (6.15)$$

where $\mathbf{K}_k^{\mathbf{x}}$ is the Kalman gain for the state, and $\mathbf{H}_k^{\mathbf{x}}$ is the Jacobian matrix of partial derivatives of f with respect to $\mathbf{x}$:

$$\mathbf{H}_k^{\mathbf{x}} = \left. \frac{\partial f(\mathbf{x}_k)}{\partial \mathbf{x}_k} \right|_{\mathbf{x}_k = \hat{\mathbf{x}}_k^-}. \quad (6.16)$$

The above algorithm can be simplified to a standard Kalman Filter (KF) by omitting the linearisation step (Eq. (6.16)) and replacing $f(\cdot)$ in Eqs. (6.10) and (6.14) with an appropriate linear operator. The KF is applied later using the surface temperature, T_3 , as measurement input for comparison with the EKF using Z'' .

6.3 Experimental

6.3.1 Setup

The experimental setup is similar to that outlined in Chapter 2, with some minor differences as described below. Experiments were carried out with a 4.4 Ah cylindrical cell (A123 Model AHR 32113 Ultra-B) with LiFePO_4 positive electrode and a graphite negative electrode. A larger cell was used in this case than in the 1-D experiment to ensure measurable 2-D effects. The properties of the cell are given in Table 6.1. The cell was fitted with four thermocouples, three on the surface and another inserted into the core via a hole which was drilled in the positive electrode end.² The thermocouple locations correspond to the model output locations described previously. Cell cycling and impedance measurements were carried out using a Biologic HCP-1005 potentiostat/booster. The impedance was measured using Galvanostatic Electrochemical Impedance Spectroscopy (GEIS) with a 200 mA peak-to-peak perturbation current. The environmental temperature was controlled with a Votsch VT4002 thermal chamber. The chamber includes a fan which runs continuously at a fixed speed during operation. Photos of the test equipment and a schematic of the experimental setup are shown in Figs. 6.4 and 6.5, respectively.

Two different cooling configurations were tested (see Fig. 6.5). In Config. 1 the right end and entire curved surface of the cell are thermally insulated, and a heat sink fixed

²Since the end of the thermocouple embedded within the cell was surrounded by a thin layer of heat shrink (to electrically isolate it from the cell current collector at the inner surface of the jelly roll), it is necessary to verify that it still provides accurate internal temperature estimates; justification for this assumption this is presented in Appendix C.

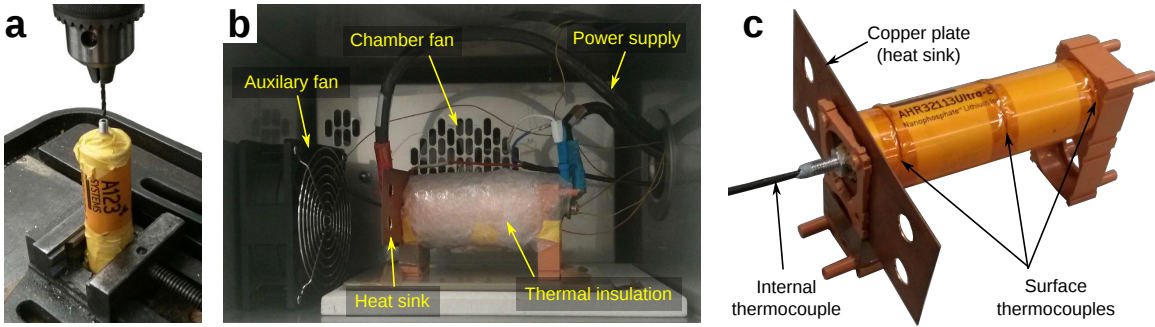


Fig. 6.4 Photos of experimental setup: (a) cell drilling procedure, (b) insulated cell (Config. 2) inside thermal chamber, (c) uninsulated cell with heat sink showing thermocouple locations.

to the left end. An additional (auxiliary) fan is placed inside the chamber as shown in Fig. 6.4b. In this case, both the built-in chamber fan and the auxiliary fan run continuously throughout the duration of the experiments. This setup is designed to achieve maximum cooling from the left end of the cell (heat sink) whilst minimising radial heat transfer. In Config. 2, only the right end of the cell is insulated, and the auxiliary fan is switched off. This setup allows for greater radial heat flux.

Table 6.1 Properties of the lithium-ion cell used for validation.

Model	A123 AHR-32113	Nominal capacity	4.4 Ah
Anode material	Graphite	Jelly-roll length (H)	100 mm
Cathode material	LiFePO_4	Jelly-roll outer radius (r_{out})	16 mm
Nominal voltage	3.3 V	Jelly-roll inner radius (r_{in})	1 mm

6.3.2 Procedure: full spectrum impedance

In order to verify that the impedance at the selected frequency was independent of SoC, full spectrum impedance measurements were carried out at a uniform cell temperature of 10°C , over a range of 10-90% SoC in intervals of 20%³. The EIS frequency range spanned 5 kHz to 0.1 Hz with 10 frequencies per decade and 3x averaging. The cell capacities at each temperature were first determined with a constant current constant voltage (CCCV) charge/discharge. The SoC was then adjusted to the required values by drawing a 1 C current. At each SoC, the cell was allowed to rest to ensure its

³The setup of Config. 2 was used for the full spectrum impedance measurements, although note that the choice between Config. 1 and 2 for this step is somewhat arbitrary since the chamber and cell temperatures are allowed to equilibrate before each measurement.

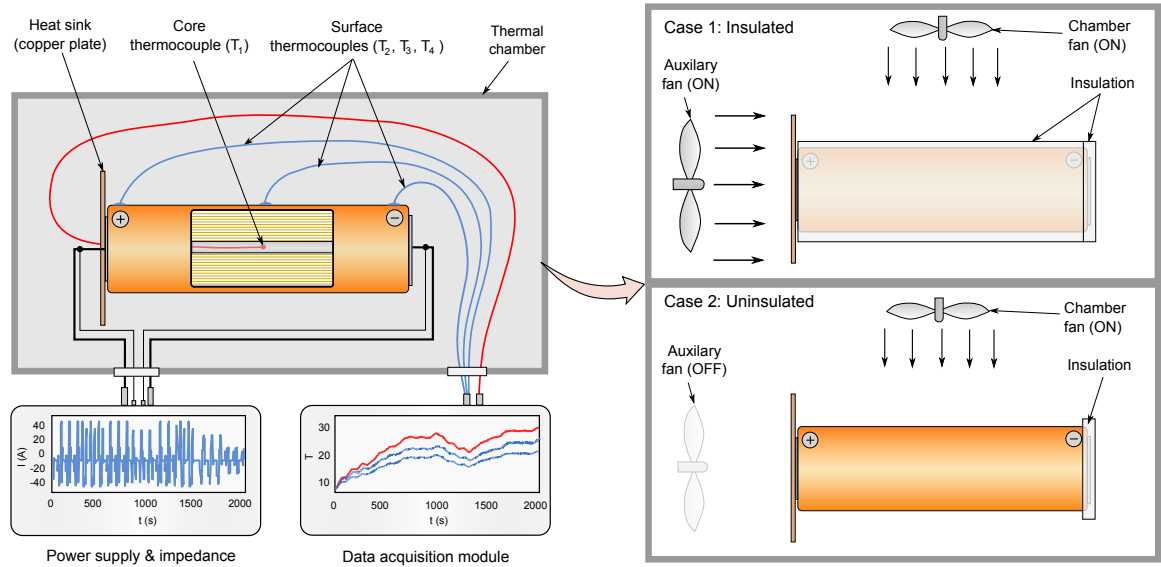


Fig. 6.5 Schematic diagram of experimental setup: *Left*: cell in chamber with cutaway view showing core and jelly roll; *right*: the two cooling configurations.

temperature had equilibrated, which typically occurred in less than 2 hrs. This was verified when the temperatures registered by the internal and surface thermocouples were within 0.2 °C and repeated impedance measurements over a 20 minute period yielded identical results.

6.3.3 Procedure: validation experiments

Test Set I (HEV drive cycles)

In the first test set, dynamic experiments were conducted using three different current excitation profiles, denoted HEV-I, HEV-II, and HEV-III. Each cycle was generated by looping over different portions of an Artemis HEV drive cycle, and scaling the applied currents to the range ± 50 A. HEV-I was used to parameterise the thermal model, and HEV-II and HEV-III were used to validate the identified parameters and to demonstrate the temperature estimation technique (see Section 6.5).

The procedure for the experiments was as follows: impedance measurements at 215 Hz were carried out every 24 s with 4 s pauses before each impedance measurement, and the four thermocouple temperatures were also monitored. Before each experiment, the SoC was adjusted to 50% by drawing a 1 C current. The temperature of the thermal chamber was set to 8 °C and the cell was allowed to rest until its temperature equilibrated before each test began.

Test Set II (constant current discharge)

Dynamic experiments were conducted using two different constant current values (4 C discharge and 6 C discharge) at three different chamber temperatures (10°C, 17.5°C, 25°C). The discharge current was applied until the cell SoC reached 5%, which occurred when the cumulative discharge ($I \times t$) reached 4.18 Ah (i.e. 4.4 Ah $\times$ 95%).

The procedure for the experiments was as follows: impedance measurements at 215 Hz were carried out every 20 s with no pause before each measurement (i.e. the impedance signal was superposed over the DC current), and the four thermocouple temperatures were monitored. Before each experiment, the SoC was adjusted to 100% by applying a 1 C charging current. The thermal chamber was set to the required initial temperature and the cell was allowed to rest until its temperature equilibrated before each test began.

6.4 Full spectrum impedance

The experiments for the 1-D problems in Part I of this thesis demonstrated independence of the impedance at 215 Hz with respect to SoC for a 26650 LiFePO₄ cell (A123 ANR26650 m1-A) over a range of temperatures from -20 to 45°C. Since the cell used in this case is from the same manufacturer and has the same chemistry, it was deemed sufficient to verify SoC independence at a single temperature close to the middle of this range. Hence, the full spectrum impedance tests were carried out at a uniform cell temperature of 10°C (over a range of 10-90% SoC in intervals of 20%). The results are shown in Fig. 6.6. It can be seen from this figure that the impedance at $f \approx 200$ Hz is approximately independent of SoC (as in the 1-D case, this is due to the fact that the frequency in this range is independent of the charge transfer and double layer capacitor resistances, which are highly dependent on SoC). The frequency for temperature evaluation was chosen to be 215 Hz, for consistency with the 1-D case.

6.5 Parameterisation and validation

The full set of thermal parameters is: ρ , c_p , k_r , k_z and the three convection coefficients (one on each end, and one on the cell curved surface), denoted by h_l , h_r and h_t (see Fig. 6.3). However, three of these parameters were known a priori from the literature: Fleckenstein et al. [28] identified values for the density, ρ , the specific heat capacity, c_p , and the radial thermal conductivity, k_r , for an identical cell using thermal impedance spectroscopy, and so these values are used in the present case. Hence, parameterisation

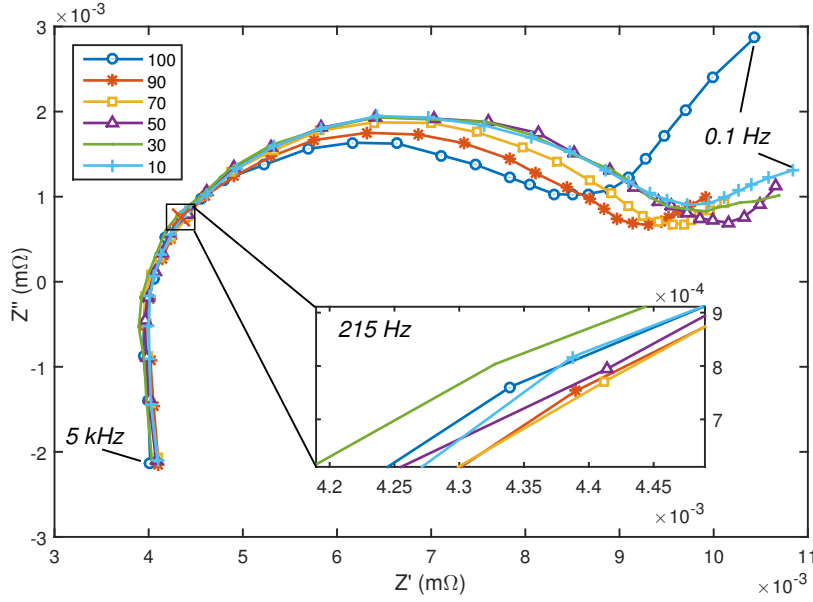


Fig. 6.6 Impedance spectra at 10°C and various states of charge over the frequency range 5 kHz to 0.1 Hz. Inset: Impedance at $f = 215$ Hz. At this frequency the impedance is approximately independent of SoC.

is only required to estimate the remaining four parameter values: the axial thermal conductivity, k_z , and the three convection coefficients: h_l , h_r and h_t .

The measurements from HEV-I (comprising cell current, voltage, and surface and core temperatures, and the chamber temperature) were used for the parameter estimation for both cooling configurations. HEV-I was deliberately chosen for the parameterization since it results in slightly higher cell temperatures than HEV-II or HEV-III, and hence ensures that the polynomial fit is applied using the largest temperature range possible. For Config. 1, all four parameters were identified. For Config. 2, the axial thermal conductivity, k_z , was assumed known a-priori, using the identified value from Config. 1 (since k_z is the same in each case), and hence it was only necessary to identify the three convection coefficient parameters.

The parameterisation was carried out using *fmincon* in Matlab to minimise the magnitude of the Euclidean distance between the measured and estimated temperatures for each of the four thermocouples. Concretely, the error between the measured (subscript ‘exp’) and model predictions (subscript ‘m’) at each time step, k , is given by,

$$\epsilon(k, \theta) = [T_{1,m}(k, \theta), T_{2,m}(k, \theta), T_{3,m}(k, \theta), T_{4,m}(k, \theta)] - [T_{1,exp}, T_{2,exp}, T_{3,exp}, T_{4,exp}], \quad (6.17)$$

and the parameters are identified by,

$$\theta^* = \arg \min_{\theta} \sum_{k=1}^{N_f} \|e(k, \theta)\|_2. \quad (6.18)$$

where N_f is the number of time steps in the cycle.

Table 6.2 presents the thermal parameters, including those known a-priori and those identified via parameterisation. The convection coefficient values are within the range expected of forced convection air cooling [114]. The left coefficient is greatest in both cases as expected due to the presence of the copper heat sink. The values of h_r and h_l are greater in Config. 1, due to the presence of the auxiliary fan, whereas the value of h_t is greater in Config. 2 since the curved surface is uninsulated. The value of k_z is ~ 55 times greater than k_r ; this is typical of cylindrical cells with wound jelly-roll constructions as discussed in earlier chapters. Uncertainty in the parameter estimation may arise due to manufacturing variability, error in the heat generation calculation (due to the omission of entropic heating), heat generation in the contact resistances between the cell and connecting wires and/or measurement uncertainty in the temperature.

Table 6.2 Thermal parameters for Configs. 1 and 2, including those known a-priori from the literature [28] and those identified using the parameterisation cycle.

Parameter	Units	Config. 1		Config. 2	
		Known	Identified	Known	Identified
ρ	kg m^{-3}	2680		2680	
c_p	$\text{J kg}^{-1} \text{K}^{-1}$	958		958	
k_r	$\text{W m}^{-1} \text{K}^{-1}$	0.35		0.35	
k_z	$\text{W m}^{-1} \text{K}^{-1}$		19.3	19.3	
h_l	W m^{-2}		155		98.2
h_r	W m^{-2}		23.3		7.2
h_t	W m^{-2}		16.9		56.2

The measured core and surface temperatures (subscript ‘exp’) and the corresponding model predictions (subscript ‘m’) for the parameterised model for Config. 1 are shown in Fig. 6.7a. The model with identified parameters was validated against the second current excitation profile, HEV-II (Fig. 6.7b). For Config. 2, HEV-I was used as the parameterisation cycle and HEV-III for validation; these results are shown in Figs. 6.7c and 6.7d respectively. Note that, for clarity, T_4 is omitted from these and subsequent plots since it is very close in value to T_3 . The root-mean-square errors (RMSE) in each case are shown in table 6.3. The errors in the validation tests are only marginally greater than those in the parameterisation tests, indicating that the estimation is satisfactory.

Table 6.3 RMS errors in the parameterisation and validation cycles for the two cooling configurations. Units: °C.

Sensor	Config. 1		Config. 2	
	Parameterisation	Validation	Parameterisation	Validation
T_1	0.353	0.659	0.384	0.458
T_2	0.255	0.448	0.213	0.282
T_3	0.245	0.434	0.209	0.279
T_4	0.188	0.310	0.176	0.234

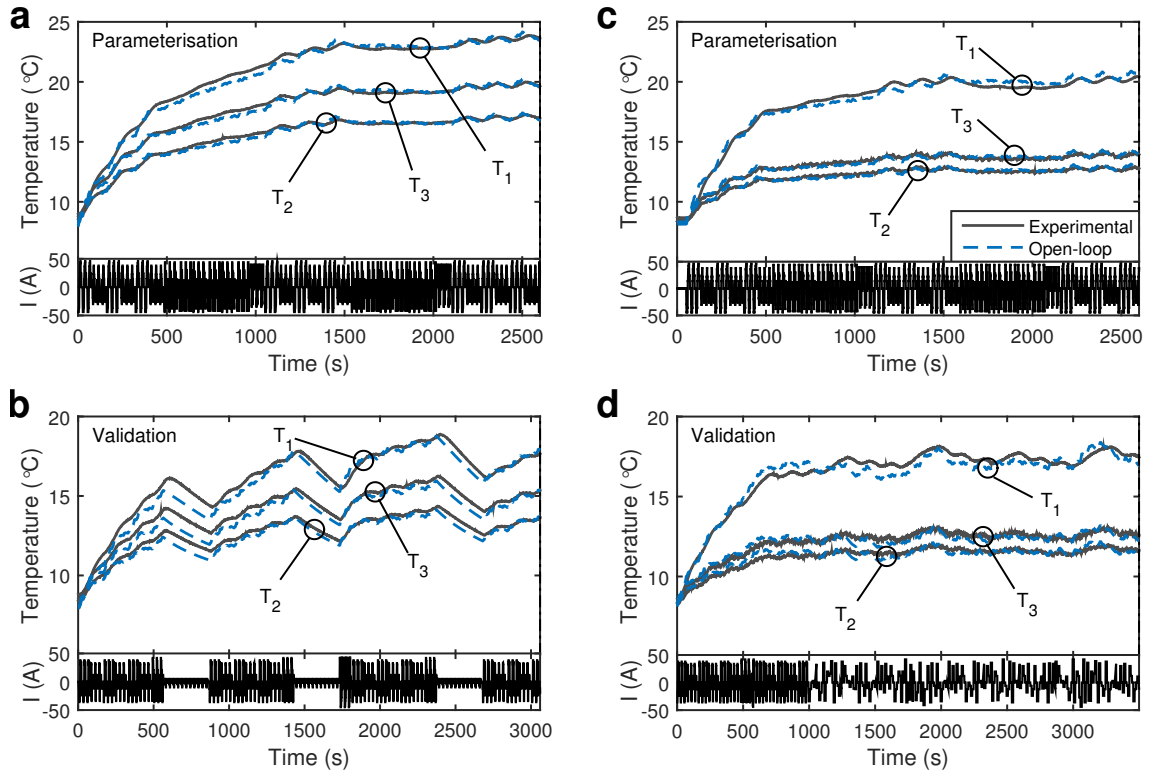


Fig. 6.7 Comparison between measured and predicted temperatures at the thermocouple locations for the parameterisation and validation cycles. a) Config. 1, parameterisation with HEV-I; b) Config. 1, validation with HEV-II; c) Config. 2, parameterisation with HEV-I; d) Config. 2, validation with HEV-III. For clarity, T_4 is omitted from these and subsequent plots since it is very close in value to T_3 .

