**ENGR7019 Engineering Dissertation Project Final Report**

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| Graphical user interface, text  Description automatically generated  Artificially Informed Driven Physics Based Battery Model Parameterisation with Particle Swarm Optimisation (PSO) method for the LG M50 dataset | | |
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# Abstract

This thesis looks to provide the first ever Julia coded PBM optimisation toolbox utilising a PSO method and DFN model, this is a revolutionary piece of open-source software which enables a user to input measured cell data for an LGM50 and determine the physical and chemical parameters of a DFN model. At a larger scale this program can look to inform SOC and SOH prediction for the LGM50 by potentially using emulated higher fidelity terminal voltage responses and provide a better approximation of the physical and chemical parameters of a battery model than experimental techniques.

The thesis firstly outlines a 6-stage methodology including literature reviews and software exploration. Then targets the 6 most sensitive parameters and confirms by performing an OAT analysis that the thickness of cathode is the most sensitive parameter for terminal voltage behaviour for a HPPC and GITT test cycle within the virtual PBM environment of an LGM50 cell.

The thesis secondly builds and deploys an artificially informed optimisation to this virtual PBM environment and can improve the fitment of terminal voltage for a WLTP by 38% from an experimentally populated dataset for the LGM50. Which achieves a voltage RMSE of 9.7mV within 8 seconds per WLTP drive cycle and complete simulation time of ~1.5 hours.

In conclusion, the thesis provides an open-source toolbox which is unique and powerful at fitting terminal voltage for an LGM50.

**Key words:** LGM50, PSO, DFN, Julia, HPPC, GITT, WLTP, RMSE and PBM

# Highlights

* The first ever Julia coded PBM parameter AI Optimisation tool using PETLION and Metaheuristic.jl which is developed completely with open-source packages to ensure wide utilisation.
* Built a working PSO method applied to a PBM optimisation for a DFN.
* User defined electrochemical dataset and custom functions for the Chen2020 LGM50 dataset within the domain of PETLION.
* Used experimental, simulated and measured data for the LGM50 to determine the validity of the developed model.

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Secondly, I want to thank HVES, who is the research group who will look to inherit my work. HVES kindly supplied the data for the LGM50 and again supported me through the challenging modelling aspects of the thesis.

Thirdly, I want to thank the Oxford Brookes Racing team. The team supported me to succeed with my thesis and allowed me to cultivate skills in EV technology. In which I could first hand see the long-term benefit of the work of my thesis and formulate the background to the opportunity.

Finally, I wish to thank my close family, in which they showed their unwavering support in the challenging moments of this thesis.

Table of Contents

[1 Abstract 3](#_Toc114513374)

[2 Highlights 4](#_Toc114513375)

[3 Acknowledgments 4](#_Toc114513376)

[4 List of Figures 7](#_Toc114513377)

[5 List of Symbols and Abbreviations 9](#_Toc114513378)

[6 Introduction and Background 10](#_Toc114513379)

[6.1 Projects aim and objectives 11](#_Toc114513380)

[6.2 Originality and Contributions 11](#_Toc114513381)

[7 Literature review 12](#_Toc114513382)

[7.1 ECM compared to P2D 12](#_Toc114513383)

[7.2 Sensitivity Analysis 13](#_Toc114513384)

[7.3 Data-driven Optimisation 14](#_Toc114513385)

[7.4 PSO Optimisation 16](#_Toc114513386)

[8 Methodology 17](#_Toc114513387)

[8.1 Objective 1 18](#_Toc114513388)

[8.2 Objective 2 18](#_Toc114513389)

[8.3 Objective 3 2](#_Toc114513390)

[8.3.1 PyBaMM 2](#_Toc114513391)

[8.3.2 PETLION 3](#_Toc114513392)

[8.4 Objective 4 3](#_Toc114513393)

[8.4.1 Pyswarm 3](#_Toc114513394)

[8.4.2 Optim.jl 3](#_Toc114513395)

[8.4.3 Metaheuristics.jl 3](#_Toc114513396)

[8.4.4 Top Level PSO model 4](#_Toc114513397)

[8.5 Objective 5 5](#_Toc114513398)

[8.6 Objective 6 5](#_Toc114513399)

[9 Results and Discussion 6](#_Toc114513400)

[9.1 Temperature sensitivity to Terminal Voltage 6](#_Toc114513401)

[9.2 Further sensitivity analysis 8](#_Toc114513402)

[9.3 AI Optimisation 12](#_Toc114513403)

[10 Conclusions 16](#_Toc114513404)

[11 References 18](#_Toc114513405)

[A.1 Detailed background 22](#_Toc114513406)

[A.2 Detailed literature review 23](#_Toc114513407)

[A.3 Methodology 30](#_Toc114513408)

[A.4 Alternative approaches 37](#_Toc114513409)

[A.5 Project limitations 38](#_Toc114513410)

[A.6 Results and discussion 39](#_Toc114513411)

[A.7 References 45](#_Toc114513412)

# List of Figures

[*Figure 1: The commonly used battery electrical equivalent circuit model* (Zhang, Xia, Li, Cao, *et al.*, 2018) 13](#_Toc114583721)

[*Figure 2: P2D Porous-Electrode model* (Plett, 2015) 13](#_Toc114583722)

[*Figure 3: Schematic of experiment-based parameter identification (Li* et al.*, 2022)* 15](#_Toc114583723)

[*Figure 4: Schematic of the multi-objective multi-step data-driven identification process (Li* et al.*, 2022)* 15](#_Toc114583724)

[Figure 5: Error distributions of the invasive experimental and data-driven parameter 16](#_Toc114583725)

[Figure 6: PSO against CSA for simulation iterations and RMSE voltage error (Li et al., 2022) 17](#_Toc114583726)

[Figure 7: Overall Project Methodology 18](#_Toc114583727)

[Figure 8: Chen2020 dataset simulating a 2C discharge comparing SPM, SPMe and DFN (Planella et al., 2022) 21](#_Toc114583728)

[Figure 9: Benchmarking of PETLION, LIONSIMBA and PyBaMM (Berliner et al., 2021) 21](#_Toc114583729)

[Figure 10: Authors PSO Top level method 23](#_Toc114583730)

[Figure 11: Overriding methodology for entire model 24](#_Toc114583731)

[Figure 12: Average Sensitivity in Temperature for GITT (a) and HPPC (b) for LCO dataset 25](#_Toc114583732)

[Figure 13: GITT (blue) and HPPC (green) RMSE voltage for temperature OAT with the orange line denoting benchmark temperature of 25°C for LCO 26](#_Toc114583733)

[Figure 14: GITT comparison of real-world LGM50 data against PETLION simulated voltage and C-rate 27](#_Toc114583734)

[Figure 15: RMSE in Terminal voltage for lp (a), ɛp (b), ln (c), kn (d), cmax,p (e) and ɛn (f) for GITT, where the Orange line denotes the focus point of the LGM50 dataset 28](#_Toc114583735)

[Figure 16: Ranking of Parameter Sensitivity for the LGM50 dataset within PETLION 30](#_Toc114583736)

[Figure 17: Global particles swarm with the fitness of the RMSE voltage at initialisation (a) and at 10th generation (b) 31](#_Toc114583737)

[Figure 18: WLTP response driven by PSO optimization 34](#_Toc114583738)

[*Figure 19: ECM against a PBM from MPC analysis (G. Florentino and M. S Trimboli, 2018)* 42](#_Toc114583739)

[Figure 20: DFN equations summarised (Li et al., 2022) 45](#_Toc114583740)

[Figure 21: Visual Comparison of different sensitivity analysis weighting magnitude of sensitivity (Andersson et al., 2022) 46](#_Toc114583741)

[Figure 22: Classification of a subset of optimization methods that has been used for PBM (Andersson et al., 2022) 47](#_Toc114583742)

[Figure 23: Process for OAT sensitivity analysis 49](#_Toc114583743)

[Figure 24: HPPC comparison of real-world LGM50 data against PETLION simulated voltage and C-rate 58](#_Toc114583744)

[Figure 25: WLTP comparison of real-world LGM50 data against PETLION simulated voltage and C-rate 58](#_Toc114583745)

[Figure 26: Time series sampled comparison for GITT, PETLION is original and Measured data is down sampled 60](#_Toc114583746)

[Figure 27: Example of Terminal Voltage changing with OAT Ln 62](#_Toc114583747)

**List of Tables**

[Table 1: Correlation and RMSE of Drive cycles from PETLION to Measured Data for LGM50 27](#_Toc114583759)

[Table 2: PSO results for PETLION Virtual Validation for GITT 32](#_Toc114583760)

[Table 3: PETLION PSO results for measure data WLTP 33](#_Toc114583761)

[Table 4: Comparison of 2D PBM methods 44](#_Toc114583762)

[Table 5: Accessed Software tools summary 50](#_Toc114583763)

[Table 6: Proposed boundary conditions for PETLION OAT for 6 strongest parameters 52](#_Toc114583764)

[Table 7: Chen2020 parameters required for PETLION DFN 54](#_Toc114583765)

[Table 8: PSO values for weighting 55](#_Toc114583766)

[Table 9: Alternatives approaches for project objectives 56](#_Toc114583767)

[Table 10: Overall Project Limitations 57](#_Toc114583768)

[Table 11: PETLION PSO results for measure data ‘GITT’ and WLTP 63](#_Toc114583769)

**List of Tables of Appendix**

# List of Symbols and Abbreviations

|  |  |
| --- | --- |
| SOC | State Of Charge |
| SOH | State Of Health |
| LCO | Lithium Cobalt Oxide |
| C-rate | Ratio of Current related to Cell Capacity |
| CC-CV | Constant Current – Constant Voltage |
| PSO | Particle Swarm Optimisation |
| LM | Levenberg-Marquardt |
| DAE’s | Differential-Algebraic System of Equations |
| BMS | Battery Management Systems |
| PBM | Physical Based Battery Model |
| HPPC | Hybrid Pulse Power Characterization |
| GITT | Galvanostatic Intermittent Titration Technique |
| WLTP | Worldwide Harmonised Light Vehicle Test Procedure |
| DOD | Depth Of Discharge |
| P2D | Pseudo-two-dimensional |
| MIL | Model In Loop |
| OCV | Open Circuit Voltage |
| PDE | Partial Differential Equations |
| SEI | Solid Electrolyte Interphase |
| BJDST | Beijing Dynamic Stress Test |
| DST | Dynamic Stress Test |
| OCP | Open Circuit Potential |
|  |  |
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# Introduction and Background

Rechargeable batteries are everywhere and can be scaled in different sizes for different applications, in instance at the Wh level they are used in mobile phones, kWh level they are in Electric Vehicles (EV) and MWh level they are used for off grid energy storage. Currently, Lithium-ion batteries are the dominant chemistry available on the market due to their high power and energy densities, but there is ongoing research to find more cost effective solutions to be more consumer focused and ensure better affordability for battery powered items (Mehta, 2022).