6.6 Test Set I: HEV drive cycles

This section presents the results of the state estimation using HEV drive cycle data as the input, starting first with the results of the impedance-temperature calibration step.

6.6.1 Impedance calibration

As discussed in Section 6.1, in the present case: (i) the imaginary, rather than the real, impedance is used as the measurement; (ii) the impedance is assumed to be directly related to the volume average temperature, $\bar{T}$; and (iii) the impedance coefficients are calibrated using data from an a-priori drive cycle, rather than by measurements at multiple uniform cell temperatures.

The calibration is achieved as follows. The current/voltage data from Config. 1, HEV-I is applied to the parameterised model (Fig. 6.8, *left*). A KF is applied to the model using the surface temperature (T_3) as measurement input⁴. The predicted $\bar{T}_m$ output from the KF (Eq. (6.4)) at each measurement step is paired with the measured Z''_{exp} value from the HEV-I experimental data. A second order polynomial fit is then applied to the Z''_{exp} vs. $\bar{T}_m$ data (Fig. 6.8, *right*). Fig. 6.8 shows that a second order fit is capable of closely approximating the measured data. As discussed in Section 2.1, an Arrhenius fit could also be obtained but the polynomial is sufficiently accurate and facilitates faster online computation.

⁴Note that the open-loop model could alternatively have been used here and is sufficient for the purpose of impedance calibration; however, the KF was applied since it further increases the model accuracy.

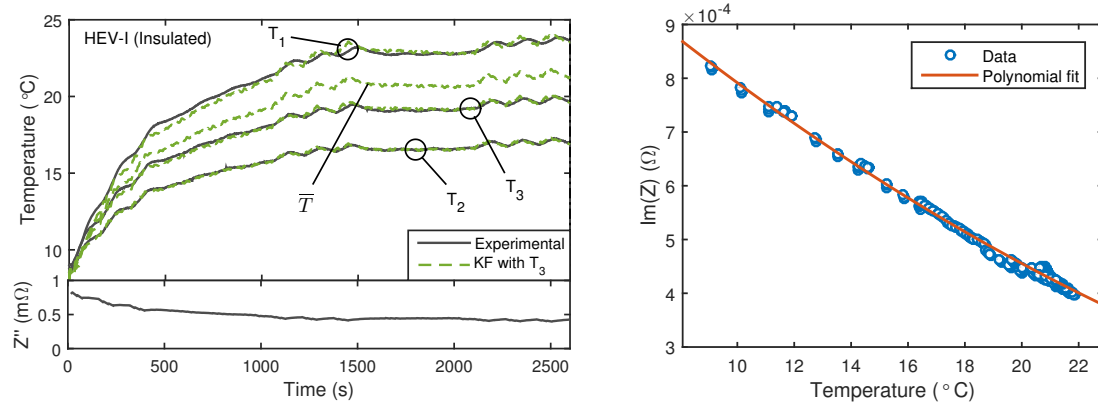


Fig. 6.8 Identification of impedance-temperature polynomial fit. *Left*: Parameterisation drive cycle results; *Right*: Resulting polynomial fit of Z'' against $\bar{T}$.

6.6.2 Results and discussion

We now compare the performance of the EKF with that of a KF based on the same thermal model but with T_3 as the measurement input rather than Z'' . T_3 was chosen for comparison since this is the location of the measurement input used in Part I for the 1-D case.

The initial state estimate provided to the battery is defined such that the battery has a uniform temperature distribution at 25 °C:

$$\hat{\mathbf{x}}_0 = \Psi^{-1}(25 - T_e), \quad (6.19)$$

where T_e is the arbitrary function for homogenising the boundary conditions (Eq. 5.50; see Section 5.2.2). The true initial battery state is a uniform temperature distribution at 8°C. The covariance matrices are calculated as $R^n = \sigma_n^2$ and $\mathbf{R}^v = \beta_v^2 \text{diag}(2, 2)$. The first tuning parameter for the EKF is chosen as $\sigma_n = 3 \times 10^{-5} \Omega$, which is a rough estimate of the standard deviation of the imaginary impedance measurement. The second tuning parameter was chosen as $\beta_v = 5 \times 10^{-3}$, by trial and error. For the KF with T_3 as measurement input the tuning parameters were chosen as $\sigma_n = 5 \times 10^{-4} \text{ }^\circ\text{C}$ and $\sigma_n = 0.05$, which are the same values as those used in the KF in Chapter 4.

Figs. 6.9 and 6.10 show the results for Config. 1 and Config. 2, respectively. For each configuration, the core and surface temperatures quickly converge to the correct values and are accurately estimated throughout the rest of the excitation profile. Fig. 6.9b shows that, for the HEV-III cycle, the EKF and KF underestimate the true temperature, in particular during periods with very low or zero applied currents. This error may be a result of a limitation in the thermal model: the heat generation term (Eq. (6.1)) only accounts for ohmic heating, whereas additional electrochemical heating may occur due to the relaxation of concentration gradients, which would result in continued internal heating after the removal of an applied load. This error may be mitigated by the inclusion of an electrochemical heat generation model, although this is beyond the scope of the current work. However, overall the performance of the method is satisfactory. Figs. 6.9c and 6.10c show 2-D contour plots of the cell at the end of the HEV-I cycle and HEV-II cycle respectively. These contour plots are generated by evaluating the cell temperature on a fine grid throughout the entire $(r-z)$ domain using the thermal model described in the previous chapter. They show that in each case, a significant radial temperature distribution develops within the cell, but in Configuration 2, a larger axial temperature gradient arises, as expected.

Figs. 6.11a-d show histogram plots of the errors in the estimates of T_1 and T_3 in each drive cycle for the EKF with Z'' and the KF with T_3 . Although the errors may include contributions from various sources (such as measurement uncertainty, variations in ambient temperature or fan flow rate, etc.), we can distinguish between impedance related and model related errors by considering the difference in error arising from the method using impedance measurement input versus surface temperature measurement input. In each case the errors are mostly peaked around a zero mean with a standard deviation in the range $0.2^\circ\text{C} - 0.7^\circ\text{C}$. The RMS error in each case is displayed in the top right corner of the plot. It can be seen that the KF with T_3 performs slightly better in most cases, with a lower offset from the zero mean and a narrower distribution. This is to be expected given the higher accuracy of the thermocouple measurement. In particular, the KF performs better in the estimate of T_3 , which is unsurprising since it uses T_3 as a measurement input. However, in general the performance of the EKF is satisfactory and comparable with that of the KF. Fig. 6.11c shows that the error distribution for the estimate of T_1 for the HEV-III cycle is multi-modal: there are peaks at ~ -0.2 and $\sim 0.5^\circ\text{C}$. This is a manifestation of the errors discussed previously arising from the limitation of the purely ohmic heat generation term.

It should be noted that the RMSE of T_1 in Table 6.3 is larger than that of the other three sensors (T_2 , T_3 and T_4). This is perhaps explained as follows: (i) the parameterization scheme minimizes the error over all four sensors; but (ii) the error in each of the three surface temperatures may be strongly correlated since the temperature gradient in the radial direction is greater than that in the axial; and hence (iii) the parameterization may be biased towards minimizing the error in the three surface temperatures at the expense of the error in the core.

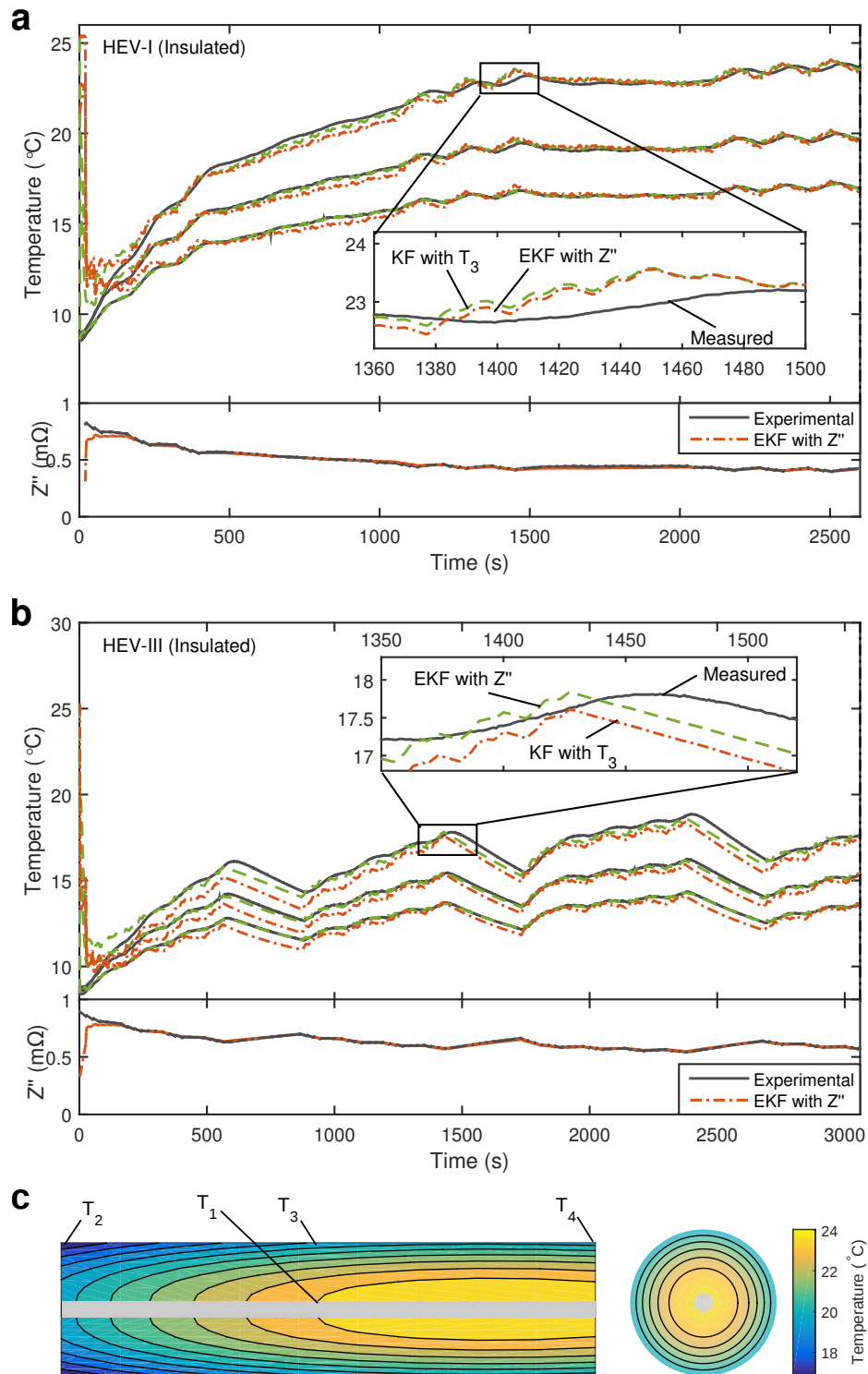


Fig. 6.9 Comparison of temperature measurements against the EKF (using Z'') and KF (using T_3) predictions for Config. 1. Plots a) and b) show the time evolution of temperature outputs for HEV-I and HEV-III respectively. The subplots beneath each main plot compare the measured impedance against the EKF state estimate of the impedance at that time step; the difference between these two values is used for the measurement update. Plot c) is a 2-D contour plot of the cell temperature distribution at the end of the HEV-I cycle ($t = 2550$ s).

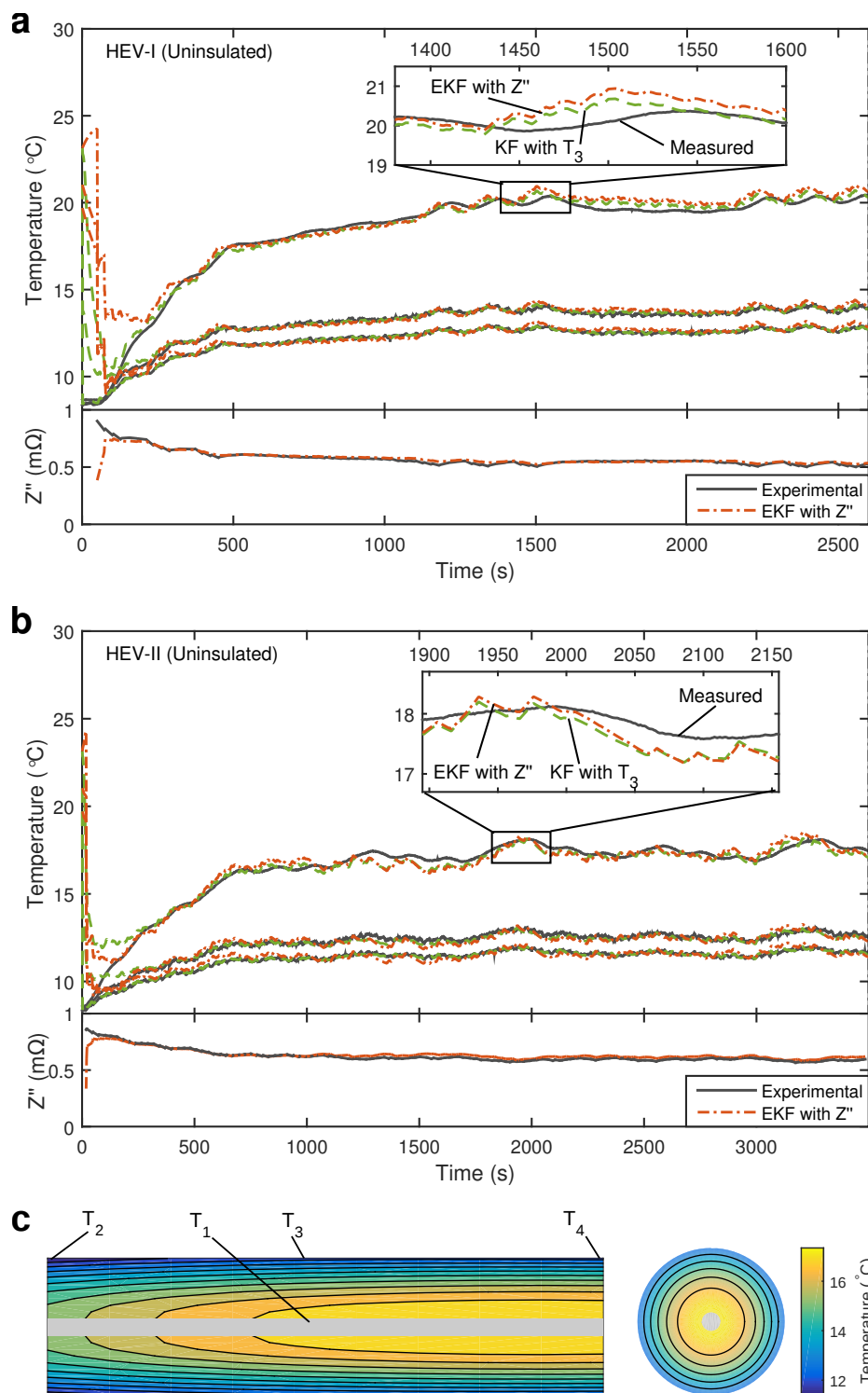


Fig. 6.10 Comparison of temperature measurements against the EKF (using Z'') and KF (using T_3) predictions for Config. 2. Plots a) and b) show the time evolution of temperature outputs for HEV-I and HEV-II respectively. The subplots beneath each main plot compare the measured impedance against the EKF state estimate of the impedance at that time step; the difference between these two values is used for the measurement update. Plot c) is a 2-D contour plot of the cell temperature distribution at the end of the HEV-II cycle ($t = 3400$ s).

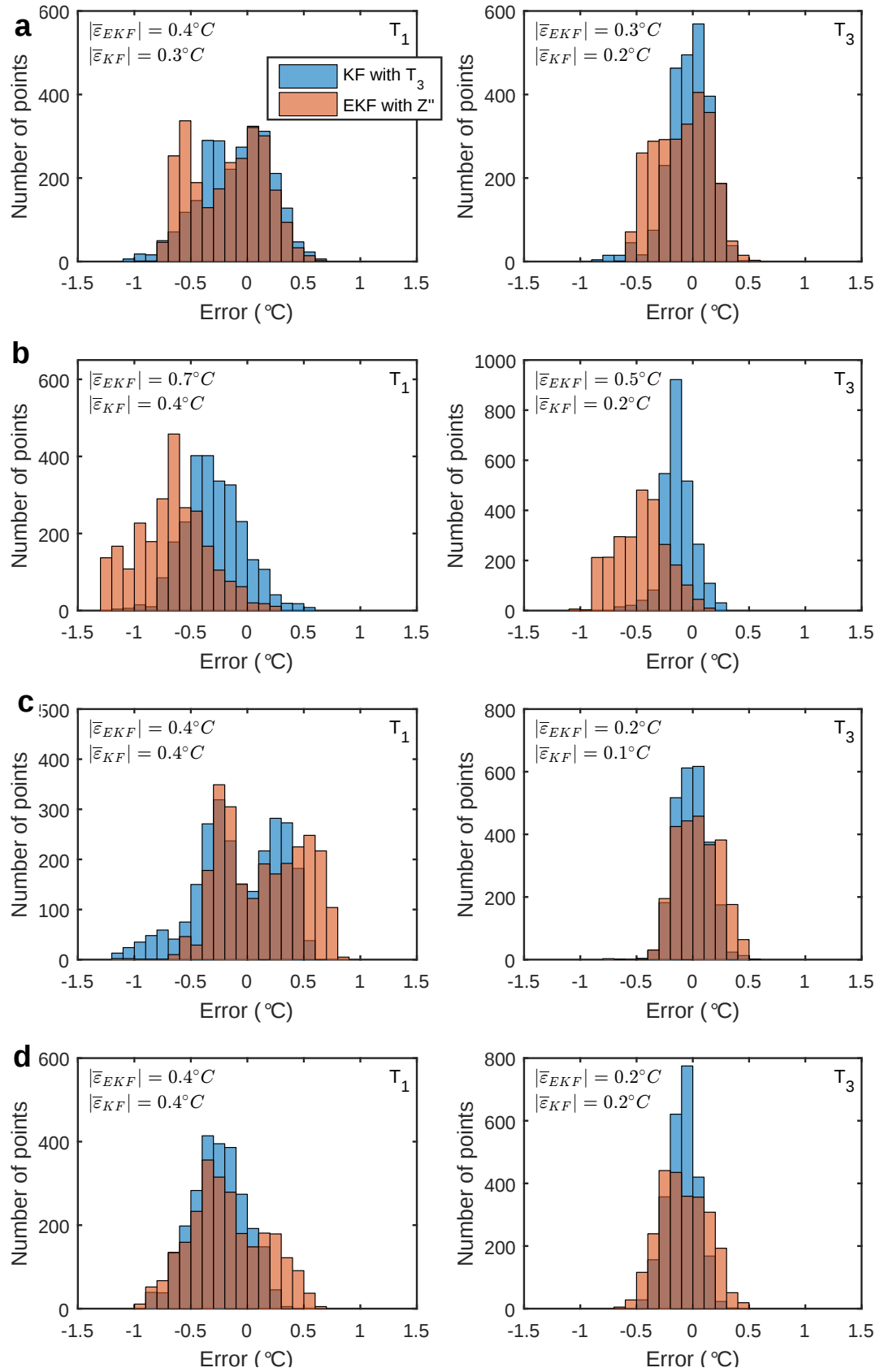


Fig. 6.11 Error analysis for Test Set I. a) Config. 1, HEV-I; b) Config. 1, HEV-III; c) Config. 2, HEV-I; d) Config. 2, HEV-II.

6.7 Test Set II: constant current discharge

This section presents the results of the method using constant current data as the input. This requires a separate impedance calibration step for each of the currents studied.

6.7.1 Impedance calibration

The calibration for Test Set II is achieved using a similar approach to that of Test Set I except that there are no rest periods applied before each impedance measurement. At each chamber temperature, the constant current discharge causes the cell temperature to increase, and so a set of impedance-temperature ($Z'' - \bar{T}$) data over a range from T_{env} to some higher temperature is obtained. For each of the two applied currents, a polynomial fit is applied to the combined impedance-temperature data from two of the experiments: at $T_{env} = 10^\circ\text{C}$ and $T_{env} = 25^\circ\text{C}$ (see Fig. 6.12). Validation experiments are then carried out using the data from the third experiment ($T_{env} = 17.5^\circ\text{C}$). In this way, the polynomial fit interpolates the data in the range of temperatures arising during the validation test.

It is apparent from these plots that the fits of the impedance under load deviate from the no-load fit; hence, the method presented here relies on calibrating the impedance under the same load as to be tested.

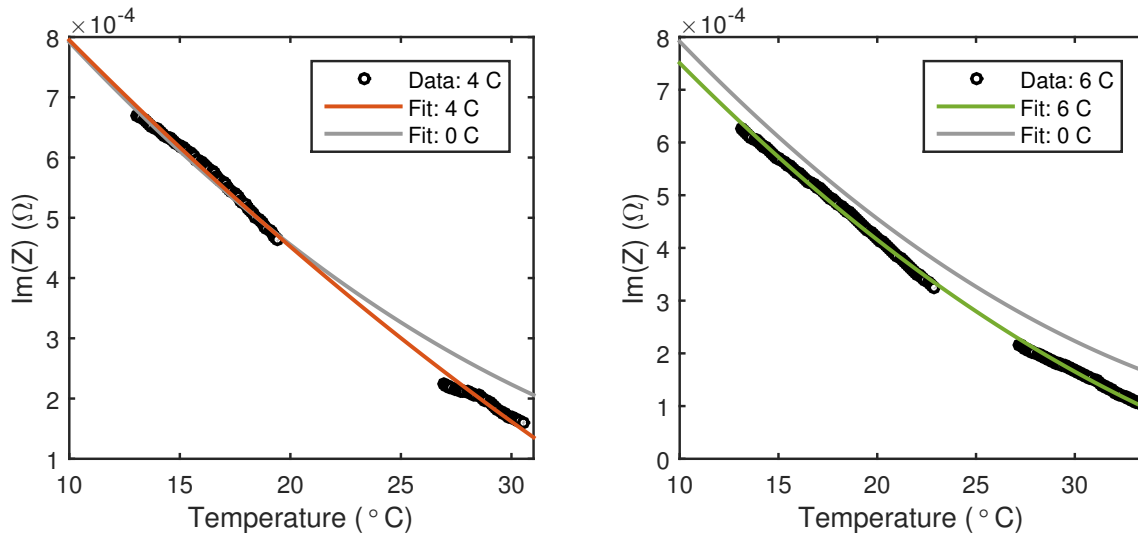


Fig. 6.12 Impedance-temperature polynomial fit for cell under superposed currents of (left) 4 C and (right) 6 C. The impedance was measured at 215 Hz. The standard (no superposed current) impedance-temperature fit is shown in grey in each plot.

6.7.2 Results and discussion

The initial state estimate provided to the battery is defined such that the battery has a uniform temperature distribution at 0 °C, i.e. $\hat{\mathbf{x}}_0 = \Psi^{-1}(-T_e)$, whereas the true initial battery state is a uniform temperature distribution at 17.5°C. The values of the tuning parameters are the same as those used in Test Set I.

Figs. 6.13 and 6.14 show the results for the 4 C and 6 C cases, respectively. For each current value, the core and surface temperatures quickly converge to the correct values and are accurately estimated throughout the rest of the excitation profile. Note that for the KF the surface temperatures (T_2 , T_3 and T_4) converge more rapidly than the core temperature, T_1 ; this is expected since T_3 is the measurement input. Overall the performance of both the EKF and KF are satisfactory; with the KF performing slightly better, as shown by the plot insets in Figs. 6.13a and 6.14a.

Figs. 6.15a and b show histogram plots of the errors in the estimates of T_1 and T_3 for each current value for the EKF with Z'' and the KF with T_3 . In each case the errors are mostly peaked around a zero mean with a standard deviation in the range 0.9°C – 2.9°C. The RMS errors are slightly larger than those of Test Set I because the cycle length is shorter in the present case, and so effect of the initial error on the overall result is greater. As with the first test set, the performance of the EKF is comparable with that of the KF, although the KF performs slightly better in general.

6.8 Conclusions

This chapter extends Hybrid Method II to problems involving 2-D thermal dynamics. An EKF using a parameterised 2-D spectral-Galerkin (SG) model with Z'' measurement input was shown to accurately predict the core temperature and multiple surface temperatures for current excitation profiles based on an Artemis HEV drive cycle. The performance of the EKF is comparable to an equivalent KF estimator using surface temperature as measurement input, although the latter is slightly superior due to the higher accuracy of the thermocouple. These results demonstrate the applicability of the hybrid method to more general scenarios than the 1-D case presented in Part I of this thesis. Furthermore, the calibration of the impedance coefficients was achieved using data from a single drive cycle, rather than by measurements at multiple uniform cell temperatures; this is advantageous over the method presented in Part I since it greatly reduces the time and effort required for the calibration step.

In order to apply the method to 2-D it was necessary to relax the definition of the impedance under non-uniform temperatures: Z'' was assumed to be related to

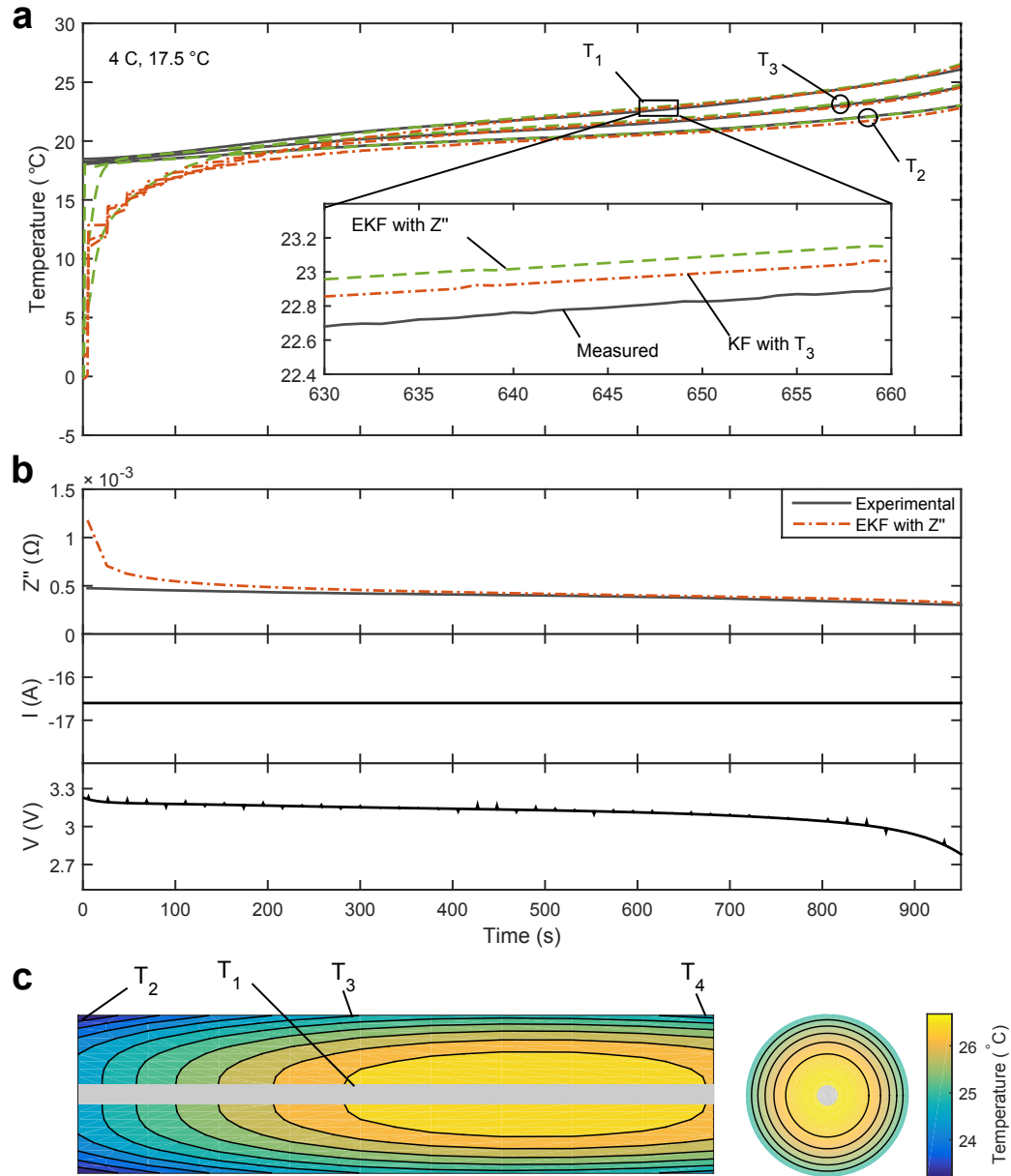


Fig. 6.13 Comparison of temperature measurements against the EKF (using Z'') and KF (using T_3) predictions under 4 C superposed currents. a) time evolution of temperature outputs. b) measured current and voltage data; and measured and predicted Z'' data. c) 2-D contour plot of the cell temperature distribution at the end of discharge (t = 940 s, SOC = 5 %).

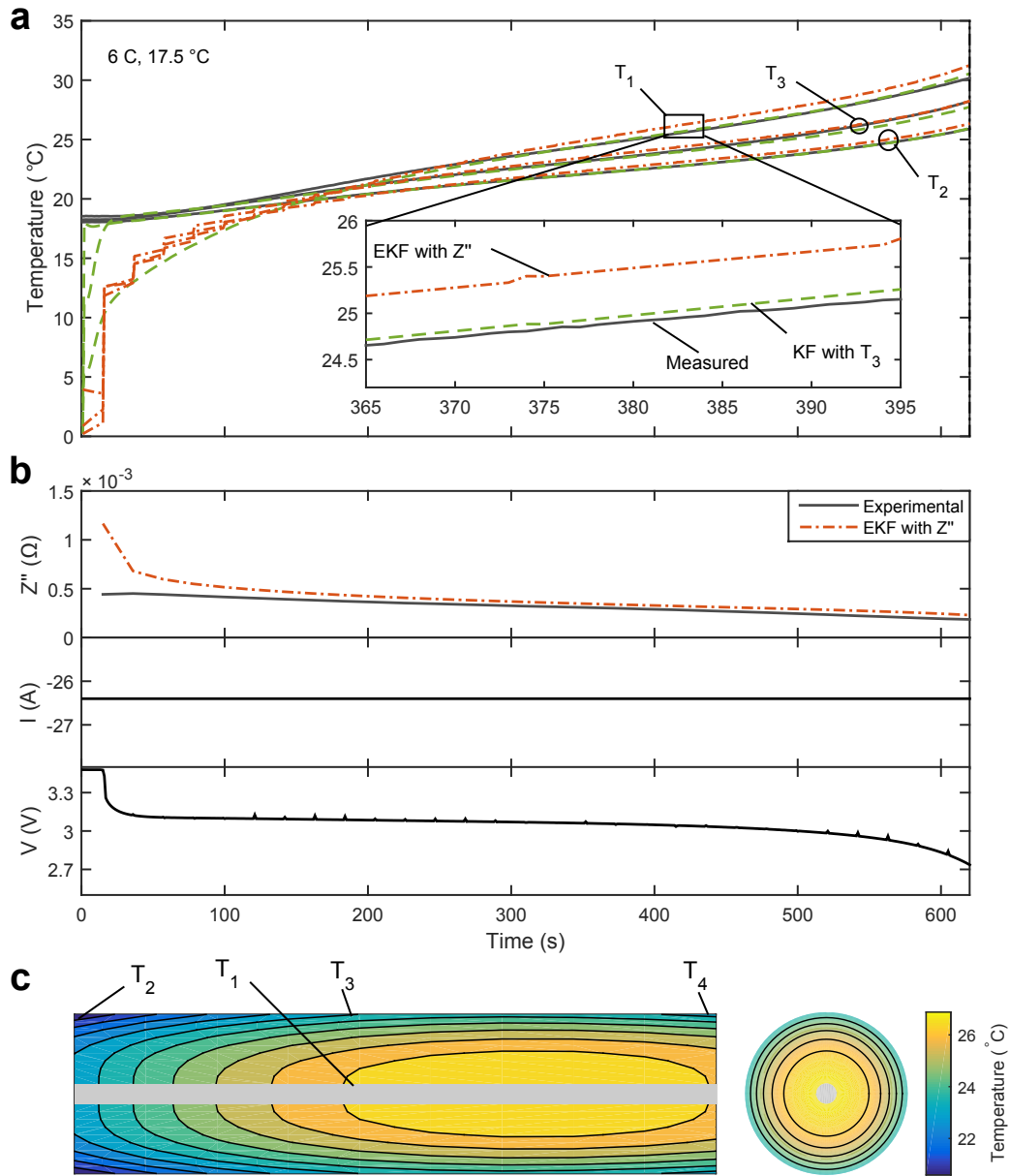


Fig. 6.14 Comparison of temperature measurements against the EKF (using Z'') and KF (using T_3) predictions under 6 C superposed currents. a) time evolution of temperature outputs. b) measured current and voltage data; and measured and predicted Z'' data. c) 2-D contour plot of the cell temperature distribution at the end of discharge (t = 615 s, SOC = 5 %).

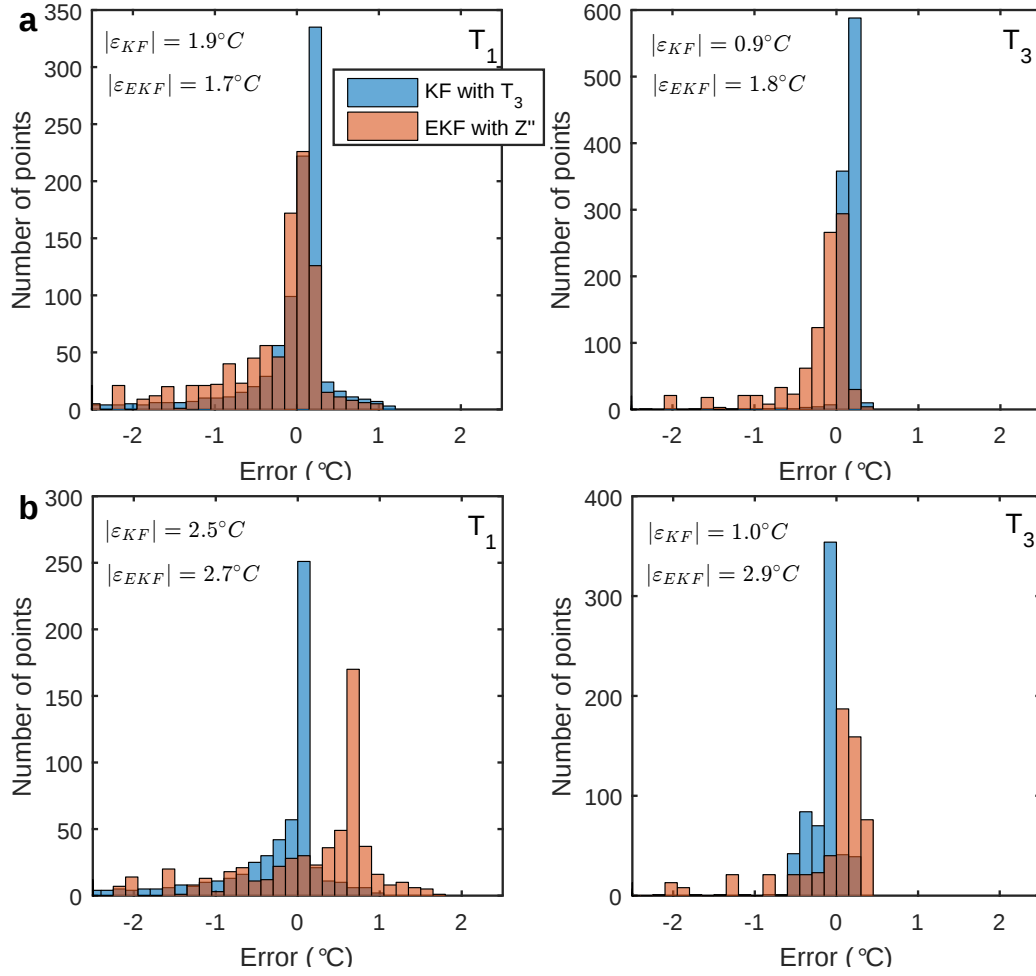


Fig. 6.15 Error analysis for Test Set II. a) 4 C; b) 6 C.

the volume-average temperature rather than the impedance-based volume average temperature used in the 1-D case. However, the resulting error is only significant for very large temperature gradients or for highly non-linear impedance-temperature correlations, and the method was shown to be acceptable in the present case.

The method was also applied to a cell under an applied constant-current load. In this case the impedance measurements were carried out superposed over the applied load; hence mitigating the need to temporarily remove the current load before taking a measurement. To achieve this, it was necessary to calibrate the impedance under the same load as to be tested; however future work could consider methods of interpolating between, or extrapolating from, a set of impedance-temperature curves at different currents to facilitate state-estimation at other current values. Alternatively, the use of impedance at higher frequencies could be investigated since these should be less

sensitive to DC current (since the charge transfer process, which is a function of current, is not measured).

Lastly, it should be noted that, similar to the 1-D case discussed in Section 3.3.2, the performance of the method is not guaranteed if a hotspot has arisen due to anomalous heat generation, and further assumptions or measurements would be necessary in this case.

Part III

Conclusions

Chapter 7

Conclusions and further work

This thesis presented a number of contributions towards impedance-based temperature monitoring of cells with internal temperature gradients. Here I present a summary of these contributions, with conclusions. Following this, recommendations of areas of potential further research are discussed.

7.1 Conclusions

The contributions of this thesis can be categorised into: (i) the introduction of novel hybrid methods for battery thermal monitoring and (ii) the development of low-order modeling methods to use with these hybrid methods.

7.1.1 Hybrid methods

Two novel hybrid methods for battery temperature monitoring were presented: (i) combining ITD with an additional surface temperature measurement (ITD/T), and (ii) combining ITD with a thermal model (ITD/TM). In each case, results were presented showing the accuracy of the method over a typical HEV drive cycle. Both methods were shown to be more accurate than standard ITD methods, since the latter merely identify the volume average temperature, or worse, treat the cell temperature as uniform.