In order to improve this the modelling of batteries is critical, as this enables a system to be better understood and optimised without the dependency of constant experiments, so multiple hypotheses can be tested and validated faster and with less capital expenditure. These modelling approaches can be applied in varying levels from just at the individual cell to discover new chemistries or to improve functional safety of a BMS by understanding the true SOC and SOH limits of large battery packs (Synopsys, 2022).

Primarily, this thesis will investigate the modelling methods at the individual cell level in the physical and chemical domain and look to build a system which can optimise and find these parameters from a well understood academic dataset called Chen2020 which is from the LG M50 (Chen *et al.*, 2020). PBM’s are vastly complex and require high computational effort to analyse the complex interactions, so the dependency on data-driven Artificial Intelligence (AI) is critical to correlate fitment of new result against a known baseline quickly and efficiently.

This form of research is completely new field, so any step which requires less computational effort or time to get high fitting results is highly advantageous to the industry.

## Projects aim and objectives

The main aim of the project is to develop an AI model that will optimise the 6 highest sensitivity physical based parameters for battery cells with a PSO method, this is achieved by focusing on what constitutes these 6 of the 26 parameters that drive cell characteristics for terminal voltage. This will be performed with the Chen2020 dataset to enable further benchmarking of the virtual cell testing to real data provided by HVES. The following are the SMART objectives to achieve the main aim:

1. Identify the primary use cases and limitations for ECM and P2D modelling.
2. Review the different sensitivity analysis parameters objectified in previous research.
3. Access different open-source PBM programmes and discuss the limitations and ease of use of each package.
4. Review the different AI and statistical based approaches for PBM, to decide what method would be suitable for the authors level of proficiency.
5. Determine which physical based parameters should be parameterised to obtain motorsport focused performance or automotive focused performance.
6. Perform AI based modelling to understand the correlation and validate the physical cell’s measurements to simulated behaviours.

## Originality and Contributions

The project aims to deliver an AI method for PBM parameter optimisation for a DFN or SPM. The author will use completely open-source tools to achieve this, to ensure that no barrier to entry is in place if other researchers wish to use the method developed for the AI PBM parameter optimisation.

The choice of PETLION is to further demonstrate originality and ingenuity, while the framework of this package is clean to use, some features are yet to be full developed compared to other more developed packages. Therefore, the author can demonstrate three key features and links that PETLION could inherit:

* Addition of more formalised drive cycle and test cycles
* Addition of Chen2020 dataset for LGM50
* Cross compatibility between PETLION and Optim.jl to integrate methods for AI and/or Statistical analysis

# **Literature review**

The following literature review will pivot of four key concepts which help to conceptualise the paper.

## ECM compared to P2D

An ECM as explained in the background uses Resistor and Capacitor (RC) networks to determine the electrical behaviour, this is done by lumping RC’s together and corresponding RC values to obtain the OCV and SOC performance for a given cell’s chemistry. In Zhang et al work it captures and discusses a few different lumped RC models of increasing order (Zhang, Xia, Li, Cao, *et al.*, 2018), pictured in *Figure 1*.

Diagram, schematic

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*Figure 1: The commonly used battery electrical equivalent circuit model* (Zhang, Xia, Li, Cao, *et al.*, 2018)

The Pseudo Two-Dimensional (P2D) Porous-Electrode model is one type of electrochemical model, which Plett covers in more depth (Plett, 2015). The fundamental of this model is that the porous material on both electrodes, is simplified to be a perfect circle in the 2D domain (*Figure 2*), the model then has multiple systems of PDE’s that govern the behaviours such as the concentration gradients at temperature, to the mechanics of how electrons flow through the separator.

Chart

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*Figure 2: P2D Porous-Electrode model* (Plett, 2015)

The systems of equations drive upwards of 26 different parameters, which are all defined in A. M. Bizeray et al’s work (A. M. Bizeray *et al.*, 2019).This is incredibly advantageous as it gives much more control to idealise the behaviour of the cell in comparison to ECM models RC values.

In conclusion, the author has shown the fundamentals and concepts of an ECM and P2D model, and the overall positives and negatives of deploying the models. The author is looking to build on how PBM are implemented but wants to emphasize the goal of the paper comes from further optimisations of the 26 parameters for PBM, as the next section (7.2) will show the challenges of measuring and validating these such parameters while A 2.1 of the appendix shows the performance advantages and a deeper dive into other cell models (A 2.2).

## Sensitivity Analysis

The importance of understanding how the 26 different parameters of a PBM perform is critical. This is done by performing a sensitivity analysis, which use sweeps of changing values for a single parameter One-At-a-Time (OAT) and measures the how the output changes from a fixed position. The 26 parameters are grouped into 4 sub categories in Li et al’s paper (Li *et al.*, 2020):

* Geometric parameters – 11 parameters
* Transport parameters – 9 parameters
* Kinetic parameters – 3 parameters
* Concentration parameters – 3 parameters

These parameters have applied boundary conditions which then are OAT calculated, the larger majority of papers have chosen to present how terminal voltage is affected. Terminal voltage is primarily chosen as this is much easier to validate to real world data sets, however Li et al’s paper does show how alternative outputs can be effected (Li *et al.*, 2020).

The highly sensitive parameters are capacity related parameters which belong primarily in the Geometric and Transport subgroups. However, the challenge becomes being able to obtain the relevant data accurately and physically for the parameters.

As shown in Figure 3, it shows a few of the methods required to obtain the parameters values for a given cell chemistry.

Diagram

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*Figure 3: Schematic of experiment-based parameter identification (Li* et al.*, 2022)*

These methods require disassembly of the cell and expensive testing equipment to obtain individual and targeted values for the PBM, which even with just a single measured data point it does not depict the full model.

In conclusion, the author has shown the purpose of sensitivity analysis, outlined what is objectified in the analysis and some of the challenges of obtaining the data. In the next section (7.3) it will show the data-driven approach to populating the parameters and contained in A 2.3 of the appendix it outlines what methods have been used from literature and which are the most sensitive parameter determined by multiple authors.

## Data-driven Optimisation

The need for data driven optimisations is critical, by looking to group parameter sets and validate the PBM. Li et al’s further work (Li *et al.*, 2022) shows this in Figure 4.

Timeline

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*Figure 4: Schematic of the multi-objective multi-step data-driven identification process (Li* et al.*, 2022)*

By integrating machine learning techniques in a multi-stage process, it enables to populate close fitting values for a respective chemistry. The primary strategy W. Li et al’s work deploys is the Cuckoo Search Algorithm (CSA) which was developed by Yang et al (X. -S. Yang and Suash Deb, 2009). The CSA is generational based algorithm which iteratively finds the optimal solution by replacing the worst solution in each new generation, the user defines the maximum number of iterations to avoid a never-ending loop.

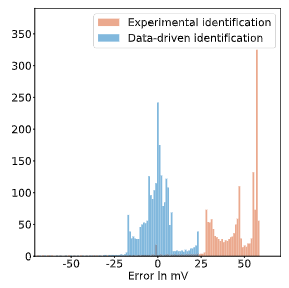


Figure : Error distributions of the invasive experimental and data-driven parameter

identification results under 2C discharge (Li et al., 2022)

Figure 5 demonstrates clearly the performance advantage of how the CSA algorithm outperforms the experimentally populated values for a 2C discharge experiment for the Voltage RMSE being reduced.

In conclusion, the author has shown one of the current approaches to populating the 26 different parameters with data-driven techniques. In the final section (0), the author will look at another alternative AI approach and state why the strategy is at the focus of this project.

## PSO Optimisation

The final aspect of the literature review is looking at the Particle Swarm Optimization (PSO) an artificial generative model developed by Kennedy and Eberhart in 1995 that simulates the thinking pattern of a swarm of animals to determine the global minimum for an objective function (J. Kennedy and R. Eberhart, 1995).

It is strongly debated what algorithms persists as AI-focused, the author views a PSO as an AI method as it based upon using artificial life to come to the decision of a global minimised result while tying an evolutionary element where generations feedback prior learning to inform the global best result, with no ability to iteratively intervene upon the solution. An interesting observation from Li et al’s work shows the difference of performance for a PSO to the CSA method described in section 7.3, this is captured in Figure 6.

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Figure : PSO against CSA for simulation iterations and RMSE voltage error (Li et al., 2022)

While convergence is faster in the quantity of simulation steps and the fitness is RMSE is reduced further than 200 iterations for a CSA, Li et al mentions that computational requirements and time are far greater compared to a PSO which is the primary benefit the author wishes to exploit with a PSO method.

In conclusion, the author has described the fundamental mechanics of the PSO and outlined the opportunity of developing this approach into a PBM and contained in the appendices (A 2.4) it elaborates further on the different optimisation techniques applied to different PBM’s and performance.

# Methodology

The overall project methodology is presented in Figure 7, where it is 6 stage process highlight where the objectives overlap in different colours. Boxes with a light-yellow shade indicate literature review tasks, light blue is accessing software tools and light red is the modelling phase.

Diagram, schematic

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Figure : Overall Project Methodology

## Objective 1

Primarily this objective was an initial literature review for ECM and P2D models, how they can be deployed on BMS’s, and comparing the performance advantages of P2D model with the disadvantages of hardware integration, which is broadly covered in the initial literature review (7.1).

In addition, this objective intended to look at what cell’s performance characteristics are desired for both motorsport and automotive applications, in which the research into cell tab plating, concentration of electrolyte and electrode material will be discussed further in the appendices (0).

## Objective 2

This objective is literature oriented, where different sensitivity analyses are reviewed. In the expectation, that the physical and chemical variables can be understood and used for Objective 5, to give what variables should be optimised for a motorsport or automotive application. Some of which is captured in the literature review before (7.2) but does not explain the limitations and assumptions needed to conduct this form of analysis.

In order for sensitivity analysis to be effective the author has to define the limits and boundaries in where sensitivity is measured, so this requires the assumption from prior experimental papers on where the boundaries must be placed (A.1 - Table 6). The author references boundaries outlined in Li et al’s work for any of the selected parameters for OAT, as this paper extensively covers this and is the inspiration for the method the author uses (Li *et al.*, 2020).

The prime limitation of this method is doing one steady state case to indicate overall sensitivity is not sufficient, the need for different dynamic cases is needed to show how strong capacity driven parameters are with changing C-rates and DOD. The author is focusing on standardised test profiles to be emulated which are within the appendices more details of the drive cycle are given (A.1).

The method in how sensitivity is measured will be done in two ways, the first being primitive to purely see whether the simulation is working by looking at the average percentage change in the terminal voltage from a known baseline. The known baseline is computed beforehand and within the parameter sweeps a nested loop will simulate the study but with the changed parameter value (A.3 - Figure 23).

The second more powerful measurement of sensitivity is Root Mean Square Error (RMSE) (1), which considers deviation from the baseline terminal voltage (Vbaseline) to simulated terminal voltage (Vsim) with parameter change within a known sample size of data points (n).

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These two methods are later applied to Objective 6 and 3 to measure how terminal voltage is affected by temperature within a pure PBM simulation and the start of the framework to developing a cost function for the AI model to optimise as an output for the overriding model. In A 3.1 it outlines potential further limitations with using the Chen2020 data set for projecting terminal voltage change with temperature change and boundary conditions required for the OAT.

## Objective 3

This objective is both be literature oriented and software focused, where the author has accessed large databases and open-source packages, understood the benefits and withdrawals of operating in the software package/database. Summarising in A.3 - Table 5 is what the author looked at initially and what the trade-offs are. Out of this process of researching and using these packages, two key packages were the strongest for PBM, which the author shows the features and how the software can be used to determine sensitivity with terminal voltage.

### PyBaMM

PyBaMM is a powerful tool which has the SPM, SPMe and DFN modelling capabilities and easy to navigate features which display graphics with little effort for the author (Figure 8).

A picture containing text, building, window

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Figure : Chen2020 dataset simulating a 2C discharge comparing SPM, SPMe and DFN (Planella et al., 2022)

Therefore, the author wants to incorporate these features to PETLION as outlined in A.3 - Table 5 it solves close to 22 times faster than PyBaMM, which is hugely advantageous when it comes to AI optimisations (Figure 9).

Table

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Figure : Benchmarking of PETLION, LIONSIMBA and PyBaMM (Berliner et al., 2021)

### PETLION

PETLION is Julia Package which can simulate a cells behaviour using a DFN model. However, due to PETLIONS fast solving speed, the author needs to be conscious of the errors that could occur when sweeping small step sizes which could be a potential limitation. In the Appendices it shows how the Chen2020 dataset can be populated into PETLION (0)

## Objective 4

This objective was literature based, where different previous research for AI and statistical based models for P2D optimisations was analysed within the initial literature review (7.3) and further details within the appendices of how these models function (A 2.2) and boundary conditions (0).

The method the author is looking create in software uses a singular objective process for optimisation, in where it performs a global search using a PSO method. Like Objective 3 the author researched and used packages with different software environments, that could provide the foundation for the author to develop the desired method. The packages mentioned were found which could have potential to do this but state their limitations.

### Pyswarm

Pyswarm is a PSO gradient free method which uses Python (Pyswarm, 2022), this has been widely used and very stable to use. However, due to choosing PETLION as the main PBM package using Pyswarm via Julia would not be efficient as it would need to be rebuilt via another environment.

### Optim.jl

Optim.jl is an Univariate and multivariate optimization tool available on Julia which includes the gradient free PSO method (Mogensen and Riseth, 2018). This performs very similarly to Pyswarm but has less examples of the package being used, so a limitation of using the package is debugging may take longer.

### Metaheuristics.jl

Metaheuristics.jl is a global focused optimisation tool available on Julia which includes singular objective functions, multi objective focused models or many objective focused models (Mejía *et al.*, 2022). It includes a PSO method which can be used if Optim.jl is not successful as further contingency.

### Top Level PSO model

Presented in Figure 10 it shows the backend of the software process with the chosen packages, which looks to build upon what Rahman et al methodology was for a PSO method (Rahman, Anwar and Izadian, 2016).

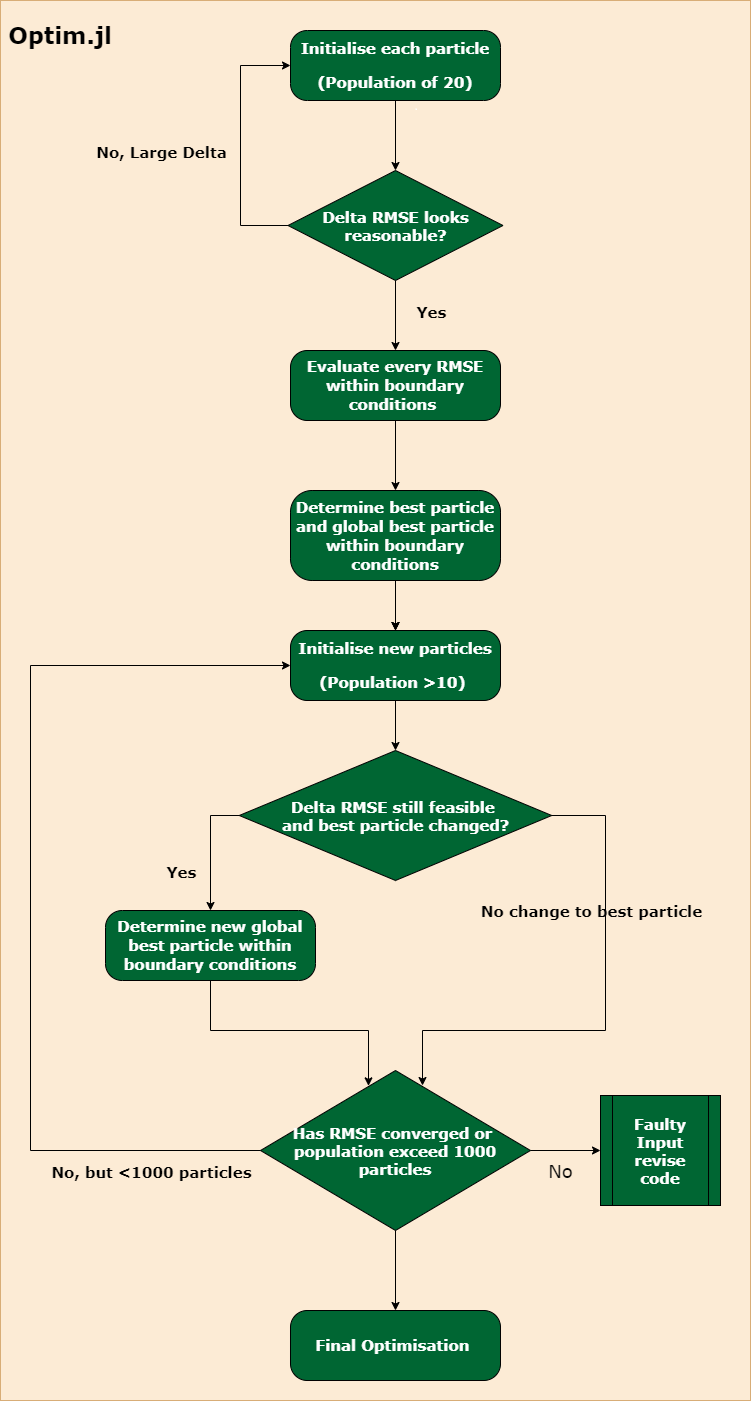


Figure : Authors PSO Top level method

## Objective 5

This objective is software based, where the initial groundwork for the model begins. As the author is looking to replicating previous sensitivity analysis for conditions of Chen2020. This work on the methodology for the inputs and extensive data required for the DAE’s to compliment the Chen2020 dataset are contained with the appendices (0).

At the conceptualisation of the project the author was torn on what narrative the model should look to answer from the initial literature reviews, hence the decision block in the overall project methodology (Figure 7). The Author has decided to focus on the automotive approach, which looks to find close fitment to terminal voltage as there is much more literature to help support the observations the author may see. As using a current or capacity related outputs as a way to see variation would require a huge number of assumptions that very little literature/journal could look to support.

## Objective 6

The last objective is software driven. This will use the work from Objective 5 and combine it to the code for the AI based optimisation tool, furthermore this will utilise real life data generated from a full life characterisation of a LG M50 cell, to help develop the model and train the AI to yield closer fitting simulations for cell behaviour. At this stage, if the model is unsuccessful the author can formatively review the short comings of the model and approach.

The overriding methodology for how the model will be developed integrating what has been researched and built from the previous objectives (Figure 11).

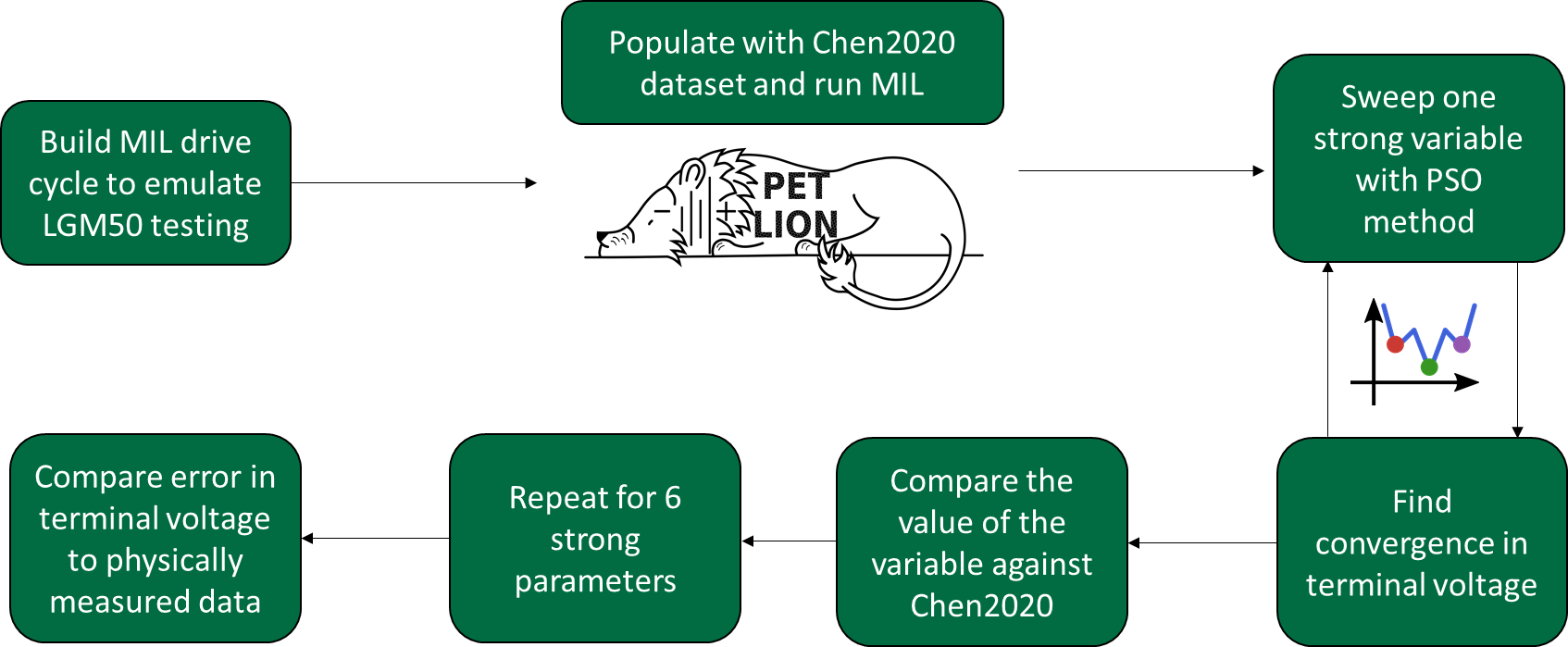


Figure : Overriding methodology for entire model

# Results and Discussion

The results and discussion are separated into three sections. Section 9.1 looks to apply the methodology conceptualised in Objective 2 to demonstrate the PBM features of PETLION with temperature dependencies. While, Section 0 looks to go further by showing more parameters and how the package being developed in made more robust, using the methodology contained in Objective 3 and Objective 5. Finally, section 9.3 looks to show how the PBM model has been integrated into methodology of Objective 5 to show the final product determined by Objective 6.