Each of the hybrid methods has unique advantages and disadvantages. ITD/T (presented in Chapter 3) does not rely on knowledge of the cell thermal properties, heat generation rates or thermal boundary conditions. However, it requires both a thermocouple and impedance measurement on each cell and so its instrumentation cost may be prohibitive. Moreover, although it overcomes the requirement for a thermal model, it still relies on a Pseudo-Steady-State temperature approximation (Section 3.2) which

introduces error when the temperature of the heat transfer fluid varies rapidly. On the other hand, ITD/TM relies on knowledge of the cell electrical/thermal properties. However, it was shown that, provided these are known or identified, the cell temperature may be estimated to high accuracy. Moreover, it requires only a single measurement input - the impedance metric - and thus has the potential to substantially reduce instrumentation costs.

In Chapter 4, ITD/TM was applied in 1-D, and in Chapter 6, it was extended to the 2-D case. In the 1-D case, an EKF was shown to accurately predict core and surface temperatures for a HEV drive cycle, and a DEKF was shown to accurately identify the convection coefficient when the latter was not provided to the model in advance. In the 2-D case, an EKF was shown to accurately predict the core temperature and the surface temperature at three different locations on the surface. Furthermore, in the 2-D case, the calibration of the impedance coefficients was achieved using data from a single drive cycle, rather than by measurements at multiple uniform cell temperatures. This greatly reduces the time and effort required for the calibration step (although it should be noted that this method could equally be applied to the calibration of the impedance in the 1-D problem). The extension to 2-D came with a compromise: the impedance was assumed to be directly related to the volume-average temperature to facilitate a computationally efficient model output. However, the resulting error is only significant for very large temperature gradients or for highly non-linear impedance-temperature correlations, and the accuracy of the results show that the assumption is acceptable in that case.

7.1.2 Low order thermal models

The second main focus of this thesis is low-order thermal modelling. Online modelling is an essential part of most battery temperature monitoring schemes, both conventional and impedance-based, and the issue of low-order thermal modelling is particularly important: a model must be efficient enough to be implementable using a low-cost micro-controller with limited computational power.

Where appropriate I used existing thermal models from the literature and incorporated them into the hybrid methods presented in this work. For instance, in Chapter 3 a simple steady-state analytical model was used since this was satisfactory to constrain the solution when provided with two measurement inputs. In Chapter 4 a 1-D cylindrical PA model first presented by Kim et al. [24] was used for the ITD/TM technique. To apply similar methods to other battery geometries additional PA models are needed. In Appendix A, two additional PA models were derived and validated: 1-D Cartesian

coordinates (suitable for simulating prismatic cells) and a 1-D annulus (an extension of the solid cylinder model to cases where the inner radial dimension is non-zero).

In order to monitor cells with more general cooling conditions – such as end cooling via liquid-coolant plates – it is necessary to use a 2-D or 3-D model. In Appendix B, PA is shown to be suitable for modelling 2-D problems with certain symmetrical boundary conditions with reasonable accuracy. However, it is unsuitable for modelling problems with more general conditions. These results justify the use of more sophisticated methods for flexible and efficient 2-D thermal modelling.

In Chapter 6, I presented and validated a computationally efficient 2-D spectral-Galerkin (SG) thermal model, which can account for different external temperatures and/or convection coefficients at each surface. This generality makes it suitable for simulating various battery cooling configurations. This model can be used in the ITD/TM scheme, as demonstrated in Chapter 6, but is also highly suited to battery modelling in conventional schemes (i.e. using thermocouple measurement inputs).

7.2 Future work

ITD is a new area of research; the initial paper by Srinivasan et al. proposing the idea was published in 2011. There are multiple challenges to be overcome to ensure the eventual implementation of impedance-based temperature monitoring systems, and hence it is rich with exciting opportunities for further work. The results of this thesis show that the method has promise, but it also highlights a number of outstanding issues worthy of further investigation. These issues are discussed in detail below.

7.2.1 Alternative thermal/electrochemical models

In this thesis, a variety of solution methods were used – analytical (Chapter 3), polynomial approximation (PA) (Chapter 4, Appendix 1, 2), and spectral-Galerkin (SG) (Chapter 5) – to model the cell thermal dynamics as part of the proposed temperature monitoring techniques. My aim in each case was to use the simplest approach possible to give sufficiently accurate results with minimal computational overhead; e.g., where PA models proved unsatisfactory spectral-Galerkin methods were employed. However, other choices are also worthy of exploration. Most notably, thermal equivalent circuit (TEC) models (discussed in Section 1.5.2) may be useful as an alternative method of modelling cell dynamics in 2 or 3 dimensions. Although some of the limitations of TECs were highlighted earlier (they only provide surface-average temperature outputs, and they have poor performance for highly transient dynamics

and/or large Biot numbers) they are much simpler and more flexible to implement than SG. Since a complete monitoring system will have various other sources of error (caused by sensor noise, model limitations, parameter uncertainty etc.), the error introduced by using a TEC rather than a more accurate model may be deemed acceptable. For instance, in Chapter 6, the limitations of the ohmic heat generation model are apparent, since it results in an under-prediction of the cell temperature during times shortly after the removal of a current load (Fig. 6.9). Incorporating electrochemical heat generation into the SG model used in this approach would be challenging; however, this could be achieved relatively easily with a TEC. Likewise, extending the model to a multi-cell system would be similarly more achievable.

Alternatively, the spectral method approach could be extended to account for non-uniform heat generation. This can be a significant source of inaccuracy if the cell is sufficiently large (e.g. $r > 16$ mm), since the current distribution (and hence the heat generation) throughout the cell can be highly non-uniform in such cases.

7.2.2 Further hybrid methods

This thesis introduced two hybrid methods for battery temperature monitoring. Method I takes advantage of having multiple sensors (impedance and a thermocouple) whilst Method II takes advantage of having a sensor and knowledge of the thermal properties (from which to construct a thermal model). However, alternative configurations could also be considered. For instance, what if the designer has all three options available, i.e. an impedance measurement, a temperature sensor, and knowledge of the cell thermal properties? How would the accuracy/observability of the system be affected in this case? How could the sensor redundancy be best exploited to enable robust temperature monitoring and/or fault detection? In short, what is the optimal configuration of temperature sensors – conventional or impedance-based – to enable robust/extensive temperature monitoring? These are all open questions, and I hope that the methods and results presented in this thesis provide groundwork for further work in this area.

7.2.3 Impedance calibration

One of the limitations of the existing method is that the impedance must be calibrated against temperature in advance of its use online. The standard approach to this was presented in Part I: the impedance was measured at multiple uniform cell temperatures and then a fit was applied to the resulting data. A faster approach was presented in

Part II, whereby the calibration was achieved using data from a single drive cycle. However, this would still require – at the very least – a thermocouple to be fitted to each cell during the calibration cycle. To avoid this it would be desirable to have a canonical impedance-temperature calibration – obtained from a single cell or a statistical analysis of a subset of cells – and then apply this fit to the remaining cells. This is challenging because the impedance-temperature behaviour of one cell is not necessarily identical to that of another cell of the same model. This is due to manufacturing variability, changes due to ageing, different storage conditions or current loading histories etc. It is possible that for certain cell models or chemistries this effect may be less severe than for the LiFePO_4 cells studied in this thesis, and so this approach may be applicable in these cases.

7.2.4 Other factors affecting impedance

As discussed in Chapter 1, the cell impedance is a function of temperature, SoC, SoH, and applied current. In this work, the dependence on factors other than temperature were neglected; however, greater accuracy could be achieved if these factors were accounted for. It would be relatively straightforward to account for SoC by implementing multiple impedance-temperature fits for different ranges of SoC - although this would make the calibration step more time intensive. Accounting for SoH is less trivial: whilst there is some experimental evidence to suggest that the impedance-temperature fit may be robust against changes with use [45] (as discussed in Chapter 1), even small changes in impedance can manifest as large errors in temperature prediction. Hence, the issue of updating or self-calibrating the fit during use is worthy of investigation. Lastly, the issue of interpreting impedance measurements under superposed DC currents is yet to be systematically investigated. Section 6.7 presented some preliminary results showing that separate impedance-temperature fits can be obtained for different superposed current loads. However, this approach was only demonstrated for constant-current loading - and a more advanced - perhaps model based - approach is needed if impedance under load is to be achieved during a highly dynamic cycle without periodically removing the applied load. Alternatively, as discussed in Section 6.8, the use of impedance at higher frequencies could be investigated since these should be less sensitive to DC current.

7.2.5 Multi-cell systems

Scaling up this approach from one cell to multi-cell systems is an important consideration. Aside from the aforementioned model selection issue (spectral versus equivalent

circuit), there is also scope to study novel hybrid methods at the multi-cell level, e.g. is there an optimal combinations of sensors (conventional and/or impedance-based) for series or series/parallel systems of cells? These and various other challenges present interesting avenues for future work.

7.2.6 On-board demonstration

The ultimate aim is to apply ITD online on a battery pack in an EV or other application. As discussed in Section 1.3.3, a recent study has already demonstrated ITD (for average internal temperature estimation) in a vehicle [55]. An interesting area for future work could involve applying the hybrid ITD approaches presented in this thesis in a similar on-board setting to enable estimation of cell internal temperature *distributions*. Such an implementation would have the potential to offer significant cost savings: As discussed in Section 1.3, the requirement for surface temperature sensors on every cell in a large pack is costly and challenging, due to requirements on positioning, thermal contacting, and wiring. On the other hand, fast cost-effective techniques for measuring battery impedance online in an application have already been demonstrated [64]. Moreover, impedance has the potential to monitor a much greater proportion of the cells in large battery packs since individual cell voltage monitoring is typically undertaken anyway for safety reasons. With parallel connected cells, voltage measurements for each individual cell cannot be decoupled and so only the average impedance of a parallel string could be measured; however, this could nonetheless be a valuable measurement input to a pack thermal model (although the accuracy of measurements required in such a case would be greater). Lastly, online impedance measurement may be required for other purposes such as SoC estimation, and so the marginal cost of utilising the acquired signals to implement one of the ITD methods proposed in this work would be minimal.

Publications

1. Robert R. Richardson, Shi Zhao, David A. Howey, "Battery internal temperature estimation by combined impedance and surface temperature measurement." *Journal of Power Sources* 265 (2014): 254-261. [Publisher copy](#)
2. Robert R. Richardson, Shi Zhao, David A. Howey, "Sensorless Battery Internal Temperature Estimation using a Kalman Filter with Impedance Measurement." *IEEE Transactions on Sustainable Energy* 6(4) (2015). [Publisher copy](#) and [Open-access pre-print](#)
3. Robert R. Richardson, Shi Zhao, David A. Howey, "On-board monitoring of 2-D spatially-resolved temperatures in cylindrical lithium-ion batteries: Part I. Low-order thermal modelling", *Journal of Power Sources*, 326 (2016): 377-388, [Open-access publisher copy](#)
4. Robert R. Richardson, Shi Zhao, David A. Howey, "On-board monitoring of 2-D spatially-resolved temperatures in cylindrical lithium-ion batteries: Part II. State estimation via impedance-based temperature sensing", *Journal of Power Sources*, 327 (2016): 726-735, [Open-access publisher copy](#)

References

- [1] SMM Alavi, CR Birkel, and DA Howey. Rechargeable battery energy storage system design. In J. Yan, editor, *Handbook of Clean Energy Systems*, pages 2801–2818. Wiley Online Library, 2015.
- [2] Ui Seong Kim, Chee Burm Shin, and Chi-Su Kim. Modeling for the scale-up of a lithium-ion polymer battery. *J. Power Sources*, 189(1):841–846, April 2009.
- [3] Neil S Spinner, Corey T Love, Susan L Rose-Pehrsson, and Steven G Tuttle. Expanding the operational limits of the single-point impedance diagnostic for internal temperature monitoring of lithium-ion batteries. *Electrochimica Acta*, 174:488–493, 2015.
- [4] Rajib Mahamud. *Advanced battery thermal management for electrical-drive vehicles using reciprocating cooling flow and spatial-resolution, lumped-capacitance thermal model*. PhD thesis, University of Nevada, 2011.
- [5] Billy Wu, Vladimir Yufit, Monica Marinescu, Gregory J. Offer, Ricardo F. Martinez-Botas, and Nigel P. Brandon. Coupled thermal-electrochemical modelling of uneven heat generation in lithium-ion battery packs. *Journal of Power Sources*, 243:544–554, June 2013.
- [6] Qingsong Wang, Ping Ping, Xuejuan Zhao, Guanquan Chu, Jinhua Sun, and Chunhua Chen. Thermal runaway caused fire and explosion of lithium ion battery. *J. Power Sources*, 208:210–224, June 2012.
- [7] Todd M Bandhauer, Srinivas Garimella, and Thomas F Fuller. A critical review of thermal issues in lithium-ion batteries. *Journal of the Electrochemical Society*, 158(3):R1–R25, 2011.
- [8] Donal P Finegan, Mario Scheel, James B Robinson, Bernhard Tjaden, Ian Hunt, Thomas J Mason, Jason Millichamp, Marco Di Michiel, Gregory J Offer, Gareth Hinds, et al. In-operando high-speed tomography of lithium-ion batteries during thermal runaway. *Nature communications*, 6, 2015.
- [9] Incident Report and Safety Board. Aircraft Incident Report, Auxiliary Power Unit Battery Fire, Japan Airlines Boeing 787-8, JA829J. Report No. PB2014-108867. Technical report, National Transport Safety Board, 2014.
- [10] British Broadcasting Corporation (BBC). Dreamliner: Boeing starts replacing 787 batteries, April 2013.

- [11] A.A. Pesaran, G H Kim, and M Keyser. Integration Issues of Cells into Battery Packs for Plug-In and Hybrid Electric Vehicles. In *EVS 24 International Battery, Hybrid and Fuel Cell Electric Vehicle Symposium*, Stavanger, Norway, 2009.
- [12] Alexander Farmann, Wladislaw Waag, Andrea Marongiu, and Dirk Uwe Sauer. Critical review of on-board capacity estimation techniques for lithium-ion batteries in electric and hybrid electric vehicles. *Journal of Power Sources*, 281:114–130, 2015.
- [13] K Amine, J Liu, and I Belharouak. High-temperature storage and cycling of c-lifepo 4/graphite li-ion cells. *Electrochemistry Communications*, 7(7):669–673, 2005.
- [14] Yancheng Zhang, Chao-Yang Wang, and Xidong Tang. Cycling degradation of an automotive lifepo 4 lithium-ion battery. *Journal of Power Sources*, 196(3):1513–1520, 2011.
- [15] Matthias Fleckenstein, Oliver Bohlen, Michael a. Roscher, and Bernard Bäker. Current density and state of charge inhomogeneities in Li-Ion battery cells with LiFePO₄ as cathode material due to temperature gradients. *J. Power Sources*, 196(10):4769–4778, January 2011.
- [16] C-K Huang, JS Sakamoto, J Wolfenstine, and S Surampudi. The limits of low-temperature performance of li-ion cells. *Journal of The Electrochemical Society*, 147(8):2893–2896, 2000.
- [17] SS Zhang, K Xu, and TR Jow. The low temperature performance of li-ion batteries. *Journal of Power Sources*, 115(1):137–140, 2003.
- [18] Jiang Fan and Steven Tan. Studies on charging lithium-ion cells at low temperatures. *Journal of The Electrochemical Society*, 153(6):A1081–A1092, 2006.
- [19] Andreas Vlahinos and Ahmad A Pesaran. Energy efficient battery heating in cold climates. Technical report, SAE Technical Paper, 2002.
- [20] Yan Ji and Chao Yang Wang. Heating strategies for li-ion batteries operated from subzero temperatures. *Electrochimica Acta*, 107:664–674, 2013.
- [21] D. Andre, M. Meiler, K. Steiner, Ch. Wimmer, T. Soczka-Guth, and D.U. Sauer. Characterization of high-power lithium-ion batteries by electrochemical impedance spectroscopy. I. Experimental investigation. *J. Power Sources*, 196(12):5334–5341, June 2011.
- [22] D Andre, M Meiler, K Steiner, H Walz, T Soczka-Guth, and DU Sauer. Characterization of high-power lithium-ion batteries by electrochemical impedance spectroscopy. ii: Modelling. *Journal of Power Sources*, 196(12):5349–5356, 2011.
- [23] Christophe Forgez, Dinh Vinh Do, Guy Friedrich, Mathieu Morcrette, and Charles Delacourt. Thermal modeling of a cylindrical LiFePO₄/graphite lithium-ion battery. *J. Power Sources*, 195(9):2961–2968, May 2010.

- [24] Youngki Kim, Jason B Siegel, and Anna G Stefanopoulou. A computationally efficient thermal model of cylindrical battery cells for the estimation of radially distributed temperatures. In *American Control Conference (ACC)*, pages 698–703, Washington, DC, 2013.
- [25] Youngki Kim, Shankar Mohan, Student Member, Jason B Siegel, Anna G Stefanopoulou, and Yi Ding. The Estimation of Temperature Distribution in Cylindrical Battery Cells Under Unknown Cooling Conditions. *IEEE Trans. Control Syst. Technol.*, pages 1–10, 2014.
- [26] Xinfan Lin, Hector E. Perez, Jason B. Siegel, Anna G. Stefanopoulou, R. Dyche Anderson, and Matthew P. Castanier. Online Parameterization of Lumped Thermal Dynamics in Cylindrical Lithium Ion Batteries for Core Temperature Estimation and Health Monitoring. *IEEE Trans. Control Syst. Technol.*, 21(5):1745–1755, September 2013.
- [27] Xinfan Lin, Hector E. Perez, Shankar Mohan, Jason B. Siegel, Anna G. Stefanopoulou, Yi Ding, and Matthew P. Castanier. A lumped-parameter electro-thermal model for cylindrical batteries. *J. Power Sources*, 257:1–11, July 2014.
- [28] Matthias Fleckenstein, Sebastian Fischer, Oliver Bohlen, and Bernard Bäker. Thermal impedance spectroscopy-a method for the thermal characterization of high power battery cells. *Journal of Power Sources*, 223:259–267, 2013.
- [29] Evgenij Barsoukov, Jee Hwan Jang, and Hosull Lee. Thermal impedance spectroscopy for li-ion batteries using heat-pulse response analysis. *Journal of power sources*, 109(2):313–320, 2002.
- [30] SJ Drake, DA Wetz, JK Ostanek, SP Miller, JM Heinzl, and A Jain. Measurement of anisotropic thermophysical properties of cylindrical li-ion cells. *Journal of Power Sources*, 252:298–304, 2014.
- [31] Patrick Keil, Klemens Rumpf, and Andreas Jossen. Thermal impedance spectroscopy for li-ion batteries with an ir temperature sensor system. In *Electric Vehicle Symposium and Exhibition (EVS27), 2013 World*, pages 1–11. IEEE, 2013.
- [32] Jan Philipp Schmidt, André Weber, and Ellen Ivers-Tiffée. A novel and precise measuring method for the entropy of lithium-ion cells: δs via electrothermal impedance spectroscopy. *Electrochimica Acta*, 137:311–319, 2014.
- [33] Jianbo Zhang, Bin Wu, Zhe Li, and Jun Huang. Simultaneous estimation of thermal parameters for large-format laminated lithium-ion batteries. *Journal of Power Sources*, 259:106–116, 2014.
- [34] Arthur J Krener and Kayo Ide. Measures of unobservability. In *Decision and Control, 2009 held jointly with the 2009 28th Chinese Control Conference. CDC/CCC 2009. Proceedings of the 48th IEEE Conference on*, pages 6401–6406. IEEE, 2009.