## Temperature sensitivity to Terminal Voltage

The author initially used the LCO dataset pre-built in PETLION to start the building the code around the framework shown in Figure 23. The Author achieved this by making two functions which worked together in the main executable script, the first being the OAT function which takes an input for the desired case and inputs the boundary conditions for the nested loop. The second being the drive cycle and data plausibility checker of the nested loop, which would eliminate unreasonable results which could exceed the performance boundaries of the cell and skew how sensitivity that parameter truly is.

Running the simulation for the temperature dependency within the LCO identified some important features to understand in the OAT approach within PETLION for advanced drive cycles (Figure 12).

|  |  |
| --- | --- |
| (a) | (b)Chart, line chart  Description automatically generated |

Figure : Average Sensitivity in Temperature for GITT (a) and HPPC (b) for LCO dataset

Figure 12a shows a large change at 323.15K (+55°C), this is due to exceeding the temperature boundaries configured for the LCO of 55°C, so at any further temperature points it outputs the same terminal voltage profile, but importantly it shows at 25°C that the average variation in terminal voltage is minimised to the original baseline simulation which is at 25°C.

Building the RMSE function (1) within Julia required some additional thought, as the main for loop uses Float64 values as the control iterator for OAT, however to calculate RMSE it needs to be sufficiently indexed to perform taking the sum of the delta voltage of the array with an integer (int) value, so the addition of a while loop was used to help reduce constraining the main for loop and allow a logical statement of the RMSE index value exceeding its last index value to end the operation. Looking at the response of RMSE voltage to temperature it does correlate to the behaviours you would see from thermal data (Figure 13).

|  |
| --- |
| (a) |

Figure : GITT (blue) and HPPC (green) RMSE voltage for temperature OAT with the orange line denoting benchmark temperature of 25°C for LCO

As ambient temperature decrease significantly it decreases the terminal voltage, this is more noticeable as SOC decreases. Therefore, error increases from the baseline simulation so it determines a higher RMSE value at low temperatures. The adverse happens at higher temperatures, terminal voltage looks to be increased marginally thus the error increases positively due to RMSE taking an absolute value (Figure 13a).

This is overall well supported by Zhang et al which has published the OCV and SOC curve with temperature for an Nickel Manganese Cobalt Oxide cell (Zhang, Xia, Li, Lai, *et al.*, 2018) and the general observations in terminal voltage with time on a 18650 Li-ion Cell by Wang (Wang, 2017).

## Further sensitivity analysis

The author built the Chen2020 dataset within the PETLION backend by utilising the dataset in 0 - Table 7 with focus on equations (5) to (9) to drive the OCV curves of the Chen2020 dataset. In Figure 14 it shows how well the terminal voltage profile of the true measured data compares the PETLION simulated result for a GITT cycle, the C-rate is well matched for both magnitude and when the pulses and rests occur.

|  |  |
| --- | --- |
| Chart  Description automatically generated | Chart, bar chart  Description automatically generated |

Figure : GITT comparison of real-world LGM50 data against PETLION simulated voltage and C-rate

The difficulty then becomes looking to match the data lengths and draw a correlation between the simulated response to the measured response to enable the use of RMSE (1). As in the measured data for the LG M50 the array lengths are upwards of 40,000 data points, while the array length that PETLION outputs is approximately 20 times smaller at ~2,000 data points, so filtering by time must be applied to truly understand the correlation between the physical and simulated responses (Table 1).

Table : Correlation and RMSE of Drive cycles from PETLION to Measured Data for LGM50

|  |  |  |
| --- | --- | --- |
| **Drive Cycle** | **Correlation in Terminal Voltage (R)** | **RMSE (mV)** |
| GITT | 0.995 | 55.8 |
| HPPC | 0.981 | 66.4 |
| WLTP | 0.989 | 16.5 |

In the appendices (A 6.1) it provides more graphics for HPPC (A 6.1 - Figure 24) and WLTP (A 6.1 - Figure 25), outlines the issue of indexing by timeseries in greater detail and potentially what the author could have done differently.

The Chen2020 dataset was OAT swept using a nested loop for the strongest parameters identified in A.3 - The boundary conditions Li et al’s identified were then implemented to the authors chosen 6 strong parameters for the OAT (Table 6)

Table 6, where the GITT RMSE results are contained in Figure 15.

|  |  |
| --- | --- |
| (a) | (b) |
| (c) | (d) |
| (e) | (f) |

Figure : RMSE in Terminal voltage for lp (a), ɛp (b), ln (c), kn (d), cmax,p (e) and ɛn (f) for GITT, where the Orange line denotes the focus point of the LGM50 dataset

Primarily observing and understanding a relationship of how the parameters measure against RMSE terminal voltage is excellent to see, but not critical. The critical element is to see that the simulation verifies the pre-allocated values (orange line) by observing the minimised RMSE in terminal voltage from a baseline simulation, this gives confidence to the author whatever optimisation tool is used on top of the environment built in PETLION that the objective function of RMSE can be minimised when looking in the determined boundaries.

The problem then becomes when looking at Figure 15a the solution to have a global minimised RMSE occurs at more than one location within the boundary condition set for that parameter, so the AI optimisation tool will need to detect the best global minimum from the one another and ensure that the authors boundary conditions are able to potentially isolate this.

Additionally seen in a large majority of Figure 15f there are regions with no points, this is primarily due to the simulation outputting a terminal voltage result which exceeds the realistic boundaries of the LGM50, as with in the drive cycle function the use of omit NaN is used to ensure the value could not affect any downstream code such as being used as a false optimal result for the papers AI approach. But this may become difficult for the AI method if it is close to the global best result or is stuck in a region where no points can compute through PETLION.

In order to determine the most sensitive parameter the author had produce a method that could fairly represent this statistic by accounting for the amount of data points run, so presented below is a method to drive a Sensitivity Index (SI) approach for the parameters OAT (2).

|  |  |
| --- | --- |
|  | () |

The author recognises that this is potentially a crude method, however, it does highlight how dynamics of a drive cycle effect the terminal voltage error from the baseline dataset of Chen2020 which does ultimately show which parameter is the most sensitive within the regardless of the boundary conditions used.

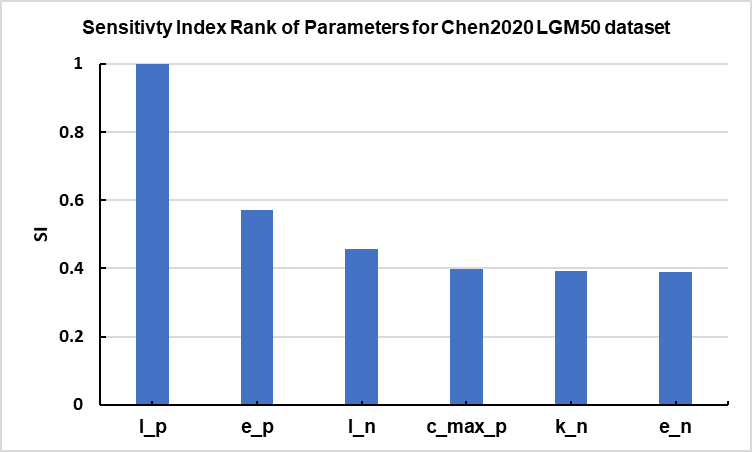


Figure : Ranking of Parameter Sensitivity for the LGM50 dataset within PETLION

The author considers the Cathode Thickness (Lp) to be the most impactful for change in RMSE voltage, this coincides well with Li et al’s paper which uses the OAT approach for a DFN (Li *et al.*, 2020) and Gao et al’s paper which uses a Monte Carlo approach for a DFN (Y. Gao *et al.*, 2021). The only parameters that are out of rank with Li et al’s paper is the Cathode Maximum Ionic Concentration (Cp,max) and Anode Reaction Rate Coefficient (Kn) which should be switched round, but critically the agreement of Lp as the most impactful parameter is there.

The Author is satisfied that the method works within PETLION and if desired this could be complete with more parameters to further gauge what impact the remaining 20 parameters would have to the PETLION model created for a LGM50.

## AI Optimisation

The author started building the PSO environment within Optim.jl, however it did not seem to compute a result, show that it was calling upon the built RMSE function nor provide any package level feedback into how to debug the issue. The attempted debugging by running manual breakpoints within Optim.jl uncovered that it did like the format of the RMSE cost function so the author reached out to the Optim.jl community to look to solve the issue, but this was not successful in find a resolution and the author did not wish to change how the RMSE would be formatted.

However, the author looked tirelessly for another package which could be more robust and pass the Voltage RMSE cost function, and found Metaheuristics.jl which a global focused optimisation tool that includes singular objective functions, or multi objective focused models (Mejía *et al.*, 2022). Fortunately, this package indeed was able to run the RMSE function, so the author could start progressing with the methodology laid out in Figure 11.

First the author focused on ensuring that the 20 particles initialised (Figure 10) could find the global best result generationally, Lp was selected initially as this is the most sensitive parameter that was addressed in Section 9.2. This was achieved by using a PETLION generated baseline of the GITT drive cycle loaded with the Chen2020 parameters to optimise (Vbaseline), while the PSO is taking Lp without an initial guess close (assigned as a random value) to Chen2020’s value but constrained within the parameter boundaries outlined in A 3.1-Table 6.

|  |  |
| --- | --- |
| (a)  C:\Users\17053998\Downloads\anim- l_p convergence.gif | (b) |

Figure : Global particles swarm with the fitness of the RMSE voltage at initialisation (a) and at 10th generation (b)

Figure 17 overall shows the progression and movement of the PSO, this is clearly evident at the 10th generation (Figure 17b) where the particle swarm is much closer to the global best (Orange point) compared to Figure 17a where the particle swarm has a large spread compared to the global best from the first initialisation. Now there is a high level of confidence that the PSO can minimise RMSE without an initial guess close to the Chen2020 dataset this was repeated for all of the remaining 5 strongest parameters.

Table : PSO results for PETLION Virtual Validation for GITT

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Parameter** | **Random Initial guess** | **RMSE best (V)** | **PSO parameter value** | **Percentage difference from Chen2020 (%)** | **Generations / Function Calls** |
| Cathode Thickness (Lp) | 9.1·10-5 | 6.68·10-10 | 7.56·10-5 | 4.7·10-7 | 272 / 5440 |
| Cathode Porosity (εp) | 0.421 | 5.26·10-10 | 0.335 | 3·10-7 | 276 / 5580 |
| Anode Thickness (Ln) | 17·10-5 | 8.52·10-5 | 8.52·10-5 | -4.7·10-7 | 269 / 5380 |
| Anode Reaction Rate Coefficient (Kn) | 3.0·10-11 | 6.18·10-10 | 5.03·10-11 | -9.2·10-6 | 245 / 4900 |
| Cathode Maximum Ionic Concentration (Cp,max) | 48741 | 4.93·10-10 | 51764 | 1.4·10-8 | 274 / 5480 |
| Anode Porosity (εn) | 0.37 | 6.08·10-10 | 0.25 | 7.2·10-7 | 272 / 5440 |

Table 2 highlights how robust this approach is due to the high fitment to the Chen2020 dataset when fed with an incorrect initial guess, while simulating purely as virtual test cycle for GITT. Each parameter was limited to 1200 seconds for it to determine the best solution so in total this took close to 2 hours for the 6 parameters. Importantly listed in Table 2 is the function calls and generations which is the number times the particles used the RMSE function to solve for fitness.

Now moving to the final stage of the AI optimisation process (Figure 11) is the ability to optimise the DFN parameter set when fed with physically measured data. As the prior step is comparing a simulation to another simulation it is expected there will be high fitment when the model is comparing against itself, so seeing from Table 1 which shows with the experimentally populated values for the Chen2020 dataset compared against true measured cell data there exists a Voltage RMSE of no less than 16.5mV so any step to decrease this RMSE will alter a parameter value.

To completely ensure this method is more versatile all 6 parameters were run together in the same objective for a WLTP drive cycle, instead of performing an individual fitness of functions on each parameter separately like before and using more dynamic data such as the WLTP. This truly presents a real case when most of critical PBM parameters for a cell are not understood, the summary results are contained in Table 3 which was limited to 3600s at an average of 8 seconds per function call.

Table : PETLION PSO results for measure data WLTP

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter** | **Random Initial guess** | **RMSE best (mV)** | **PSO parameter value** | **Percentage difference from Chen2020 (%)** |
| Cathode Thickness (Lp) | 9.1·10-5 | 9.78 | 8.05·10-5 | -6.54 |
| Cathode Porosity (εp) | 0.421 | 0.3 | 10.4 |
| Anode Thickness (Ln) | 17·10-5 | 10·10-5 | -17.4 |
| Anode Reaction Rate Coefficient (Kn) | 3.0·10-11 | 2.5·10-11 | -50.3 |
| Cathode Maximum Ionic Concentration (Cp,max) | 48741 | 52000 | -0.45 |
| Anode Porosity (εn) | 0.37 | 0.2 | 20 |

This improved the fitment of Voltage by 38% from the benchmark established from Table 1 for a WLTP with the experimentally applied. However, it is important to comment on the changes of parameter values with the largest being Kn at 50.3% (Table 3). This is due to the anode reaction rate coefficient understood from Chen2020 dataset not been correctly input into PETLION due to using a different unit. The voltage profile for the PSO generated WLTP is found in Figure 18, which highlights the better capture of dynamics when compared to A 6.1 - Figure 25.

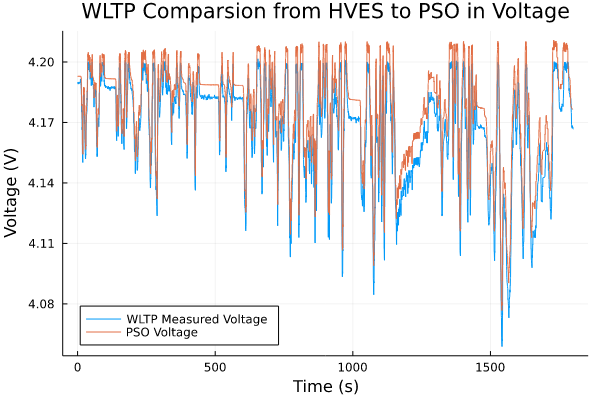


Figure : WLTP response driven by PSO optimization

To provide further validation this was repeated for a GITT drive cycle and is contained in the appendices (A 6.3) which follows the same conclusions presented for the WLTP.

# Conclusions

The author has clearly outlined and delivered upon all of the objectives contained in the whole project methodology (Figure 7) to achieve in developing an Artificial Intelligent Driven Physics Based Battery Model Parameterisation with a PSO method for the LG M50 dataset. This was achieved by extensively reviewing close to 30 papers published on topics such as PBM, AI modelling and Sensitivity analysis. With all battery focused content being within the previous 7 years and including 12 papers that have been published in 2022. This truly highlights the advanced nature of this field of research in PBM optimisation with AI methods with new literature to help inform and back up the results of this thesis.

The PETLION environment the author built achieved a high level of correlation and marginal error in terminal voltage response for multiple different drive cycles (Table 1) for the Chen2020 data set. In addition to this the OAT approach developed in tandem with PETLION clearly showed the versatility of using Voltage RMSE as an objective function (Figure 15) to determine a minimised result for all of the 6 strongest parameters indicated from literature (A 2.3). Using the ranking system developed by the author (2) to determine the sensitivity index for all 6 parameters (Figure 16) for both HPPC and GITT cases aligns well with the observations seen in the literature covered (A 2.3).

The PSO method (Figure 10) built within the PETLION environment produced excellent fitness to the singular objective function of terminal voltage when purely training with virtually generated data (Figure 17) and additionally showed how robust the approach is when the initial guess is a random starting point contained within a realistic boundary for the parameter (Table 2).

The final stage of the PSO validation methodology (Figure 11) was then applied to real measured data to verify that this model can accurately determine the parameters. This did encounter problems with the how the input of measured data is presented to the objective function, however it was able to minimise the RMSE voltage by 38% for a WLTP (Table 3) providing a better fit for terminal voltage for the LGM50 which is a huge success from the authors perspective.

Computationally this was able to perform a WLTP function call every ~8 seconds with ~300 seconds of pre-allocation for the PETLION Jacobian PBM model so in total to achieve a RMSE of 9.78mV it takes under 1.5 hours to simulate completely. Which is ~10 times faster than Li et al’s CSA approach on a system which has 26 cores, against the author which has not utilised multi-threading and achieves a better result for voltage RMSE with less data (Li *et al.*, 2022).

However, not every aspect of this thesis was successful, from the initial concept of being able to use Optim.jl it was not possible due to having software integration problems but was mitigated by changing to Metaheuristics.jl and the conditioning and matching of time series provided a higher RMSE error than expected (Table 1) so using an alternative technique such as Dynamic Time Warping could potential solve this issue and make input condition more robust (Müller, 2007).

In conclusion, the author is delighted that a completely unique PBM AI optimisation toolbox which produces high fitting terminal voltage responses for an LGM50 has been produced and will look to release this project toolbox on GitHub after the submission of the thesis.

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1. Detailed background

The use of software packages such as MATLAB and Python are popular within academia and industry, but it does not offer the fastest execution of looped commands and has financial barriers for using the advanced optimisation features of MATLAB. This is why Julia was created to enhance performance by using Just-In-Time Compilation of code which is on the level of compiling of C-code, is completely open-source and its ideal use case is for data science and machine learning (Bezanson *et al.*, 2017). Additionally, the syntax and package management are simple to navigate in comparison to Python.

The primary advantages to developing a PBM optimisation toolbox is to reduce the dependency of needing experimentally obtained values to drive a PBM, as only needing to perform the minimal test cycles which are required for battery pack development and characterisation ensures that cost and time is kept to a minimum. Pictured in Figure 3 it shows the long process of testing and obtaining parameter values at the half cell level, and this proven by reviewing the Chen2020 dataset it demonstrates that the experimental and statistical methods used to observe parameters only achieve medium levels fitment for simple discharge cases of 46mV for a C/2 experiment when applied to a DFN model (Chen *et al.*, 2020).

Which when compared to the levels of fitment for an AI-driven DFN model pictured in Figure 4 this approach can achieve close to ~10mV for test cycles such as a WLTP when only fed an OCP and electrolyte concertation equations which is a reduce amount of testing resource compared to fulfilling the stages seen in Figure 3 (Li *et al.*, 2022). This is the reason why the author wanted to focus on developing this thesis, to use the powerful tools of data science and AI optimisations.

1. Detailed literature review

This section looks to continue the literature review and provides more detail on the advantages to PBM modelling (A 2.1), what PBM methods are available (A 2.2) and AI methods have been used (A 2.4).

* 1. Advantages of PBM modelling

The overriding consensus from R. Zhang et al work, the key limitation using this approach is the time required to obtain the data to accurately depict the chemical behaviour, as the level of fitting to physical data is critical. Likewise, Y. Zheng et al agrees by looking at the Electrochemical model based approach, it out performs ECM in the SOC estimation (Zheng *et al.*, 2018). However, Y. Zheng et al does helpfully explain that the level of complexity is higher, which will make it less advantageous for lower fidelity online based solvers

This can be seen more prominently when looking at how the models are deployed onto a simulated BMS. From Trimboli’s and Florentino’s work from the University of Colorado (G. Florentino and M. S Trimboli, 2018) shows by deploying Model Predictive Control (MPC) measures to both PBM and ECM models that the performance benefit for PBM is significant (Figure 19).