- [35] Xinfan Lin, Anna G Stefanopoulou, Jason B Siegel, and Shankar Mohan. Temperature estimation in a battery string under frugal sensor allocation. In *ASME 2014 Dynamic Systems and Control Conference*, pages V001T19A006–V001T19A006. American Society of Mechanical Engineers, 2014.
- [36] Shriram Santhanagopalan, Premanand Ramadass, and John Zhengming Zhang. Analysis of internal short-circuit in a lithium ion cell. *Journal of Power Sources*, 194(1):550–557, 2009.
- [37] Chi-Yuan Lee, Shuo-Jen Lee, Ming-Shao Tang, and Pei-Chi Chen. In situ monitoring of temperature inside lithium-ion batteries by flexible micro temperature sensors. *Sensors*, 11(10):9942–9950, 2011.
- [38] Madhu Santosh K Mutyala, Jingzhou Zhao, Jianyang Li, Hongen Pan, Chris Yuan, and Xiaochun Li. In-situ temperature measurement in lithium ion battery by transferable flexible thin film thermocouples. *Journal of Power Sources*, 260:43–49, 2014.
- [39] Chi-Yuan Lee, Huan-Chih Peng, Shuo-Jen Lee, I Hung, Chien-Te Hsieh, Chuan-Sheng Chiou, Yu-Ming Chang, Yen-Pu Huang, et al. A flexible three-in-one microsensor for real-time monitoring of internal temperature, voltage and current of lithium batteries. *Sensors*, 15(5):11485–11498, 2015.
- [40] Chi-Yuan Lee, Sheng-Ming Chuang, Shuo-Jen Lee, I-Ming Hung, Chien-Te Hsieh, Yu-Ming Chang, and Yen-Pu Huang. Flexible micro sensor for in-situ monitoring temperature and voltage of coin cells. *Sensors and Actuators A: Physical*, 232:214–222, 2015.
- [41] Nora Martiny, Alexander Rheinfeld, Jan Geder, Yuxi Wang, Werner Kraus, and Andreas Jossen. Development of an all kapton-based thin-film thermocouple matrix for in situ temperature measurement in a lithium ion pouch cell. *Sensors Journal, IEEE*, 14(10):3377–3384, 2014.
- [42] Rengaswamy Srinivasan, Bliss G. Carkhuff, Michael H. Butler, and Andrew C. Baisden. Instantaneous measurement of the internal temperature in lithium-ion rechargeable cells. *Electrochimica Acta*, 56(17):6198–6204, July 2011.
- [43] Rengaswamy Srinivasan. Monitoring dynamic thermal behavior of the carbon anode in a lithium-ion cell using a four-probe technique. *J. Power Sources*, 198:351–358, January 2012.
- [44] Jan Philipp Schmidt, Stefan Arnold, André Loges, Daniel Werner, Thomas Wetzels, and Ellen Ivers-Tiffée. Measurement of the internal cell temperature via impedance: evaluation and application of a new method. *J. Power Sources*, 243:110–117, June 2013.
- [45] L.H.J. Raijmakers, D.L. Danilov, J.P.M. van Lammeren, M.J.G. Lammers, and P.H.L. Notten. Sensorless battery temperature measurements based on electrochemical impedance spectroscopy. *J. Power Sources*, 247:539–544, February 2014.

- [46] J.G. Zhu, Z.C. Sun, X.Z. Wei, and H.F. Dai. A new lithium-ion battery internal temperature on-line estimate method based on electrochemical impedance spectroscopy measurement. *Journal of Power Sources*, 274:990–1004, January 2015.
- [47] P Suresh, AK Shukla, and N Munichandraiah. Temperature dependence studies of ac impedance of lithium-ion cells. *Journal of applied electrochemistry*, 32(3):267–273, 2002.
- [48] D.P. Abraham, E.M. Reynolds, E. Sammann, a.N. Jansen, and D.W. Dees. Aging characteristics of high-power lithium-ion cells with $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ and $\text{Li}_4/3\text{Ti}_5/3\text{O}_4$ electrodes. *Electrochim. Acta*, 51(3):502–510, October 2005.
- [49] Yancheng Zhang and Chao-Yang Wang. Cycle-Life Characterization of Automotive Lithium-Ion Batteries with LiNiO_2 Cathode. *Journal of The Electrochemical Society*, 156(7):A527, 2009.
- [50] Yannic Troxler, Billy Wu, Monica Marinescu, Vladimir Yufit, Yatish Patel, Andrew J. Marquis, Nigel P. Brandon, and Gregory J. Offer. The effect of thermal gradients on the performance of lithium-ion batteries. *Journal of Power Sources*, (247):1018–1025, June 2013.
- [51] PG Balakrishnan, R Ramesh, and T Prem Kumar. Safety mechanisms in lithium-ion batteries. *Journal of Power Sources*, 155(2):401–414, 2006.
- [52] Ortal Haik, Svetlana Ganin, Gregory Gershinsky, Ella Zinigrad, Boris Markovsky, Doron Aurbach, and I Halalay. On the thermal behavior of lithium intercalated graphites. *Journal of The Electrochemical Society*, 158(8):A913–A923, 2011.
- [53] Zonghai Chen, Yan Qin, Jun Liu, and K Amine. Lithium difluoro (oxalato) borate as additive to improve the thermal stability of lithiated graphite. *Electrochemical and Solid-State Letters*, 12(4):A69–A72, 2009.
- [54] Reinhold Koch and Andreas Jossen. Temperature Measurement of Large Format Pouch Cells with Impedance Spectroscopy. *EVS28 International Electric Vehicle Symposium and Exhibition*, pages 1–9, 2015.
- [55] Luc HJ Raijmakers, Dmitri L Danilov, Joop PM van Lammeren, Thieu JG Lammers, Henk Jan Bergveld, and Peter HL Notten. Non-zero intercept frequency: an accurate method to determine the integral temperature of li-ion batteries. *IEEE Transactions on Industrial Electronics*, 63(5):3168–3178, 2016.
- [56] Robert R. Richardson, Peter T. Ireland, and David A. Howey. Battery internal temperature estimation by combined impedance and surface temperature measurement. *J. Power Sources*, 265:254–261, May 2014.
- [57] Robert R Richardson and David A Howey. Sensorless Battery Internal Temperature Estimation using a Kalman Filter with Impedance Measurement. *IEEE Transactions on Sustainable Energy*, 6(4), 2015.

- [58] Robert Richardson, Shi Zhao, and David A Howey. On-board monitoring of 2-d spatially-resolved temperatures in cylindrical lithium-ion batteries: Part ii. state estimation via impedance-based temperature sensing. *Journal of Power Sources*, Article in press, 2016.
- [59] Christoph R Birkel and DA Howey. Model identification and parameter estimation for lifepo4 batteries. 2013.
- [60] SMM Alavi, CR Birkel, and DA Howey. Time-domain fitting of battery electrochemical impedance models. *Journal of Power Sources*, 288:345–352, 2015.
- [61] Adrien Mathieu Bizeray, Stephen R Duncan, and David Alastair Howey. Li-ion battery state estimation using a pseudo two-dimensional electrochemical model-based extended kalman filter with temperature and degradation effects. In *Meeting Abstracts*, volume 1, pages 85–85. The Electrochemical Society, 2015.
- [62] A Bizeray, S Duncan, David Howey, et al. Advanced battery management systems using fast electrochemical modelling. In *Hybrid and Electric Vehicles Conference 2013 (HEVC 2013)*, IET, pages 1–6. IET, 2013.
- [63] A Bizeray, S Zhao, SR Duncan, and DA Howey. Lithium-ion battery thermal-electrochemical model-based state estimation using orthogonal collocation and a modified extended Kalman filter. *Journal of Power Sources*, 296:400–412, November 2015.
- [64] David A Howey, Paul D Mitcheson, Senior Member, Vladimir Yufit, Gregory J Offer, and Nigel P Brandon. On-line measurement of battery impedance using motor controller excitation. *IEEE Trans. Veh. Technol.*, 63(6):2557–2566, 2014.
- [65] Nigel Brandon, Paul Mitcheson, David A. Howey, Vladimir Yufit, and Gregory J. Offer. Battery Monitoring in Electric Vehicles, Hybrid Vehicles and other Applications, 2012.
- [66] Wangxin Huang and Jaber Abu Qahouq. An Online Battery Impedance Measurement Method Using DC-DC Power Converter Control. *IEEE Trans. Ind. Electron.*, 0046(c):1–1, 2014.
- [67] Reinhold Koch and Andreas Jossen. Speed optimized multisine stimuli for electrochemical impedance spectroscopy with a switched mode excitation. In *Vehicle Power and Propulsion Conference (VPPC), 2014 IEEE*, pages 1–6. IEEE, 2014.
- [68] Robert Koch and Andreas Jossen. Impedance spectroscopy for battery monitoring with switched mode amplifiers. In *Power Electronics and Motion Control Conference and Exposition (PEMC), 2014 16th International*, pages 496–501. IEEE, 2014.
- [69] Yong-Duk Lee, Sung-Yeul Park, and Soo-Bin Han. Online embedded impedance measurement using high-power battery charger. *Industry Applications, IEEE Transactions on*, 51(1):498–508, 2015.

- [70] Paul Robertson. Battery Diagnostic System and Complex Impedance Measurement Algorithm. *EVS28 International Electric Vehicle Symposium and Exhibition*, 2015.
- [71] Matteo Muratori, Ning Ma, Marcello Canova, and Yann Guezennec. A model order reduction method for the temperature estimation in a cylindrical li-ion battery cell. In *ASME 2010 Dynamic Systems and Control Conference*, pages 633–640. American Society of Mechanical Engineers, 2010.
- [72] Matteo Muratori, Marcello Canova, Yann Guezennec, Giorgio Rizzoni, Energia Politecnico, and Via Lambruschini. A Reduced-Order Model for the Thermal Dynamics of Li-Ion Battery Cells. In *6th IFAC Symposium Advances in Automotive Control*, pages 10–15, Munich, Germany, 2010.
- [73] Valentin Roscher, Matthias Schneider, Phillip Durdaut, Nico Sassano, Sergej Pereguda, Eike Mense, and Karl-Ragnar Riemschneider. Synchronisation using wireless trigger-broadcast for impedance spectroscopy of battery cells. In *Sensors Applications Symposium (SAS), 2015 IEEE*, pages 1–6. IEEE, 2015.
- [74] Gi Heon Kim, Ahmad Pesaran, and Robert Spotnitz. A three-dimensional thermal abuse model for lithium-ion cells. *Journal of Power Sources*, 170(2):476–489, 2007.
- [75] Ahmad a. Pesaran. Battery thermal models for hybrid vehicle simulations. *Journal of Power Sources*, 110(2):377–382, August 2002.
- [76] W. B. Gu and C. Y. Wang. Thermal-Electrochemical Modeling of Battery Systems. *Journal of The Electrochemical Society*, 147(8):2910, 2000.
- [77] Venkat Srinivasan and C. Y. Wang. Analysis of Electrochemical and Thermal Behavior of Li-Ion Cells. *Journal of The Electrochemical Society*, 150(1):A98, 2003.
- [78] WJ Minkowycz, Ephraim M Sparrow, and Jayathi Murthy. *Handbook of numerical heat transfer*. Wiley Online Library, 1988.
- [79] Xuesong Li, Fan He, and Lin Ma. Thermal management of cylindrical batteries investigated using wind tunnel testing and computational fluid dynamics simulation. *J. Power Sources*, 238:395–402, September 2013.
- [80] Xinfan Lin, Hector E Perez, Jason B Siegel, Anna G Stefanopoulou, Yi Ding, and Matthew P Castanier. Parameterization and Observability Analysis of Scalable Battery Clusters for Onboard Thermal Management. In *Les Rencontres Scientifiques d’IFP Energies nouvelles*, number December, 2011.
- [81] Nicolas Damay, Christophe Forgez, Marie-Pierre Bichat, Guy Friedrich, and Alejandro Ospina. Thermal modeling and experimental validation of a large prismatic Li-ion battery. *IECON 2013 - 39th Annual Conference of the IEEE Industrial Electronics Society*, pages 4694–4699, November 2013.

- [82] Haifeng Dai, Letao Zhu, Jiangong Zhu, Xuezhe Wei, and Zechang Sun. Adaptive Kalman filtering based internal temperature estimation with an equivalent electrical network thermal model for hard-cased batteries. *Journal of Power Sources*, 293:351–365, 2015.
- [83] Fan He and Lin Ma. Thermal management of batteries employing active temperature control and reciprocating cooling flow. *International Journal of Heat and Mass Transfer*, 83:164–172, 2015.
- [84] R. Wrobel and P. H. Mellor. A General Cuboidal Element for Three-Dimensional Thermal Modelling. *IEEE Transactions on Magnetics*, 46(8):3197–3200, August 2010.
- [85] PH Mellor, D Roberts, and DR Turner. Lumped parameter thermal model for electrical machines of tefc design. In *IEE Proceedings B (Electric Power Applications)*, volume 138, pages 205–218. IET, 1991.
- [86] Nick Simpson, Rafal Wrobel, and Phil H Mellor. A general arc-segment element for three-dimensional thermal modeling. *Magnetics, IEEE Transactions on*, 50(2):265–268, 2014.
- [87] Fang Qi, Alexander Stippich, Moritz Guettler, Markus Neubert, and Rik W De Doncker. Methodical considerations for setting up space-resolved lumped-parameter thermal models for electrical machines. In *Electrical Machines and Systems (ICEMS), 2014 17th International Conference on*, pages 651–657. IEEE, 2014.
- [88] Nick Simpson, Rafal Wrobel, and Phil H Mellor. An accurate mesh-based equivalent circuit approach to thermal modeling. *Magnetics, IEEE Transactions on*, 50(2):269–272, 2014.
- [89] K. Shah, S.J. Drake, D.a. Wetz, J.K. Ostanek, S.P. Miller, J.M. Heinzl, and a. Jain. An experimentally validated transient thermal model for cylindrical Li-ion cells. *Journal of Power Sources*, 271:262–268, December 2014.
- [90] K Shah and A Jain. Modeling of steady-state and transient thermal performance of a li-ion cell with an axial fluidic channel for cooling. *International Journal of Energy Research*, 39(4):573–584, 2015.
- [91] K Shah, SJ Drake, DA Wetz, JK Ostanek, SP Miller, JM Heinzl, and A Jain. Modeling of steady-state convective cooling of cylindrical li-ion cells. *Journal of Power Sources*, 258:374–381, 2014.
- [92] David W Hahn and M Necati Ozisik. *Heat conduction*. John Wiley & Sons, 2012.
- [93] Latif M. Jiji. *Heat Conduction*. Springer, 2009.
- [94] Jan Taler and Piotr Duda. *Solving direct and inverse heat conduction problems*. Springer Science & Business Media, 2010.
- [95] Jie Shen, Tao Tang, and Li-Lian Wang. *Spectral Methods: Algorithms, Analysis and Applications*. Springer, 2011.

- [96] Lloyd N Trefethen. *Spectral methods in MATLAB*, volume 10. Siam, 2000.
- [97] Venkat R. Subramanian, Vinten D. Diwakar, and Deepak Tapriyal. Efficient Macro-Micro Scale Coupled Modeling of Batteries. *Journal of The Electrochemical Society*, 152(10):A2002, 2005.
- [98] Paul W. C. Northrop, Venkatasailanathan Ramadesigan, Sumitava De, and Venkat R. Subramanian. Coordinate Transformation, Orthogonal Collocation, Model Reformulation and Simulation of Electrochemical-Thermal Behavior of Lithium-Ion Battery Stacks. *Journal of The Electrochemical Society*, 158(12):A1461, 2011.
- [99] Long Cai and Ralph E. White. Lithium ion cell modeling using orthogonal collocation on finite elements. *Journal of Power Sources*, 217:248–255, November 2012.
- [100] P. W. C. Northrop, M. Pathak, D. Rife, S. De, S. Santhanagopalan, and V. R. Subramanian. Efficient Simulation and Model Reformulation of Two-Dimensional Electrochemical Thermal Behavior of Lithium-Ion Batteries. *Journal of the Electrochemical Society*, 162(6):A940–A951, 2015.
- [101] Robert Richardson, Shi Zhao, and David A Howey. On-board monitoring of 2-d spatially-resolved temperatures in cylindrical lithium-ion batteries: Part i. low-order thermal modelling. *Journal of Power Sources*, Article in press, 2016.
- [102] Mohinder S Grewal. *Kalman filtering*. Springer, 2011.
- [103] Hongwen He, Rui Xiong, Xiaowei Zhang, Fengchun Sun, and JinXin Fan. State-of-charge estimation of the lithium-ion battery using an adaptive extended kalman filter based on an improved thevenin model. *IEEE Transactions on Vehicular Technology*, 60(4):1461–1469, 2011.
- [104] Domenico Di Domenico, Anna Stefanopoulou, and Giovanni Fiengo. Lithium-ion battery state of charge and critical surface charge estimation using an electrochemical model-based extended kalman filter. *Journal of dynamic systems, measurement, and control*, 132(6):061302, 2010.
- [105] Jaemoon Lee, Oanyong Nam, and BH Cho. Li-ion battery soc estimation method based on the reduced order extended kalman filtering. *Journal of Power Sources*, 174(1):9–15, 2007.
- [106] Gregory L Plett. Sigma-point kalman filtering for battery management systems of lipb-based hev battery packs: Part 1: Introduction and state estimation. *Journal of Power Sources*, 161(2):1356–1368, 2006.
- [107] Gregory L Plett. Sigma-point kalman filtering for battery management systems of lipb-based hev battery packs: Part 2: Simultaneous state and parameter estimation. *Journal of Power Sources*, 161(2):1369–1384, 2006.
- [108] Gregory L Plett. Extended kalman filtering for battery management systems of lipb-based hev battery packs: Part 1. background. *Journal of Power sources*, 134(2):252–261, 2004.

- [109] Gregory L Plett. Extended kalman filtering for battery management systems of lipb-based hev battery packs: Part 2. modeling and identification. *Journal of power sources*, 134(2):262–276, 2004.
- [110] Gregory L Plett. Extended kalman filtering for battery management systems of lipb-based hev battery packs: Part 3. state and parameter estimation. *Journal of Power sources*, 134(2):277–292, 2004.
- [111] Haifeng Dai, Letao Zhu, Jiangong Zhu, Xuezhe Wei, and Zechang Sun. Adaptive kalman filtering based internal temperature estimation with an equivalent electrical network thermal model for hard-cased batteries. *Journal of Power Sources*, 293:351–365, 2015.
- [112] Jinlei Sun, Guo Wei, Lei Pei, Rengui Lu, Kai Song, Chao Wu, and Chunbo Zhu. Online internal temperature estimation for lithium-ion batteries based on kalman filter. *Energies*, 8(5):4400–4415, 2015.
- [113] Kailong Liu, Kang Li, and Jing Deng. A novel hybrid data-driven method for li-ion battery internal temperature estimation. In *Control (CONTROL), 2016 UKACC 11th International Conference on*, pages 1–6. IEEE, 2016.
- [114] Frank P. Incropera and David P. De Witt. *Fundamentals of Heat and Mass Transfer*. Wiley, 6th edition, 2007.
- [115] Erwin Kreyszig. *Advanced engineering mathematics*. John Wiley & Sons, 2010.
- [116] B.V. Ratnakumar, M.C. Smart, L.D. Whitcanack, and R.C. Ewell. The impedance characteristics of Mars Exploration Rover Li-ion batteries. *J. Power Sources*, 159(2):1428–1439, September 2006.
- [117] Jun Huang, Zhe Li, and Jianbo Zhang. Dynamic electrochemical impedance spectroscopy reconstructed from continuous impedance measurement of single frequency during charging/discharging. *Journal of Power Sources*, 273:1098–1102, 2015.
- [118] Jun Huang, Hao Ge, Zhe Li, and Jianbo Zhang. Dynamic electrochemical impedance spectroscopy of a three-electrode lithium-ion battery during pulse charge and discharge. *Electrochimica Acta*, 176:311–320, 2015.
- [119] Michel André. The artemis european driving cycles for measuring car pollutant emissions. *Science of the total Environment*, 334:73–84, 2004.
- [120] D Bernardi, E Pawlikowski, and J Newman. A General Energy Balance for Battery Systems. *J. Electrochem. Soc.*, 132(1):5–12, 1985.
- [121] C R Birkl and D A Howey. Model identification and parameter estimation for LiFePO₄. In *IET Hybrid and Electric Vehicles Conference 2013 (HEVC 2013)*, pages 1–6, 2013.
- [122] Hussam Khasawneh, John Neal, Marcello Canova, and Yann Guezennec. Analysis of heat-spreading thermal management solutions for lithium-ion batteries. In *ASME 2011 International Mechanical Engineering Congress and Exposition*, pages 421–428, 2011.