Graphical user interface

Description automatically generated

*Figure 19: ECM against a PBM from MPC analysis (G. Florentino and M. S Trimboli, 2018)*

Figure 19 shows an ECM over-projecting discharge performance, which will cause faster degradation for individual cells and ECM under-projects the true performance in charging. However, this approach of MPC on PBM is not that deployable to hardware BMS’s as computational time is significant, which L. Zhang et al states in their conclusion for ECM models against PBM, that the computational time for a PBM is upwards of “9600 seconds” versus a “negligible amount of time” for ECM models (Zhang *et al.*, 2017).

* 1. More PBM methods

PBM’s come in many forms in varying levels of complexity, a journal compose by Planella et al provides an excellent insight into what model is appropriate to the use case and how the models function (Planella *et al.*, 2022). Comprised in Table 4 is an overview of an SPM, SPMe and DFN.

Table : Comparison of 2D PBM methods

|  |  |  |  |
| --- | --- | --- | --- |
| **Model** | **General Concept** | **Positives** | **Negatives** |
| SPM | The Single Particle Model (SPM), looks solely at the interaction between the positive and negative electrode, negating any electrolyte dynamics. | * Robust and simplest model of three ideas of:   + Lithium transportation   + Thermodynamic relationship of lithium concentration and electrode potential   + Overpotential required * Smallest number of parameters required (17) * Widely used and has been built on a BMS (Hwang *et al.*, 2022) | * Does not perform well in very high dynamic events * Does not capture the true effects of the electrolyte which helps inform more advanced ageing or SEI models * Does not include ohmic losses or concentration overpotentials for the electrodes or electrolyte |
| SPMe | The Single Particle Model with Electrolyte dynamics (SPMe), it performs like an SPM but with more equations for electrolyte and separator mechanisms. | * Robust and moderately simple model when compared to a DFN * Has a good fitment to a DFN when looking at terminal voltage (Figure 8) * Has potential at been built as a more advanced MPC for a BMS. | * Does not perform well in very high dynamic events * 26 parameters required to drive DAE’s, which is more than a SPM * Does not capture the spatial variations across the electrode |
| DFN (P2D) | The Doyle-Fuller-Newton (DFN) or also known as P2D, builds upon the SPMe with its electrolyte dynamics but introduces more perfectly round particles which is getting closer to the true microstructure of a cell. | * Computationally affordable when compared to running microstructure focused models * A DFN performs very well in high dynamic problems, so best utilised for drive cycle correlations to measured data * Has potential at been built as a more advanced MPC for a BMS, in comparison to a microstructure focused model | * The most complex non microstructure focused model. * 26 parameters required to drive DAE’s, which is more than a SPM * Still only considers the cell in two-dimensions, which there are other microstructure focused models which capture the behaviour in 3D (Homogenised model) |

Diving deeper into the mechanics of the DFN model it is formalised and bounded by the dimensions of the electrodes, separator and particle size. Complementing these physical boundaries of the DFN model, is 5 key aspects of the model that allow the terminal voltage to be characterised stating the PDAE’s and boundaries that drive each aspect, these equations (Figure 20) are carried and simplified from the original paper produced by Doyle, Fuller and Newman (Doyle, Fuller and Newman, 1993).

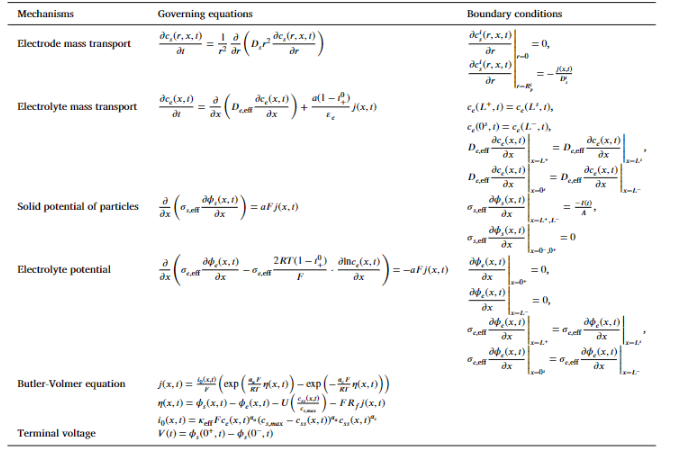


Figure : DFN equations summarised (Li et al., 2022)

* 1. Sensitivity Analysis

An extensive review by Andersson et al displays the different forms of sensitivity analysis conducted for PBM. Andersson et al selected 5 papers to visually compare how these papers concluded the most sensitivity parameters (Figure 21):

* DFN – Local – OAT (Li *et al.*, 2020)
* DFN + Thermal – Local –OAT (Liu *et al.*, 2020)
* DFN – Global – Monte Carlo + Partial Correlation (Y. Gao *et al.*, 2021)
* DFN + Thermal – Local – OAT (Vazquez-Arenas *et al.*, 2014)
* DFN – Local –OAT (Y. Bi and S. -Y. Choe, 2018)

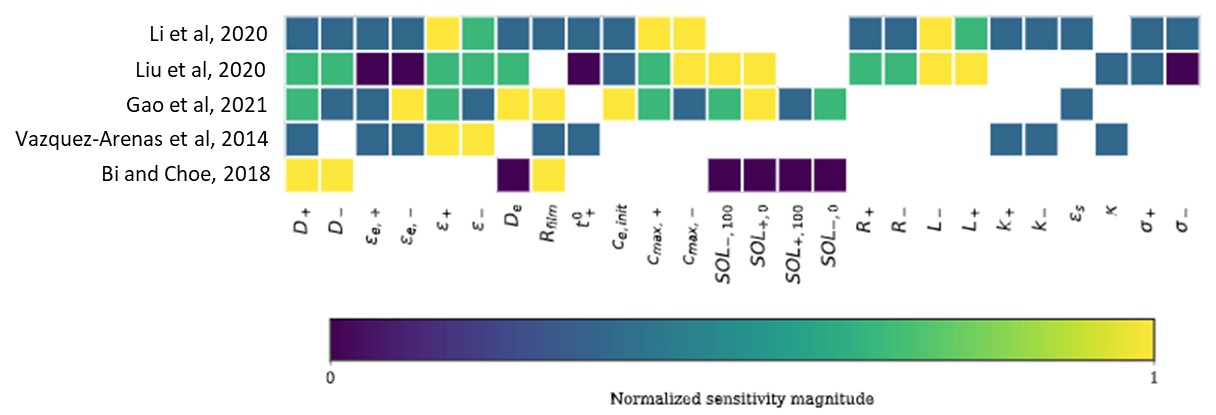


Figure : Visual Comparison of different sensitivity analysis weighting magnitude of sensitivity (Andersson et al., 2022)

It is interesting to see that the different authors weights of which parameter is the sensitivity differ from one another while performing in a similar PBM environment of the DFN, however it highlights that different target of interest and different input drive cycles can influence sensitivity to particular parameters.

While there is no definitive rank that is agreed among these authors, it highlights 6 major parameters that the author can look to perform a separate sensitivity analysis.

|  |  |  |
| --- | --- | --- |
| * Cathode Thickness (Lp) | * Anode Thickness (Ln) | * Cathode Maximum Ionic Concentration (Cp,max) |
| * Cathode Porosity (εp) | * Anode Porosity (εn) | * Anode Reaction Rate Coefficient (Kn) |

* 1. AI methods

Then Andersson et al covers extensively the AI methods that have been deployed to PBM’s and summaries how the methods give the users choice for either fast convergence, high fidelity for global optima or fewer iterations required (Figure 22).

Table

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Figure : Classification of a subset of optimization methods that has been used for PBM (Andersson et al., 2022)

The author identified 5 potential papers that interested the author to explore on how well the models performed and what differentiates them from one another:

* DFN with GA (Li *et al.*, 2022)
* SPMe with PSO (Fan, 2020)
* DFN with PSO (Rahman, Anwar and Izadian, 2016)
* ECM with PSO-LM (Shen and Li, 2017)
* SPM/DFN with LM (Santhanagopalan, Guo and White, 2007)

Li et al’s paper focused on 20 parameters in two steps using a CSA method, optimising the most sensitive 7 parameters first then optimising the remaining in a second set with the first identified parameters (Figure 4). Li et al was able to achieve an RMSE of 10mV-12.7mV which outperformed the experimental dataset of an RMSE between 31.4mV-50.1mV for a 2C discharge case and WLTP, the time taken to achieve these results was 15 hours using 26 cores which is a huge amount of computational resource and time. Li et al paper reflected that “A major step would be analysing the sensitivity of the thermal and physical parameters to voltage and temperature measurement” (Li *et al.*, 2022).

Fan’s paper focused on the 26 parameters in two steps using a PSO method, which targeted 20 parameters in the first step, then 6 parameters focusing on the activation energy. Fan’s paper was able to achieve an RMSE of 14.1-33.4mV for the US06, DST and BJDST drive cycle compared to real measured data at 45°C and 0°C. Fan concluded that the RMSE increase is due to extending the study to include more temperature, this was all achieved within 74 mins using a 40 core system (Fan, 2020).

Rahman et al’s paper focused on just 4 parameters for both the diffusivity of solid electrodes (Ds) and electrode reaction rates (K), this was achieved by deploying a PSO method. Rahman et al’s focused on objectifying the RMSE voltage for both a healthy battery cell and over-discharge battery cell with the AI method, this shows good visual correlation for terminal voltage and shows the powerfulness of using PBM to target degradation models (Rahman, Anwar and Izadian, 2016).

Shen and Li’s paper focused on 7 fitment parameters for an empirical Electrical model, using a PSO-LM method to perform a global and local search pattern to obtain an optimal fitness of terminal voltage. Shen and Li explained the difficulty of building the Jacobian matrix even for 7 parameters so this deterred the author from following this method. Regardless, Shen and Li was able to get good fitment to a 3C charge but did not publish any data regarding RMSE values (Shen and Li, 2017).

Santhanagopalan et al’s paper focused on 5 parameters of a hybrid SPM and DFN model, using a LM method to locally search the optimal fitness for terminal voltage performance. Again the paper explains the difficulty of building the Jacobian matrix to drive the optimisation for terminal voltage and only present the graphical fitment rather than publishing the RMSE voltage, again this further deters the author from embarking into the LM method due to the shear complexity (Santhanagopalan, Guo and White, 2007).

Summarizing the reviewed methods, the PSO method is the fastest method computationally and can provide good fitment when compared to a GA, while a GA can provide a solution which coverages faster and more detail so that is the key benefit to using a GA. However, the author wishes to utilise the minimized computational time and resource to ensure it is not a hinderance for other users to use the developed toolbox.

2. Methodology

The appendix methodology is divided into three sections outlining in greater detail the boundary conditions needed for the OAT analysis (A 3.1), the equations required to drive the PETLION environment for the LGM50 () and the PSO method initialization (A 3.3).

A screenshot of a computer

Description automatically generated with medium confidence

Figure : Process for OAT sensitivity analysis

Table 5: Accessed Software tools summary

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Package / Database** | **Code Language** | **Overall Concept** | **Positives** | **Negatives** |
| PETLION  (Berliner *et al.*, 2021) | Julia | High-performance simulations of the pseudo-2D porous electrode theory (PET) model in Julia   * Built for efficient controls, parameter estimation, and other complex battery simulations using the rigorous PET model * Runs a full charge or discharge with 301 DAEs in ~3 ms on a laptop with 1 MB total memory usage * Includes thermal and aging modes | * Fastest solving speed with lowest requirements (22 times faster than PyBaMM, 38 times faster than LIONSIMBA) * Thermal analysis model * P2D DFN model | * Smaller community to PyBaMM so code-based problems are slower to fix. * Author has to develop more features for drive cycles, sensitivity and cell parameter sets. * Overall, less features to PyBaMM |
| PyBaMM  (Sulzer *et al.*, 2021) | Python *(\*Julia via PyCall)* | PyBaMM (Python Battery Mathematical Modelling) solves physics-based electrochemical DAE models by using state-of-the-art automatic differentiation and numerical solvers.   * The Doyle-Fuller-Newman model can be solved in under 0.1 seconds, while the reduced-order Single Particle Model and Single Particle Model with electrolyte can be solved in just a few milliseconds. * Additional physics can easily be included such as thermal effects, fast particle diffusion, 3D effects, and more. * All models are implemented in a flexible manner, and a wide range of models and parameter sets (NCA, NMC, LiCoO2, ...) are available. * There is also functionality to simulate any set of experimental instructions, such as CCCV or GITT, or specify drive cycles. | * Fast solving speed for multiple models (~113ms) * Wide range of cell datasets to use * SPM and SPMe models included with a P2D DFN model * Drive cycle analysis methods included * Large active coding community and backing for the project, so plenty of help debugging issues. | * Slower solving speed to PETLION * Julia PyBaMM via PyCall is still in development so bug fixes required and will have a slower computational speed due to pulling request through PyCall |
| LIONSIMBA  (Torchio *et al.*, 2016) | MATLAB | LIONSIMBA provides a simulation environment for Li-ion cells. The specific modelling approach uses electrochemical pseudo two-dimensional (P2D) model which is represented by means of Partial Differential and Algebraic Equations (PDAEs). | * P2D DFN model for PBM * Open-source access to the code itself | * Slowest solving time of ~463ms for a full soultion * Using a code base which is not open source, so less adoption in research. * Model cannot be reused for different * No features for aging * Very small community of users, so debugging potentially was harder. |
| ARTISTIC  (Lombardo *et al.*, 2022) | Online | The tool links several cell manufacturing parameters and the resulting electrode microstructure. The models used account for three main steps of electrode manufacturing: the slurry phase, drying, and electrode calendaring. All microstructures generated through the platform are shared among all users, making the platform an open and collaborative database linking manufacturing conditions and simulated electrode microstructures. | * Highly advanced methods for simulating electrode behaviour in 3D * Plenty of methods accounting for calendar aging to determine electrode behaviour * A platform that does not require any coding experience to obtain high level data. * Large community of high-level industry and universities contributing data openly. | * No real correlation to optimising a P2D DFN or SPM model, solely just electrode level studies * If data was useful an API would have to built to pull the data across to PBM model. |

* 1. OAT and Temperature Dependency

The boundary conditions Li et al’s identified were then implemented to the authors chosen 6 strong parameters for the OAT (Table 6)

Table : Proposed boundary conditions for PETLION OAT for 6 strongest parameters

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Unit** | **Boundary Condition** | **Max Step size** |
| Cathode Thickness (Lp) | m | [6·10-5  - 20·10-5] | 1·10-6 |
| Cathode Porosity (εp) | - | [0.3 - 0.5] | 0.001 |
| Anode Thickness (Ln) | m | [6·10-5 - 20·10-5] | 1·10-6 |
| Anode Reaction Rate Coefficient (Kn) | m2.5mol0.5s | [1·10-11 - 20·10-11] | 1·10-12 |
| Cathode Maximum Ionic Concentration (Cp,max) | mol m-3 | [4.8·104 - 5.2·104] | 100 |
| Anode Porosity (εn) | - | [0.2 - 0.5] | 0.001 |

The LCO dataset pre-built into PETLION has which allows the input of temperature to influence the OCV curves for both the positive and negative electrodes, these functions are fit using polynomial fitment from measured data. For the LGM50 this has been completed different temperature conditions, which is what the O’regan2022 dataset accomplishes (O’Regan *et al.*, 2022) (3)(4).

|  |  |
| --- | --- |
|  | () |
|  | () |

This is the prime disadvantage with using the Chen2020 dataset as it does not include temperature dependency to terminal voltage, so this the reason why the author will not complete a temperature dependency study due to wanting to focus solely on parameter identification which the Chen2020 dataset is excellent benchmark for this. Even Chen et al saw voltage RMSE’s between 36-46mV for complete discharge events in their P2D models so this dataset can be considered as a helping benchmark for the PSO to look to optimise further (Chen *et al.*, 2020).

* 1. Equations and data for LGM50 into PETLION

The equations required to populate PETLIONS DFN for the Chen2020 dataset are listed below (5-7). In order to build an OCV curve it requires to be fitted as function of the stoichiometry () between the lithium concertation of electrode () against the maximum lithium concertation of electrode () which is shown below:

|  |  |
| --- | --- |
|  | () |

Inputting stoichiometry for the positive electrode into (6) gives the OCV profile of the positive electrode (Chen *et al.*, 2020, p. 202):

|  |  |
| --- | --- |
|  | () |

Inputting stoichiometry for the negative electrode into (7) gives the OCV profile of the negative electrode (Chen *et al.*, 2020, p. 202):

|  |  |
| --- | --- |
|  | () |

Secondly the model requires the electrolyte ionic diffusivity () to be stated with the reference to the electrolyte concertation () changes:

|  |  |
| --- | --- |
|  | () |

Finally, the electrolyte ionic conductivity () is defined like (8) and uses electrolyte concertation:

|  |  |
| --- | --- |
|  | () |

Summarised in Table 7 is the values and equations to drive PETLIONS DFN for the Chen2020 dataset.

Table : Chen2020 parameters required for PETLION DFN

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter** | **Unit** | **Positive Electrode** | **Separator** | **Negative Electrode** |
| Current Collector Thickness | m | 16·10-6 | - | 12·10-6 |
| Electrode Thickness | m | 75.6·10-6 | 12·10-6 | 85.2·10-6 |
| Electrode Length | m | 1.58 |  |  |
| Electrode Width | m | 6.5·10-2 |  |  |
| Mean Particle Radius | m | 5.22·10-6 | - | 5.86·10-6 |
| Electrolyte Volume Fraction | % | 33.5 | 47 | 25 |
| Active Material Volume Fraction | % | 66.5 | - | 75 |
| Bruggeman exponent | - | 2.43 | 2.57 | 2.91 |
| Solid Phase Lithium Diffusivity | m2 s-1 | 1.48·10-15 | - | 1.74·10-15 |
| Solid Phase Electronic Conductivity | S m-1 | 0.18 | - | 215 |
| Maximum Concentration | mol m-3 | 51765 | - | 29583 |
| Stoichiometry at 0% SOC | - | 0.9084 | - | 0.0279 |
| Stoichiometry at 100% | - | 0.2661 | - | 0.9014 |
| Electrolyte Ionic Diffusivity | m2 s-1 | Using (8) | | |
| Electrolyte Ionic Conductivity | S m-1 | Using (9) | | |
| Transference number | - | - | 0.2594 | - |
| Initial Electrolyte Concentration | mol m-3 | - | 1000 | - |
| Open Circuit Voltage | V | Using (6) | - | Using (7) |
| Activation Energy | J mol-1 | 17.8·103 | - | 35.0·103 |
| Reaction Rate | A m-2  (m3 mol-1)1.5 | 3.42·10-6 | - | 6.48·10-6 |

* 1. Initialization of PSO

The critical equations that are implemented into the different software packages mentioned in Objective 4 are derived from Kennedy and Eberhart conceptualisation of the PSO method (J. Kennedy and R. Eberhart, 1995).

|  |  |
| --- | --- |
|  | (10) |

Equation (10) describes the velocity of the particles with respect to the location (x) of the best particle (pbest) and global best particle (gbest). This uses inertia weighting factors (ω) to increase or slow the overall velocity projection of the particle, the learning rates (C) from the pbest and gbest and r is considered to be process noise which follows a uniform gaussian distribution.

|  |  |
| --- | --- |
|  | (11) |

Equation (11) is the update of position for the particle with reference to new velocity determined (10). This happens iteratively to create a generational aspect of the algorithm and find the best fitness to the objective function, which for this paper is the Voltage RMSE.

The PSO in all cases used the following values found in Table 8. The author recognises that these values could potentially be tuned further to have faster convergence, but the author was more concerned on seeing the overall output of algorithm in the environment of PETLION.