-
- [123] Eric A Wan and Alex T Nelson. Dual extended Kalman filter methods. In *Kalman filtering and neural networks*, pages 123–173. Wiley, New York, NY, 2001.
 - [124] E. H. Doha and A. H. Bhrawy. An efficient direct solver for multidimensional elliptic Robin boundary value problems using a Legendre spectral-Galerkin method. *Computers and Mathematics with Applications*, 64(4):558–571, 2012.
 - [125] Anthony Jarrett and Il Yong Kim. Design optimization of electric vehicle battery cooling plates for thermal performance. *Journal of Power Sources*, 196(23):10359–10368, December 2011.

Appendix A

Polynomial Approximation: application to other geometries

The PA model employed in Chapter 4 was originally introduced and validated by Kim et al. [24], and applies to a 1-D solid cylinder. PA models are well suited to the ITD/TM approach since they are computationally efficient but provide an expression for the temperature distribution throughout the domain of interest, which is necessary for accurately calculating the impedance.

To apply similar methods to other battery geometries we require additional PA models. Here two additional PA models are derived and validated: 1-D Cartesian coordinates (suitable for simulating prismatic cells) and a 1-D annulus (an extension of the solid cylinder model to cases where the inner radial dimension is non-zero). In each case, the PA model derivation is presented and the model is validated by comparison in the frequency domain with the corresponding analytical solution of the 1D heat equation.

A.1 1-D Cartesian

Since prismatic cells consist of layers of anode/separator/cathode, the thermal conductivity in the thickness direction is often one or two orders of magnitude greater than that in the planar direction. Thus, if the cooling configuration provides uniform heat removal from the x faces then it may be reasonable to assume a 1D heat conduction problem. Although this is less likely to occur in practice than in the case of small cylindrical cells, certain studies have proposed and experimentally validated 1-D thermal models in the simulation of prismatic cells [72]. Specifically, in [72] a physically based reduced order thermal model was developed by applying the Laplace transform to the 1D heat equation and reducing to a low- order linear model using the

singular perturbation method. However, this model was only applied using constant surface temperature (Dirichlet) boundary conditions, which are unlikely to occur in practice. Therefore, the PA model presented in this section has advantages over the model in [72], since it achieves similar accuracy and computational efficiency, whilst being readily applicable to convection boundary conditions.

Thermal model

The cell thermal model (shown in Fig. A.1) is given by the following 1-D BVP [92]:

$$\rho c_p \frac{\partial T(x, t)}{\partial t} = k \frac{\partial^2 T(x, t)}{\partial x^2} + \frac{Q(t)}{V_b} \quad (\text{A.1})$$

where ρ , c_p and k are the density, specific heat capacity and thermal conductivity respectively, V_b is the cell volume, and Q is the heat generation rate. The boundary conditions are given by:

$$\left. \frac{\partial T(x, t)}{\partial x} \right|_{x=L} = -\frac{h}{k}(T(L, t) - T_\infty(t)) \quad (\text{A.2a})$$

$$\left. \frac{\partial T(x, t)}{\partial x} \right|_{x=0} = 0 \quad (\text{A.2b})$$

where T_∞ is the temperature of the heat transfer fluid, and h is the convection coefficient.

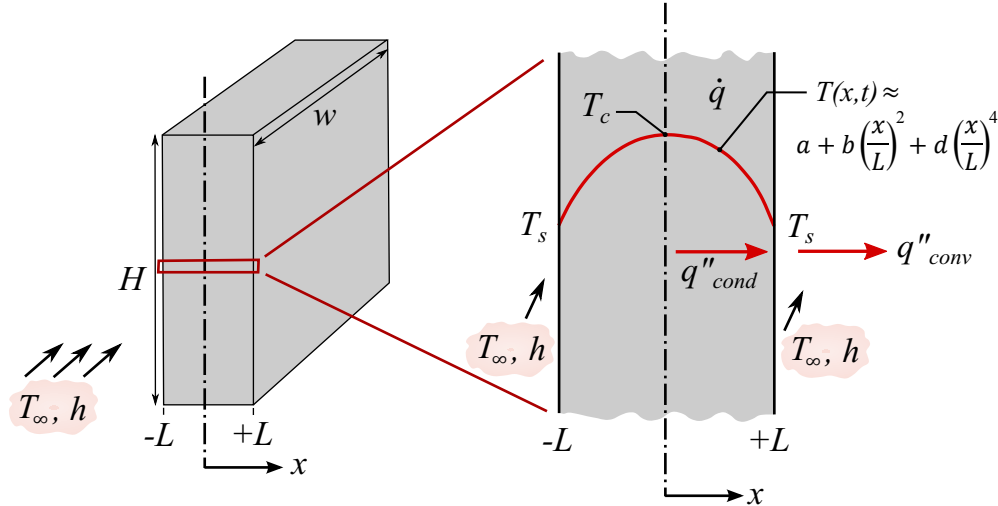


Fig. A.1 Schematic of prismatic cell geometry for the thermal model.

Polynomial Approximation

First, we assume the temperature distribution can be expressed in the form

$$T(x, t) = a(t) + b(t) \left(\frac{x}{L}\right)^2 + d(t) \left(\frac{x}{L}\right)^4, \quad (\text{A.3})$$

which satisfies the constraint of zero heat flux at the core as required. As discussed in Chapter 4, we note that other forms of polynomial may also give a reasonable solution [92]. The core and surface temperatures are then given by:

$$T_{core} = a(t), \quad T_{surf} = a(t) + b(t) + d(t) \quad (\text{A.4})$$

The two states of the model are the volume averaged temperature $\bar{T}$ and temperature gradient $\bar{\gamma}$:

$$\bar{T} = \frac{1}{L} \int_0^L T dx, \quad \bar{\gamma} = \frac{1}{L} \int_0^L \left(\frac{\partial T}{\partial x}\right) dx \quad (\text{A.5})$$

Substituting Eq. (A.3) into Eqs. (A.5) and integrating, yields:

$$\bar{T} = a(t) + \frac{b(t)}{3} + \frac{d(t)}{5}, \quad \bar{\gamma} = \frac{b(t)}{L} + \frac{d(t)}{L} \quad (\text{A.6})$$

Rearranging Eqs. (A.4) and (A.6), the time-varying constants are found to be:

$$\begin{aligned} a(t) &= T_{surf} - L\bar{\gamma} \\ b(t) &= \frac{15\bar{T}}{2} - \frac{15T_{surf}}{2} + 6L\bar{\gamma} \\ d(t) &= \frac{15T_{surf}}{2} - \frac{15\bar{T}}{2} - 5L\bar{\gamma} \end{aligned} \quad (\text{A.7})$$

Substituting (A.7) in (A.3), the temperature distribution can be expressed as a function of $\bar{T}$, $\bar{\gamma}$, and the cell surface temperature, T_{surf} :

$$T(r, t) = T_{surf} - L\bar{\gamma} + \left[\frac{15\bar{T}}{2} - \frac{15T_{surf}}{2} + 6L\bar{\gamma} \right] \left(\frac{x}{L}\right)^2 + \left[\frac{15T_{surf}}{2} - \frac{15\bar{T}}{2} - 5L\bar{\gamma} \right] \left(\frac{x}{L}\right)^4 \quad (\text{A.8})$$

By obtaining the volume-average of Eq. (A.1) and of its partial derivative with respect to x ,

$$\frac{1}{L} \int_0^L \left(\rho c_p \frac{\partial T(x, t)}{\partial t} - k \frac{\partial^2 T(x, t)}{\partial x^2} - \frac{Q(t)}{V_b} \right) dx = 0 \quad (\text{A.9a})$$

$$\frac{1}{L} \int_0^L \frac{\partial}{\partial x} \left(\rho c_p \frac{\partial T(x, t)}{\partial t} - k \frac{\partial^2 T(x, t)}{\partial x^2} - \frac{Q(t)}{V_b} \right) dx = 0 \quad (\text{A.9b})$$

the PDE is reduced to two ODEs:

$$\rho c_p L^2 \frac{d\bar{T}}{dt} + 15k\bar{T} + 8Lk\bar{\gamma} - 15kT_{surf} - \frac{L^2 Q}{V_b} = 0 \quad (\text{A.10a})$$

$$\rho c_p L^2 \frac{d\bar{\gamma}}{dt} + \frac{90k}{L} \bar{T} + 60k\bar{\gamma} - \frac{90k}{L} T_{surf} = 0 \quad (\text{A.10b})$$

Using Eq. (A.2a), the surface temperature can be expressed as

$$T_{surf} = \frac{15k\bar{T} + 8Lk\bar{\gamma} + LhT_\infty}{24k + r_{out}h} \quad (\text{A.11})$$

Thus, a two-state thermal model consisting of two ODEs is given by:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \quad (\text{A.12})$$

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \quad (\text{A.13})$$

where $\mathbf{x} = [\bar{T}, \bar{\gamma}]^T$, $\mathbf{u} = [Q, T_\infty]^T$ and $\mathbf{y} = [T_{core}, T_{surf}]^T$ are state, inputs and outputs respectively. The system matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ are defined as:

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} \frac{-15hk}{L\rho c_p(15k+Lh)} & \frac{-90hk}{L^2 c_p \rho(15k+Lh)} \\ \frac{8hk}{c_p \rho(15k+Lh)} & \frac{-60k(3k+Lh)}{L^2 c_p \rho(15k+Lh)} \end{bmatrix} \\ \mathbf{B} &= \begin{bmatrix} \frac{1}{\rho c_p V_b} & 0 \\ \frac{15hk}{L c_p \rho(15k+Lh)} & \frac{90hk}{L^2 c_p \rho(15k+Lh)} \end{bmatrix} \\ \mathbf{C} &= \begin{bmatrix} \frac{15k}{15k+Lh} & \frac{8Lk}{15k+Lh} - L \\ \frac{15k}{15k+Lh} & \frac{8Lk}{15k+Lh} \end{bmatrix} \\ \mathbf{D} &= \begin{bmatrix} 0 & \frac{Lh}{15k+Lh} \\ 0 & \frac{Lh}{15k+Lh} \end{bmatrix}. \end{aligned} \quad (\text{A.14})$$

The frequency domain response of this system, $\mathbf{H}(s)$, (which is analysed in Section A.1) is calculated by

$$\mathbf{H}(s) = \mathbf{D} + \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}, \quad (\text{A.15})$$

where $s = j\omega$ and $\mathbf{I}$ is the identity matrix.

Analytical Solution

An analytical solution to the 1D heat Eq. (A.1) in the frequency domain is found by transforming the time-domain PDE into an equivalent ODE problem in the frequency domain. The transformed BVP is given by,

$$a^2 T(x, s) = \frac{d^2 T(x, s)}{dx^2} + \frac{1}{k} Q(s), \quad (\text{A.16})$$

with boundary conditions,

$$\left. \frac{dT(x, s)}{dx} \right|_{x=L} = -\frac{h}{k} (T(L, s) - T_\infty(s)), \quad (\text{A.17a})$$

$$\left. \frac{dT(x, s)}{dx} \right|_{x=0} = 0, \quad (\text{A.17b})$$

where $a^2 = s\alpha^{-1}$ and $Q(s)$ is the transform of $Q(t)$.

The solution to Eq. (A.16) is of the form [72]:

$$T(x, s) = \frac{1}{ka^2} Q(s) + C_1(s) \cosh(ax) + C_2(s) \sinh(ax) \quad (\text{A.18})$$

The temperatures at the centre and surface of the cell are found by evaluating the solution at $x = 0$ and $x = \pm L$, respectively.

$$T_{core}(s) = \frac{Q(s)}{a^2 k V_b} + \frac{h (Q(s) - a^2 k V_b T_\infty)}{a^2 k V_b (h \cosh(aL) + a k \sinh(aL))}, \quad (\text{A.19})$$

$$T_{surf}(s) = \frac{\sinh(aL)Q(s) + a V_b h \cosh(aL) T_\infty}{a V_b (h \cosh(aL) + a k \sinh(aL))}. \quad (\text{A.20})$$

Eqs. (A.19) and (A.20) can be interpreted as the outputs of a continuous time dynamic system [72], where $\mathbf{u}(t) = [Q(t), T_\infty(t)]^T$ and $\mathbf{y}(t) = [T_{core}(t), T_{surf}(t)]^T$, such that the

solution of the BVP is equivalent to the impulse response of the system:

$$\begin{bmatrix} T_{core}(t) \\ T_{surf}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{11}(s) & \mathbf{H}_{12}(s) \\ \mathbf{H}_{21}(s) & \mathbf{H}_{22}(s) \end{bmatrix} \begin{bmatrix} Q(t) \\ T_{\infty}(t) \end{bmatrix} \quad (\text{A.21})$$

where the $\mathbf{H}$ matrix is formed by the transfer functions:

$$\mathbf{H}_{11}(s) = \frac{1}{a^2 k V_b} - \frac{h}{a^2 k V_b (h \cosh(aL) + ak \sinh(aL))} \quad (\text{A.22})$$

$$\mathbf{H}_{12}(s) = \frac{\sinh(aL)}{a V_b (h \cosh(aL) + ak \sinh(aL))} \quad (\text{A.23})$$

$$\mathbf{H}_{21}(s) = \frac{h}{h \cosh(aL) + ak \sinh(aL)} \quad (\text{A.24})$$

$$\mathbf{H}_{22}(s) = \frac{h \cosh(aL)}{h \cosh(aL) + ak \sinh(aL)} \quad (\text{A.25})$$

This system of transfer functions gives frequency responses for the analytical solution results plotted in Fig. A.2. In principle, it is possible to obtain an analytical solution in the time domain by obtaining the inverse transform of the above equations. However, this is not necessary in this case, since our goal is to compare the frequency response of the above system to the response of the PA model over the desired frequency range.

Lastly, we note that impedance-temperature detection (ITD) can also be applied to the present model in a similar manner to those employed in Chapter 4 for cylindrical cells. For a prismatic cell with thickness L the real part of the admittance can be expressed as

$$Y' = \frac{1}{L} \int_0^L (a_1 + a_2 T(x) + a_3 T(x)^2) \quad (\text{A.26})$$

Substituting Eq. (A.8) into Eq. (A.26), the real admittance can be expressed as a function of T_{surf} , $\bar{T}$, and $\bar{\gamma}$

$$\begin{aligned} Y' = & a_3 + a_2 \bar{T} + \frac{3a_1 T_{surf}^2}{7} - \frac{6a_1 \bar{T} T_{surf}}{7} + \frac{10a_1 \bar{T}^2}{7} \\ & - \frac{16a_1 L T_{surf} \bar{\gamma}}{21} + \frac{128a_1 L^2 \bar{\gamma}^2}{315} + \frac{16a_1 L \bar{T} \bar{\gamma}}{21} \end{aligned} \quad (\text{A.27})$$

Frequency analysis

Lastly, we analyze the error associated with the polynomial approximation by comparing the frequency response of the PA model to the frequency response of a full analytical solution of Eq. (A.1).

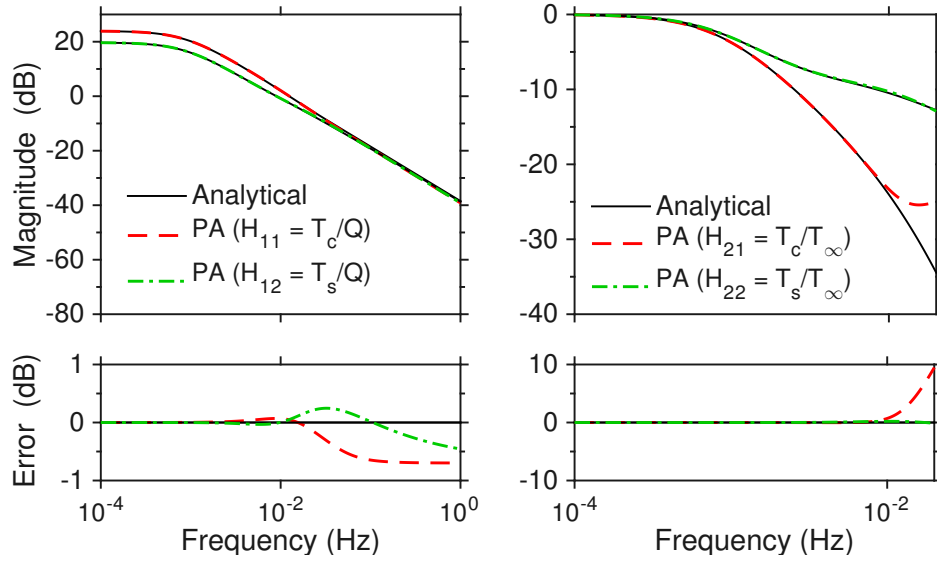


Fig. A.2 Comparison of frequency responses of the analytical solution and the polynomial approximation.

Fig. A.2 shows the impact of changes in heat generation on T_{core} and T_{surf} (H_{11} and H_{21} respectively), and the impact of changes in cooling fluid temperature T_∞ on T_{core} and T_{surf} (H_{12} and H_{22} respectively), for each model along with the error relative to the analytical solution.

The responses for all four cases are satisfactory over a broad frequency range, with a similar performance to that of the cylindrical PA model discussed in Section 4.2.

A.2 1-D annulus

In practice, so-called cylindrical cells are actually annular in geometry (i.e. they contain a hole along the central axis), and so neglecting the central hole may result in inaccuracies. Here we extend the cylindrical model presented in Chapter 4 to the case of an annulus. Although the derivation of the model is more involved, the resulting model has two states and is thus equally efficient to that of the solid cylinder.

Thermal model

The cell thermal model (shown in Fig. A.3) is given by the following 1-D BVP: [92]:

$$\rho c_p \frac{\partial T(r, t)}{\partial t} = k \frac{\partial^2 T(r, t)}{\partial r^2} + \frac{k}{r} \frac{\partial T(r, t)}{\partial r} + \frac{Q(t)}{V_b} \quad (\text{A.28a})$$

where ρ , c_p and k are the density, specific heat capacity and thermal conductivity respectively, V_b is the cell volume, and Q is the heat generation rate. The boundary conditions are given by:

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=r_{out}} = -\frac{h}{k} (T(r_{out}, t) - T_{\infty}(t)) \quad (\text{A.28b})$$

$$\left. \frac{\partial T(r, t)}{\partial r} \right|_{r=r_{in}} = 0 \quad (\text{A.28c})$$

where T_{∞} is the temperature of the heat transfer fluid, and h is the convection coefficient.