Table : PSO values for weighting

|  |  |
| --- | --- |
| **Parameter** | **Value** |
| C1 | 2 |
| C2 | 2 |
| ω | 0.8 |

1. Alternative approaches

Table : Alternatives approaches for project objectives

|  |  |  |  |
| --- | --- | --- | --- |
| **Objective** | **Summary of Objective** | **Alternative Approaches** | **Reason to be rejected** |
| 1 | Literature review of ECM against P2D modelling | Look to focus on an SPMe model which has the trade-off having reduced complexity and overall better fitment to terminal voltage compared to an ECM. | A DFN is the superior model when coming to P2D level studies. So using a SPMe may have less parameters required but comes at the penalty of fidelity of terminal voltage responses at high dynamics which is what the author wants to demonstrate against an ECM |
| 2 | Literature review of different sensitivity analysis | Look to use the Monte Carlo method of random sampling to minimise RMSE which potentially could provide | There are more papers demonstrating the OAT approach which will make easier to identify similarities of the authors discoveries compared to the Monte Carlo Approach |
| 3 | Software tool analysis of physical based battery | Look to build a completely independent PBM model and focus | This is too ambitious for the author to complete alone and would require a team of high-level personnel to achieve this. There are plenty of good tools available (PETLION and PyBaMM) which have communities of users to solve issues that the author encounters |
| 4 | Literature review of AI and statistical modelling approaches | Use a genetic algorithm rather than using a PSO method, as a genetic algorithm can find results which more minimise further than a PSO. | The author wants to utilise a more time and resource efficient algorithm such as the PSO at the potential penalty of a result which could be minimised further |
| 5 | Decision of focus of application of model | Using a motorsport approach which looks to find high fitment to high current demand, which is looking at finding what parameters can be pushed to achieve high dynamics | This was not possible when modelling for a PBM and attempting to get fitness to current and build an objective function for improvement in current performance was not possible as OCV / OCP is the true output characteristic of the cell that most academic papers are looking for in parametrisation. |
| 6 | Development and validation of AI based physical battery model | Using Python packages due to the wider adoption and use in the software engineering compared to Julia | Julia is specifically built to perform as a Data Science and Machine learning tool versus Python which is more of a general-purpose software tool. Additionally highlighted in Figure 9 is the benefit of using a Julia designed PBM package which is ~20 times faster than a Python Package. |

1. Project limitations

Table : Overall Project Limitations

|  |  |  |  |
| --- | --- | --- | --- |
| **Area of Project** | **Limitation** | **Potential Changes to Project** | **Overall Outcome** |
| AI Optimisation method (8.4.4) | At the conceptualisation of the project there was the intent of building a PSO-LM method which combines a global and local approach for optimisation, but this was too ambitious for the author after diving into the literature analysis of building the needed Jacobian Structure to run it (A 2.4) | If the author can use the PSO within PETLION that would be sufficient to be an artificially focused optimisation tool so would still address the main aims of the projects | Utilised a PSO method which proved to be very effective |
| Drive cycles for OAT sensitivity  (9.1) | The Author could not get the WLTP drive cycle to be run due to the performance limits of the Linux machine used, this means a potential benchmark tool is lost to compare to literature to truly understand how powerful the OAT tool is. | Ensure more literature can look to support the outcomes of the model for the sensitivity of parameters or include a simpler discharge cycle | Found enough literature to confirm the authors observations in parameter sensitivity without the supporting need of simpler drivecycles |
| AI Optimisation tools  (8.4) | Was unable to use Optim.jl which is considered to the standard for Optimisations tools within Julia, due to having PETLION integration issues. | Look for a contingency piece of Julia software to use instead or change to a pure statistical analysis which would not meet the objectives | Used Metaheuristics.jl for the PSO method, which was able to integrate with PETLION so retained the overall objectives |
| Timeseries Manipulation  (A 6.1) | When down sampling the data of HPPC and GITT it incurred a larger than expected RMSE error in voltage, which made it a less viable to use for the input of an optimisation | Would completely revisit how to condition the input data for the PSO method with alternative methods such as DTW (A 6.1) | Fortunately, was able to use the WLTP drive cycle which was not affected by down sampling and could run the PSO model and realistic use case |

1. Results and discussion

The Appendix results and discussion is divided into three sections, which looks to provide more data and detail for how drive cycles performed in the environment of PETLION to real data (A 6.1), further analysis of the sensitivity analysis performed within PETLION (A 6.2) and the issues encountered with the PSO method for the PBM (A 6.3).

* 1. Drive cycles analysis

As seen in Figure 14 for the GITT drive cycle, the HPPC (Figure 24) and WLTP (Figure 25) drive cycles have been emulated and compared to measured LGM50 data below.

|  |  |
| --- | --- |
|  |  |

Figure : HPPC comparison of real-world LGM50 data against PETLION simulated voltage and C-rate

|  |  |
| --- | --- |
|  |  |

Figure : WLTP comparison of real-world LGM50 data against PETLION simulated voltage and C-rate

Figure 24 shows the HPPC test cycle comparison of PETLION’s simulated voltage response and the measured LGM50 data, there are some key problems with the voltage profile due to not responding dynamically to the high C pulses and the different timing of pulses seen on the C-rate profile. This is due to the measured HPPC profile being SOC controlled so once the 5% of SOC has been discharged it moves on to the relaxation period irrespective of the time required to remove 5% SOC, whereas PETLION is purely time controlled and used a mean time observed from the measured data for the relaxation period. This explains the large RMSE presented in Table 1 PETLION due to the delay in C-rate deployment. PETLION does have specifiable SOC boundaries within simulate commands, but it is not advanced enough to determine a change in SOC per stage of the HPPC. It is additionally noted that each HPPC simulation takes 4 seconds to complete.

Figure 25 shows the WLTP drive cycle comparison of PETLION’s simulated voltage response and the measured LGM50 data, the way this was achieved by using the C-rate profile from the measured LGM50 data for every 500ms and is input into the simulate function and bounded by the time of drive cycle. This provided an excellent comparison of how the PETLION built DFN responds to measured data as the C-rate profiles are identical. From Table 1 it highlights a good level of RMSE fitment of 16.5mV but there is still some room for improvement at capturing the dynamics in terminal voltage.

The author was surprised with the larger than expected RMSE values for HPPC and GITT, but this is due to the method applied to correlate the datasets as RMSE requires the array lengths to be the same (1) and when plotting the datasets, they have a good level of fit visually. The author used a timeseries focused approach at matching similar events together by timeseries and down sampling the largest array to the smallest array length, this was okay for WLTP as that had a continuous time sample.

However, it became problematic for GITT and HPPC as PETLION would only provide data in where significant changes in current or voltage occurred and would stretch the time sample to show the next large event, this is best demonstrated looking at the sampled data of the GITT test cycle for the measured (Down sampled) and PETLION simulated response (Original) (Figure 26).

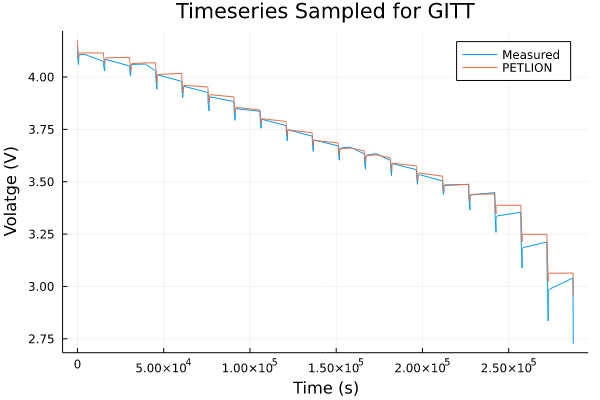


Figure 26: Time series sampled comparison for GITT, PETLION is original and Measured data is down sampled

As the voltages are miss-matched this greatly effects RMSE, which is the key objective that is being optimised with the PSO. So, using WLTP is preferred as this has a good match to the measured data when sampled for the PSO, but for validation GITT can be used to further demonstrate the ability to minimise a voltage profile.

For the author to improve this aspect of the thesis potentially using Dynamic Time Warping (Müller, 2007) which looks find the optimal matching of data points from two differently sampled time series could potential solve this issue and make input condition more robust and less susceptible to bad fitment.

* 1. Sensitivity Analysis

Unfortunately, running the WLTP drive cycle in the OAT condition was not possible, due to exceeding the authors dedicated RAM limits by attempting to store and simulate the true C-rate response of the drive cycle. This was done by allocating the ‘simulate!’ current control function to be directly fed by the array of the measured data, as per ‘simulate!’ outputs a minimum of 40 results regardless of time specified, so inputting an array of 4,000 unique C-rate points means in one simulation of a WLTP the data length for a single output variable is ~600,000, then iterating through ~150 OAT points would be ~72MB of memory required for just storing a single variable in a nested loop. This highlighted one key flaw of using a high dynamic drive cycles such as WLTP with the method conceptualised and environment of PETLION, so had to discount the use WLTP for further OAT analysis due to the values being stored globally via the ‘push!’ function.

Running the GITT and HPPC drive cycles did complete the OAT analysis, however it did present some challenges the author had not foreseen in the initial methodology presented in Figure 23. Within the environment of PETLION allocating a chosen variable to OAT within a function it just physically stored the initial parameter value rather than allowing the model to be influenced by a new value contained within the nested loop, this meant that the item of ‘p.θ[:variable]’ had to allocated every time a new variable was simulated rather than housing it under variable name that the OAT function could look to identify inside the nested loop. Which meant the simulations had to have manual changes and reduced the potential to automate the process without the need of an API or Macro.

While in Figure 12b it shows the same behaviours but shows missing datapoints this is due to the datapoint for temperature producing a terminal voltage response which is not plausible, the check performed for this is ensuring the maximum terminal voltage does not exceed 5V and if a minimum is below 2V. The Author allowed ±0.5V on the boundaries for the cells, which gives enough space for high dynamics but can omit ‘NaN’ for any results which give wildly unrealistic values.

In Figure 26 it shows an example of all the terminal voltage profiles with the influence of Ln being swept from 6·10-5 to 20·10-5.

Chart

Description automatically generated

Figure : Example of Terminal Voltage changing with OAT Ln

If the author could revisit this aspect of the thesis again, the implementation of attempting to solve more in functions and reducing the need of populating locally results would have improved the ability to allow the WLTP drive cycle to be included in the OAT analysis which would have provided an excellent insight into how dynamics can greatly fluctuate RMSE voltage response.

* 1. PSO analysis

Continuing from section 9.3 further analysis was conducted on a GITT test cycle. As determined in A 6.1 there is an issue with RMSE being correctly obtained from down sampling data for GITT and HPPC so this primarily is to further prove that the PSO will look to continually reduce RMSE for any voltage profile. This again was run for 3600s with an average function call of 0.2s for a complete GITT cycle with a single core system (A 6.3 - Table 11).

Table : PETLION PSO results for measure data ‘GITT’ and WLTP

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **Random Initial guess** | **RMSE best (mV)** | **PSO parameter value (GITT)** | **Percentage difference from Chen2020**  **(% - GITT)** | **PSO parameter value**  **(WLTP)** | **Percentage change GITT to WLTP (%)** |
| Cathode Thickness (Lp) | 9.1·10-5 | 38.5 | 10·10-5 | -32.2 | 8.05·10-5 | 19.8 |
| Cathode Porosity (εp) | 0.421 | 0.5 | 49.3 | 0.3 | 40 |
| Anode Thickness (Ln) | 17·10-5 | 10·10-5 | 3.1 | 10·10-5 | 0 |
| Anode Reaction Rate Coefficient (Kn) | 3.0·10-11 | 2.5·10-11 | 50.3 | 2.5·10-11 | 0 |
| Cathode Maximum Ionic Concentration (Cp,max) | 48741 | 49754 | 3.8 | 52000 | -4.5 |
| Anode Porosity (εn) | 0.37 | 0.2 | -1.9 | 0.2 | 0 |

With an 31% improvement on voltage RMSE fitment from the Chen2020 experimentally obtained on the Sampled GITT cycle, it is still apparent that regardless of the quality voltage profile the PSO method will find a significantly better fitment for the 6 strongest parameters of a DFN.

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