Polynomial Approximation

The PA model assumes a temperature distribution of the form

$$T(r, t) = a(t) + b(t) \left(\frac{r - r_{in}}{r_{out} - r_{in}} \right)^2 + d(t) \left(\frac{r - r_{in}}{r_{out} - r_{in}} \right)^4, \quad (\text{A.29})$$

which satisfies the constraint of zero heat flux at the core as required. As discussed in Chapter 4, we note that other forms of polynomial may also give a reasonable solution [92]. The core and surface temperatures are then given by:

$$T_{core} = T(r = r_{in}) = a(t), \quad (\text{A.30})$$

$$T_{surf} = T(r = r_{out}) = a(t) + b(t) + d(t) \quad (\text{A.31})$$

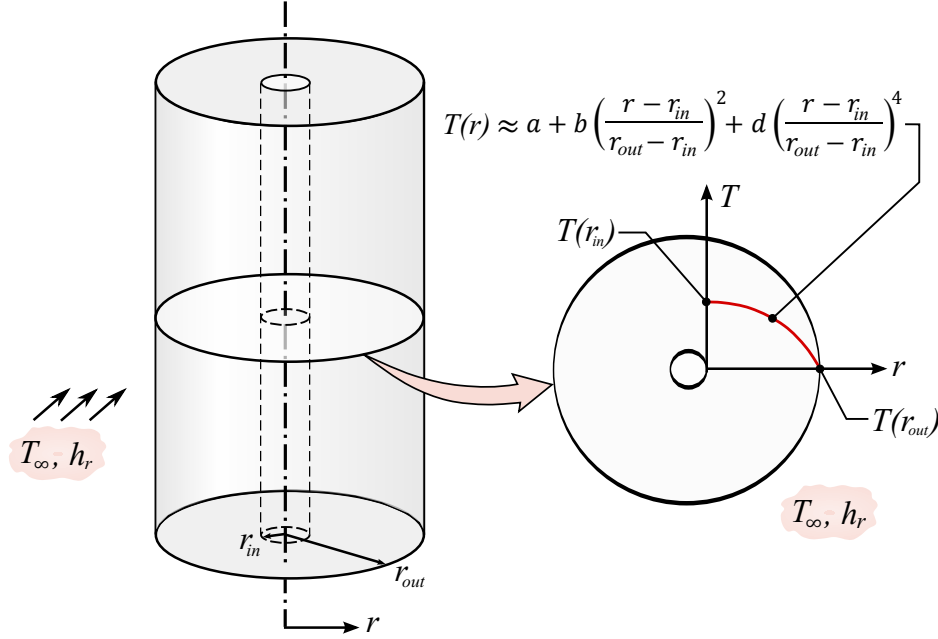


Fig. A.3 Schematic of annular cell geometry for the thermal model.

The two states of the model are the volume averaged temperature $\bar{T}$ and temperature gradient $\bar{\gamma}$:

$$\bar{T} = \frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r T dr, \quad \bar{\gamma} = \frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r \left(\frac{\partial T}{\partial r} \right) dr. \quad (\text{A.32})$$

Substituting Eq. (A.29) into Eqs. (A.32) and integrating, yields:

$$\bar{T} = \frac{r_{in} - r_{out}}{r_{in}^2 - r_{out}^2} (a (r_{in} + r_{out}) + 150b (r_{in} + 3br_{out}) + 60d (r_{in} + 5dr_{out})), \quad (\text{A.33})$$

$$\bar{\gamma} = -\frac{2}{r_{in}^2 - r_{out}^2} \left(\frac{br_{in}}{3} + \frac{2br_{out}}{3} + \frac{dr_{in}}{5} + \frac{4dr_{out}}{5} \right). \quad (\text{A.34})$$

Solving the simultaneous Eqs. (A.31), (A.33) and (A.34), the time-varying constants, a , b , and d are reduced to algebraic expressions involving $\bar{T}$, $\bar{\gamma}$ and the surface temperature, T_{surf} . Thus, the temperature distribution (Eq. (A.29)) is likewise a function of $\bar{T}$, $\bar{\gamma}$ and T_{surf} . By obtaining the volume-average of Eq. (A.28a) and of its partial derivative with respect to x , the PDE is reduced to two ODEs:

$$\frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r \left(\rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial r^2} - \frac{k}{r} \frac{\partial T}{\partial r} - \frac{Q}{V_b} \right) dr = 0 \quad (\text{A.35})$$

$$\frac{2}{r_{out}^2 - r_{in}^2} \int_{r_{in}}^{r_{out}} r \frac{\partial}{\partial r} \left(\rho c_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial r^2} - \frac{k}{r} \frac{\partial T}{\partial r} - \frac{Q}{V_b} \right) dr = 0 \quad (\text{A.36})$$

Using Eq. (A.28b), the surface temperature can be expressed as

$$T_{surf} = \frac{k}{h} \left(T_{\infty} - \frac{\partial T}{\partial r} \Big|_{r=r_{out}} \right) \quad (\text{A.37})$$

where

$$\frac{\partial T}{\partial r} \Big|_{r=r_{out}} = 6(r_{in} + r_{out}) \cdot \frac{14r_{in}(\bar{T} - T_{surf}) + 16r_{out}(\bar{T} - T_{surf}) + \bar{\gamma}(5r_{out}^2 - 11r_{in}^2 + 6r_{in}r_{out})}{13r_{in}^3 - 6r_{in}^2r_{out} - 3r_{in}r_{out}^2 - 4r_{out}^3} \quad (\text{A.38})$$

Thus, a two-state thermal model consisting of two ODEs is then given by:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \\ \mathbf{y} &= \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \end{aligned} \quad (\text{A.39})$$

where $\mathbf{x} = [\bar{T}, \bar{\gamma}]^T$, $\mathbf{u} = [Q, T_{\infty}]^T$ and $\mathbf{y} = [T_{core}, T_{surf}]^T$ are state, inputs and outputs respectively, and $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ are the system matrices.

The frequency domain response of this system, $\mathbf{H}(s)$, is calculated by

$$\mathbf{H}(s) = \mathbf{D} + \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} \quad (\text{A.40})$$

where $s = j\omega$ and $\mathbf{I}$ is the identity matrix.

Analytical Solution

An analytical solution to Eq. (A.28a) in the frequency domain is found by transforming the time-domain PDE into an equivalent ODE problem in the frequency domain. The transformed BVP is given by:

$$a^2 T(r, s) = \frac{d^2 T(r, s)}{dr^2} + \frac{1}{r} \frac{dT(r, s)}{dr} + \frac{1}{k} Q(s) \quad (\text{A.41})$$

with boundary conditions given by,:

$$\frac{dT(r, s)}{dr} \Big|_{r=r_{out}} = -\frac{h}{k} (T(r_{out}, s) - T_{\infty}(s)), \quad (\text{A.42a})$$

$$\left. \frac{dT(r, s)}{dr} \right|_{r=r_{in}} = 0, \quad (\text{A.42b})$$

where $a^2 = s\alpha^{-1}$ and $Q(s)$ is the transform of $Q(t)$.

The final solution was found to be:

$$T(r, s) = \frac{1}{ka^2} Q(s) + C_1(s) J_0(ar) + C_2(s) Y_0(ar) \quad (\text{A.43})$$

where J_0 and Y_0 are 0th order Bessel functions of the first and second kind respectively; and C_1 and C_2 (found by evaluating the boundary conditions, Eqs. (A.42a) and (A.42b)) are

$$C_1 = \frac{h(Q - T_\infty a^2 k) \mu_1}{a(a^2 k^2 \mu_1 \mu_5 + ak(h\mu_3 - ak\mu_2) \mu_4 - ahk\mu_1 \mu_6)}, \quad (\text{A.44a})$$

$$C_2 = \frac{h(Q - T_\infty a^2 k) \mu_4}{k(a^2(ak\mu_2 - h\mu_3) \mu_4 + a^2 h\mu_1 \mu_6 - a^3 k\mu_1 \mu_5)}, \quad (\text{A.44b})$$

where $\mu_1 = Y_1(ar_{in})$, and $\mu_2 = Y_1(ar_{out})$, $\mu_3 = Y_0(ar_{out})$, $\mu_4 = J_1(ar_{in})$, $\mu_5 = J_1(ar_{out})$ and $\mu_6 = J_0(ar_{out})$.

The core and surface temperatures are found by evaluating the solution at $r = r_{in}$ and $r = r_{out}$, respectively. This results in a continuous time dynamic system, which can be expressed as

$$\begin{bmatrix} T_{core}(t) \\ T_{surf}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{11}(s) & \mathbf{H}_{12}(s) \\ \mathbf{H}_{21}(s) & \mathbf{H}_{22}(s) \end{bmatrix} \begin{bmatrix} Q(t) \\ T_\infty(t) \end{bmatrix} \quad (\text{A.45})$$

where $\mathbf{H}$ is a matrix of transfer functions consisting of the coefficients of Q and T_∞ in the expressions for T_{core} and T_{surf} . The solution of the BVP is equivalent to the impulse response of this system. This system of transfer functions gives frequency responses for the analytical solution results plotted in Fig. A.4. As before, we note that impedance-temperature detection (ITD) can also be applied to the annulus model in a similar manner to that employed in Chapter 4 for the solid cylinder.

Frequency analysis

Lastly, we analyze the error associated with the polynomial approximation by comparing the frequency response of the PA model to the frequency response of a full analytical solution of Eq. (A.28a). The parameters of the model are the same as those used for the solid cylinder analysis in Section 4.2 except that the inner radius is set to $r_{in} = 5$ mm, thus defining an annulus with radius ratio of ~ 0.4

Fig. A.4 shows the impact of changes in heat generation on T_{core} and T_{surf} ($\mathbf{H}_{11}$ and $\mathbf{H}_{21}$ respectively), and the impact of changes in cooling fluid temperature T_{∞} on T_{core} and T_{surf} ($\mathbf{H}_{12}$ and $\mathbf{H}_{22}$ respectively), for the PA model along with the error relative to the analytical solution. The responses for all four cases are satisfactory over a broad frequency range, with a similar performance to that of the PA model for a solid cylinder discussed in Section 4.2.

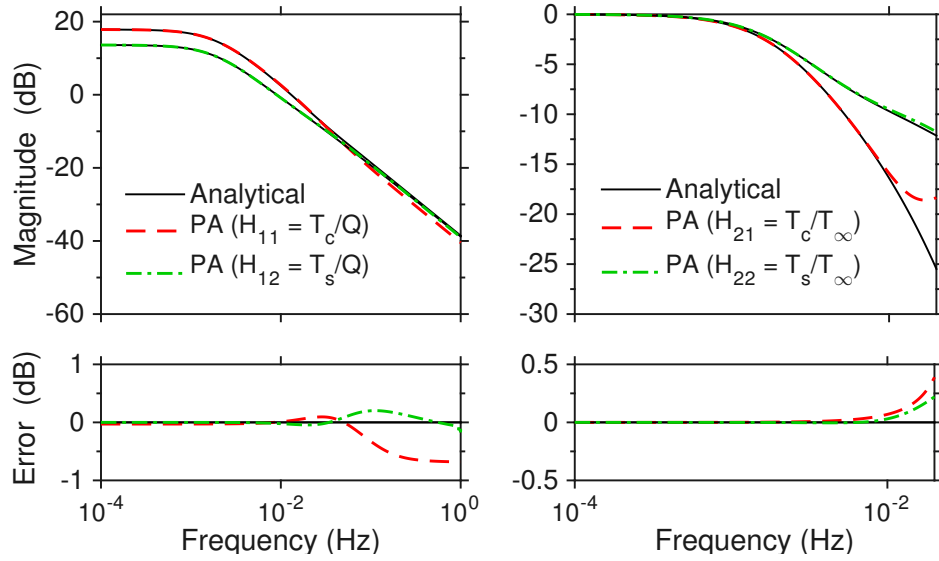


Fig. A.4 Comparison of frequency responses of the analytical solution and the PA model.

Appendix B

Polynomial Approximation: application to 2-D problems

In this appendix, a transient 2-D thermal model based on the PA approach is presented. PA is shown to be suitable for modelling 2-D problems with certain symmetrical boundary conditions with reasonable accuracy. However, as discussed in Section 1.5, it is unsuitable for modelling problems with more general conditions. The limitations outlined in Section 1.5, along with the results presented here, should serve to justify the use of the spectral-Galerkin method presented in Chapter 5 for flexible and efficient 2-D thermal modelling.

Overview

PA methods have been used extensively for 1D heat transfer problems, usually for cases involving symmetric boundary conditions or semi-infinite domains [93]. However, there is limited literature on the application of PA to multi-dimensional problems. Taler [94] presents some examples of PA applied to steady-state 2-D thermal problems; however, to the best of my knowledge there are no such studies examining transient problems. Here, I present a transient 2-D cylinder model with symmetric boundary conditions (i.e. the boundary conditions on opposite faces are either equal or one of them is zero). For such a case, it is possible to formulate a PA model which gives reasonable results under certain conditions. The performance of the model is investigated by comparison in the frequency domain with a high order numerical solution - a spectral-Galerkin

model with $N_s = 225$ states¹. The model is also compared against a low-order SG method ($N_s = 4$) to highlight the superiority of the SG method in this case.

Thermal Model

The model (shown in Fig. B.1) consists of the heat equation for 2D unsteady heat conduction in a cylinder, given by the following Boundary Value Problem (BVP) [93]:

$$\rho c_p \frac{\partial T(r, z, t)}{\partial t} = k_r \frac{\partial^2 T(r, z, t)}{\partial r^2} + \frac{k_r}{r} \frac{\partial T(r, z, t)}{\partial r} + k_z \frac{\partial^2 T(r, z, t)}{\partial z^2} + \frac{Q(t)}{V_b} \quad (\text{B.1})$$

where ρ and c_p are the density and specific heat capacity respectively, k_r and k_t are the thermal conductivities in the r and z directions, V_b is the cell volume, and Q is the heat generation rate. The boundary conditions are given by:

$$\left. \frac{\partial T}{\partial r} \right|_{r=r_{out}} = -\frac{h_r}{k_r} (T(r_{out}, z, t) - T_\infty(t)) \quad (\text{B.2a})$$

$$\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0 \quad (\text{B.2b})$$

$$\left. \frac{\partial T}{\partial z} \right|_{z=H} = -\frac{h_z}{k_z} (T(r, H, t) - T_\infty(t)) \quad (\text{B.2c})$$

$$\left. \frac{\partial T}{\partial z} \right|_{z=0} = 0 \quad (\text{B.2d})$$

where T_∞ is the temperature of the heat transfer fluid, and h_r and h_z are the convection coefficients in the r and z directions. Note that H is used to denote *half* the cell height (in contrast to its use as the total height elsewhere in this thesis) since this is more convenient for the presentation of this particular model.

¹Validation against an exact analytical solution would perhaps have been more elegant but - since such a solution is particularly involved for transient 2-D problems with anisotropic properties [91] - I have opted instead to use a high order numerical method. Since the numerical method can achieve arbitrary accuracy, in practice this choice has no discernible effect.

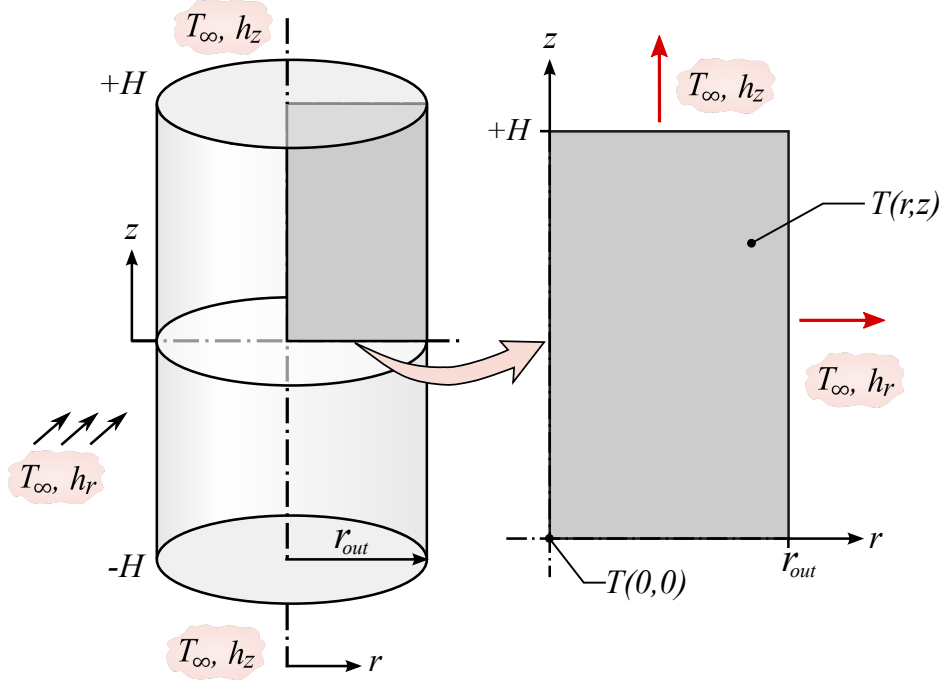


Fig. B.1 Schematic of cylindrical cell geometry for the thermal model.

Polynomial Approximation

A reduced order model is developed using a polynomial approximation of Eq. (B.1). The model assumes a temperature distribution of the form

$$\begin{aligned}
 T(r, z, t) = & a(t) + b(t) \left(\frac{r}{r_{out}} \right)^2 + c(t) \left(\frac{r}{r_{out}} \right)^3 + d(t) \left(\frac{z}{H} \right)^2 \\
 & + e(t) \left(\frac{z}{H} \right)^3 + f(t) \left(\frac{r^2 z^3}{r_{out}^2 H^3} \right) + g(t) \left(\frac{r^3 z^2}{r_{out}^3 H^2} \right)
 \end{aligned} \tag{B.3}$$

This polynomial is capable of satisfactorily approximating the temperature distribution including the constraint of zero heat flux in both the r and z directions at the axes of symmetry. The terms $r^2 z^3$ and $r^3 z^2$ are required to allow the gradient of the temperature w.r.t a given direction to vary along the orthogonal direction. The temperatures at selected locations are given by:

$$T(0, 0) = a \tag{B.4a}$$

$$T(r_{out}, 0) = a + b + c \tag{B.4b}$$

$$T(0, H) = a + d + e \tag{B.4c}$$

$$T(r_{out}, H) = a + b + c + d + e + f + g \tag{B.4d}$$

The three states of the model are the volume averaged temperature $\bar{T}$, and the volume averaged temperature gradient in the r and z directions, $\bar{\gamma}_r$ and $\bar{\gamma}_z$:

$$\bar{T} = \frac{2}{r_{out}^2 H} \int_0^L \int_0^{r_{out}} r T \, dr \, dz \quad (B.5)$$

$$\bar{\gamma}_r = \frac{2}{r_{out}^2 H} \int_0^L \int_0^{r_{out}} r \left(\frac{\partial T}{\partial r} \right) \, dr \, dz \quad (B.6)$$

$$\bar{\gamma}_z = \frac{2}{r_{out}^2 H} \int_0^L \int_0^{r_{out}} r \left(\frac{\partial T}{\partial z} \right) \, dr \, dz \quad (B.7)$$

Substituting Eq. (B.3) into Eqs. (B.5) - (B.7) and integrating, yields:

$$\bar{T} = a + \frac{b}{2} + \frac{2c}{5} + \frac{d}{3} + \frac{e}{4} + \frac{2f}{15} + \frac{g}{8} \quad (B.8)$$

$$\bar{\gamma}_r = \frac{8b + 9c + 3f + 2g}{6r_{out}} \quad (B.9)$$

$$\bar{\gamma}_z = \frac{10d + 10e + 4f + 5g}{10H} \quad (B.10)$$

Rearranging Eqs. (B.4a-B.4d) and (B.8-B.10), the time-varying constants are found to be:

$$\begin{aligned} a(t) &= \frac{1}{5} \left(8\bar{T}_H - T_{0,H} - 28\bar{T} - 2T_{r_{out},0} + 28\bar{T}_{r_{out}} - 7H\bar{\gamma}_z - 12r_{out}\bar{\gamma}_r \right) \\ b(t) &= \frac{1}{5} \left(6T_{0,H} + 2\bar{T}_H + 168\bar{T} - 8T_{r_{out},0} - 168\bar{T}_{r_{out}} - 8H\bar{\gamma}_z + 72r_{out}\bar{\gamma}_r \right) \\ c(t) &= 3T_{r_{out},0} - 2\bar{T}_H - 28\bar{T} - T_{0,H} + 28\bar{T}_{r_{out}} + 3H\bar{\gamma}_z - 12r_{out}\bar{\gamma}_r \\ d(t) &= \frac{1}{5} \left(52\bar{T} - 72\bar{T}_H - 6T_{0,H} + 18T_{r_{out},0} + 8\bar{T}_{r_{out}} + 63H\bar{\gamma}_z - 12r_{out}\bar{\gamma}_r \right) \\ e(t) &= \frac{1}{5} \left(12T_{0,H} + 64\bar{T}_H - 24\bar{T} - 16T_{r_{out},0} - 36\bar{T}_{r_{out}} - 56H\bar{\gamma}_z + 24r_{out}\bar{\gamma}_r \right) \\ f(t) &= 3T_{0,H} + 6\bar{T}_H + 4\bar{T} - 9T_{r_{out},0} - 4\bar{T}_{r_{out}} - 9H\bar{\gamma}_z + 6r_{out}\bar{\gamma}_r \\ g(t) &= \frac{1}{5} \left(32T_{r_{out},0} - 8\bar{T}_H - 72\bar{T} - 24T_{0,H} + 72\bar{T}_{r_{out}} + 32H\bar{\gamma}_z - 48r_{out}\bar{\gamma}_r \right) \end{aligned} \quad (B.11)$$

where $T_{r_{out},0}$ and $T_{0,H}$ are the cell temperatures at $T(r_{out}, 0)$ and $T(0, H)$, and $\bar{T}_{r_{out}}$ and $\bar{T}_H$ are the area averaged temperatures at the curved surface ($r = r_{out}$) and ends

($z = \pm H$) of the cell:

$$\bar{T}_{r_{out}} = \int_0^H T(r_{out}, z) dz, \quad \bar{T}_H = \frac{2}{r_{out}^2} \int_0^{r_{out}} r T(r, H) dr \quad (\text{B.12})$$

Substituting Eq. (B.11) into (B.3), it can be seen that the temperature distribution is a function of $\bar{T}$, $\bar{\gamma}_r$, $\bar{\gamma}_z$, $T_{r_{out},0}$, $T_{0,H}$, $\bar{T}_{r_{out}}$ and $\bar{T}_H$.

By obtaining the volume-average of Eq. (B.1) and of its partial derivative with respect to r and z (note that the factor of $2/r_{out}^2 H$ is omitted in each case since it does not affect the result), the PDE is reduced to three ODEs:

$$\begin{aligned} \int_0^L \int_0^{r_{out}} r \left(\rho c_p \frac{\partial T}{\partial t} - k_r \frac{\partial^2 T}{\partial r^2} - \frac{k_r}{r} \frac{\partial T}{\partial r} - k_z \frac{\partial^2 T}{\partial z^2} - \frac{Q}{V_b} \right) dr dz &= 0 \\ \int_0^L \int_0^{r_{out}} r \frac{\partial}{\partial r} \left(\rho c_p \frac{\partial T}{\partial t} - k_r \frac{\partial^2 T}{\partial r^2} - \frac{k_r}{r} \frac{\partial T}{\partial r} - k_z \frac{\partial^2 T}{\partial z^2} - \frac{Q}{V_b} \right) dr dz &= 0 \\ \int_0^L \int_0^{r_{out}} r \frac{\partial}{\partial z} \left(\rho c_p \frac{\partial T}{\partial t} - k_r \frac{\partial^2 T}{\partial r^2} - \frac{k_r}{r} \frac{\partial T}{\partial r} - k_z \frac{\partial^2 T}{\partial z^2} - \frac{Q}{V_b} \right) dr dz &= 0 \end{aligned} \quad (\text{B.13})$$

The boundary conditions are now used to identify $T_{r_{out},0}$, $T_{0,H}$, $\bar{T}_{r_{out}}$ and $\bar{T}_H$ in terms of the model states and inputs. The boundary conditions at the axes of symmetry (Eq. (B.2b) and (B.2c)) have already been satisfied implicitly by the form of the polynomial. The boundary conditions at the surfaces (Eq. (B.2a) and (B.2d)) are continuous functions of r and z respectively. The area-average of these 2 equations is obtained in order to obtain 2 discrete boundary conditions:

$$\frac{1}{H} \int_0^H \frac{dT(r_{out}, z)}{dz} dz = \frac{-h_r}{k_r} (\bar{T}_{r_{out}} - T_\infty) \quad (\text{B.14})$$

$$\frac{2}{r_{out}^2} \int_0^{r_{out}} r \frac{dT(r, H)}{dr} dr = \frac{-h_z}{k_z} (\bar{T}_H - T_\infty) \quad (\text{B.15})$$

In order to constrain the solution it is necessary to impose two additional boundary conditions. These were obtained by enforcing the boundary conditions at the points $(r_{out}, 0)$ and $(0, H)$:

$$\frac{dT(r_{out}, 0)}{dr} = \frac{-h_r}{k_r} (\bar{T}_{r_{out}} - T_\infty) \quad (\text{B.16})$$

$$\frac{dT(0, H)}{dz} = \frac{-h_z}{k_z}(\bar{T}_H - T_\infty) \quad (\text{B.17})$$

Solving Eqs. (B.14) and (B.15), gives

$$\bar{T}_{r_{out}} = \left(\frac{h_r}{k_r} + \frac{20}{r_{out}} \right) \left[\frac{1}{H} \left(6 H \bar{\gamma}_r + \frac{20 H \bar{T}}{r_{out}} \right) + \frac{T_\infty h_r}{k_r} \right] \quad (\text{B.18})$$

$$\bar{T}_H = \left(\frac{h_z}{k_z} + \frac{12}{H} \right) \left[\frac{1}{r_{out}^2} \left(6 r_{out}^2 \bar{\gamma}_z + \frac{12 r_{out}^2 \bar{T}}{H} \right) + \frac{T_\infty h_z}{k_z} \right] \quad (\text{B.19})$$

Similar results are obtained for $T(r_{out}, 0)$ and $T(0, H)$, by solving Eqs. (B.16) and (B.17).

Thus, a three-state thermal model consisting of three ODEs is then given by:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \\ \mathbf{y} &= \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \end{aligned} \quad (\text{B.20})$$

where $\mathbf{x} = [\bar{T} \ \bar{\gamma}_r \ \bar{\gamma}_z]^T$, $\mathbf{u} = [Q \ T_\infty]^T$ and $\mathbf{y} = [T_{0,0} \ T_{r_{out},0} \ T_{0,H} \ T_{r_{out},H}]^T$ are state, inputs and outputs respectively, and $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ are the system matrices. The frequency response of this system is given by $\mathbf{H}(s) = \mathbf{D} + \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}$, where $s = j\omega$ and $\mathbf{I}$ is the identity matrix.

Results and discussion

In this section, the frequency response of the PA model is compared against a baseline solution obtained by using an SG model with a large number of states ($N_s = 225$). Specifically, the impact of changes in heat generation on $T_{0,0}$, given by the transfer function $H(s) = T_{0,0}(s)/q(s)$, is examined. This is calculated using Eq. (B.20), using only the rows and columns of the $\mathbf{B}$ and $\mathbf{C}$ matrices corresponding to the heat generation input and $T_{0,0}$ output.

The parameters chosen are the same as those in the frequency domain analysis in Section B, except that the inner radius is set to zero (since the PA model is applied to a solid cylinder). A variety of different Biot numbers ($Bi = hr_{out}/k$) are obtained by varying the magnitude of the convection coefficients on each side. Convection coefficients of $h = \{10, 50, 100, 200\} \text{ Wm}^{-2}$ are chosen, resulting in Biot numbers of $Bi = \{0.48, 2.40, 4.80 \text{ and } 9.62\}$, respectively. The results are also compared against a low-order SG method ($N_s = 4$ states)

Fig. B.2 shows the magnitude of the frequency response in the range $f = 1 \times 10^{-4}$ to 1×10^0 for each of the four Biot numbers, along with the error of PA model and the 4-state SG model relative to the high fidelity solution.

These plots show that the PA model agrees well with the high-fidelity solution at low frequencies but becomes inaccurate at higher frequencies. The 4-state SG model shows a similar trend but with a smaller error across almost all frequencies and Biot numbers. Unlike the SG method, in the case of PA, there is no principled way of increasing the order to the model to improve its accuracy, and so the SG method is clearly more suitable in this case. Moreover, the PA model is limited to problems with symmetric boundary conditions such as the one considered here, whereas the SG method can be applied to much more general cases (as demonstrated in Chapter 5).

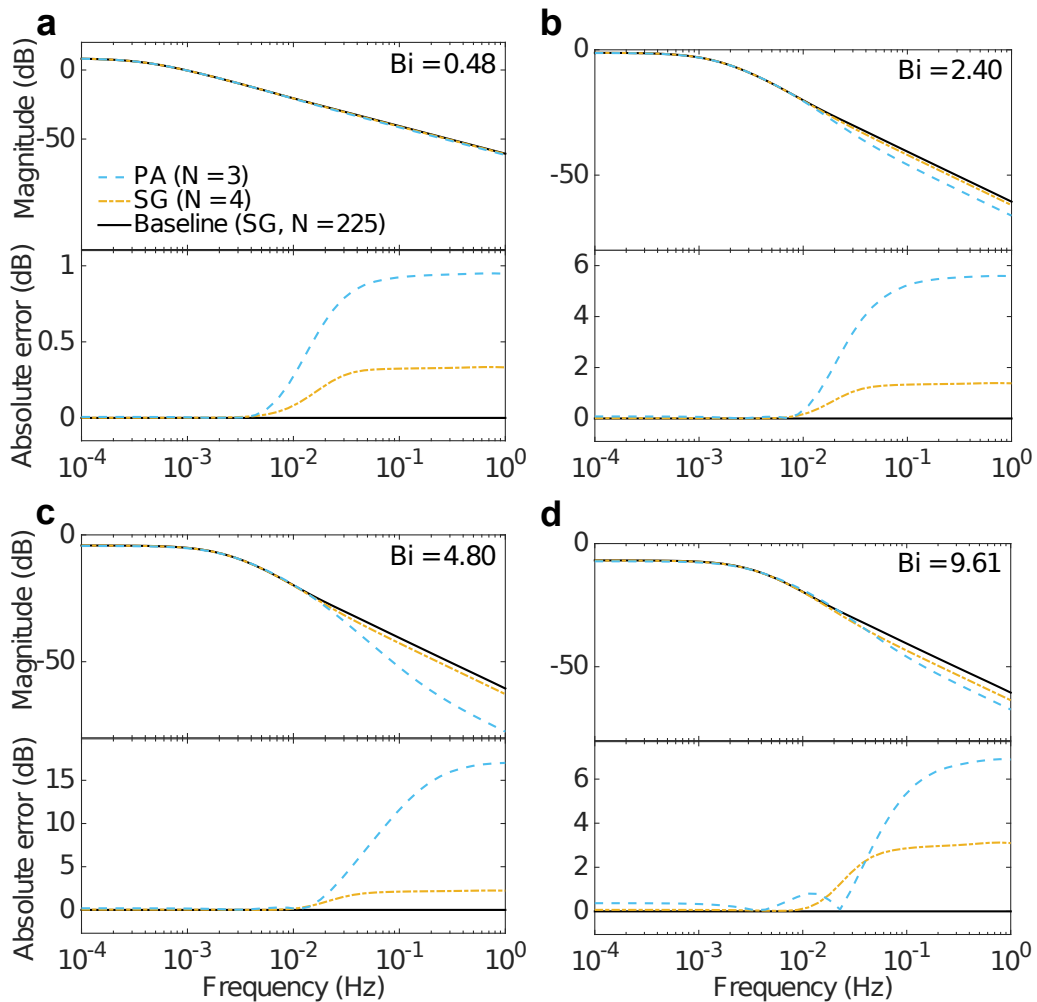


Fig. B.2 Frequency response, $T_{0,0}(s)/q(s)$, of the PA method for a range of Biot number conditions as indicated, compared with the equivalent response from a 4 state SG method. A large order ($N_s = 225$) SG method is used as the baseline solution.

Appendix C

Modelling assumptions

This appendix analyses the assumptions made in the thermal modelling and experimental measurements throughout this thesis. The first section discusses the validity of neglecting physical features in the thermal model, such as the aluminium case and tabs. The second section provides analysis supporting the assumption that the internal thermocouple gives accurate temperature measurements.

Case and tabs

It is clear that by reducing the cell thermal model to a 1-D or 2-D heat equation, several physical features are neglected, in particular the aluminium case and tabs. As discussed in Section 1.5, such simplifying assumptions are often necessary to achieve the desired computational efficiency for online modelling. We show here the calculations for the 26650 cell; the 32113 cell gives similar results, since the material properties and the ratios of the materials are similar.

Case

The following points support the assumption that the impact of the case on the thermal behaviour of the cell is minor:

- (i) The thermal capacitance of the case is:

$$\begin{aligned} C_{p, \text{case}} &= \rho c_p V = \rho c_p (2\pi r L + \pi r^2) t_c \\ &= (2700)(0.91)(2\pi \times 0.026 \times 0.065 + \pi \times 0.026^2)(1 \times 10^{-3}) \quad (\text{C.1}) \\ &= 0.013 \text{ J kg}^{-1} \text{ K}^{-1}, \end{aligned}$$

which is small relative to that of the overall cell ($C_{p, \text{cell}} = 84.6 \text{ Jkg}^{-1}\text{K}^{-1}$). Hence, the ratio: $(C_{p, \text{case}} : C_{p, \text{cell}}) \sim 1.5 \times 10^{-4}$.

- (ii) The radial thermal resistance through the case wall is

$$R_{\text{case}} = t_c(2\pi r_{\text{out}}L) = (1 \times 10^{-3})(2\pi \times 0.026 \times 0.065) = 1.3 \times 10^{-5} \text{ KW}^{-1}, \quad (\text{C.2})$$

which is small relative to the radial thermal conductivity through the cell

$$R_{\text{cell}} = \ln(r_{\text{out}}/r_{\text{in}})/(2\pi Lk) = \ln(0.026/0.001)/(2\pi \times 0.065 \times 0.4) = 15.7 \text{ KW}^{-1}. \quad (\text{C.3})$$

Hence the ratio, $(R_{\text{case}} : R_{\text{cell}}) \sim 1 \times 10^{-6}$.

- (iii) The axial thermal conductivity along the wall of the case ($k = 237 \text{ KW}^{-1}$) is of a similar order to the axial thermal conductivity of the cell jelly roll ($k = 70 \text{ KW}^{-1}$), and, since the case is quite thin ($\sim 1\text{mm}$) it could be treated as simply an extra layer in the jelly roll structure, (with appropriately modified values of the homogenised thermal properties).

Of course, the above three pieces of information are not sufficient to guarantee that the effect of the case is negligible and hence there remains the possibility that some non-negligible effects still exist, as we discuss below.

Tabs

The following points support the assumption that the tabs (which consist of thin strips of copper fixed to the ends of the cell) have minimal impact on cell thermal dynamics:

- (i) The thermal capacitance of each tab is

$$\begin{aligned} C_{p, \text{tabs}} &= \rho c_p V \\ &= (8.8 \times 10^{-3}) \times (0.39) \times (0.01 \times 0.001 \times 0.05) \\ &= 1.7 \times 10^{-3} \text{ Jkg}^{-1}\text{K}^{-1} \end{aligned} \quad (\text{C.4})$$

which is small relative to that of the overall cell, hence the ratio, $(C_{p, \text{tabs}} : C_{p, \text{cell}}) \sim 2 \times 10^{-5}$.

- (ii) The cross sectional area of the tabs is small ($A_{\text{tab}} = 0.01 \times 0.001$) and hence the thermal resistance along the plane of the tabs is relatively large

$$R_{\text{tabs}} = k_t L_t / A_t = 401 \times 0.05 / 1 \times 10^{-5} = 2 \times 10^6 \text{ KW}^{-1} \quad (\text{C.5})$$

which would minimise heat flux out of the cell.

Again, the above does not conclusively prove that the effect of the tabs is negligible, but merely provides evidence to support of this. In particular it is possible that the tabs conduct some additional heat away from the cell, but this would only be fully elucidated by a high fidelity simulation.

Thermocouple

Since the end of the thermocouple embedded within the cell was surrounded by a thin layer of heat shrink (to electrically isolate it from the cell current collector at the inner surface of the jelly roll), it is necessary to verify that it still provides accurate internal temperature estimates.

To achieve this, we verify that the thermal resistance between the ends of the thermocouple and the ambient chamber environment (which we denote R_{tc}) is significantly greater than the thermal resistance between the ends of the thermocouple and the internal portion of the cell with which it is in contact, i.e. through the heat shrink wall (which we denote R_{hs}). R_{tc} can be approximated using a thermal equivalent circuit where $R_{tc} = L/kA = 2.1 \times 10^4 \Omega$, where the length and cross sectional area of the thermocouple are $L = 32.5 \text{ mm}$ (circa. half the length of the cell) and $A_c = \pi(0.13)^2 \text{ mm}^2$, and the thermal conductivity is $k = 24 \text{ Wm}^{-1}\text{K}^{-1}$ (the mean of chromel and aluminel, the materials in a K-type thermocouple). Next, R_{hs} is found to be $R_{hs} = L/kA = 200 \Omega$ where the thickness of the heat shrink is $L = 0.2 \text{ mm}$, the cross-sectional area in contact with the thermocouple on one side and the cell jelly roll on the other is approximated as $A_c = 2^2 \text{ mm}^2$; and the thermal conductivity of the heat shrink material (PTFE) is $k = 0.25 \text{ Wm}^{-1}\text{K}^{-1}$. Hence the ratio ($R_{tc} : R_{hs}$) is large (~ 62), and hence there will not be a significant temperature drop between the jelly roll core and the thermocouple at that point.

Although the above analysis supports the assumptions made in the thesis, a rigorous validation would require a more involved approach (e.g. using a high fidelity finite element model of the setup). Hence, we must emphasise that it is possible that these physical features had some non-negligible effects on the thermal behaviour of the cell, but that their effects were simply captured by fitting the free parameters of the model.