Parameter Identifications of Electrochemical NCA/Gr.SiOx Battery Cell Model Using Scaled Data from BEV Experiments

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ABSTRACT: Not all Li-on cells have the same material properties, and the electrochemical cell model parameters (based on the DFN or P2D approach) cannot be used universally in different cells. The cell model must be calibrated before being scaled to a complete pack level for vehicle simulation. This work presents an approach to optimize the electrochemical NCA/Gr.-SiOx Li-ion cell model under transient driving cycles. The cell data is scaled from a dual-motor, long-range Tesla Model Y experiment with a 75-kWh battery (Panasonic 21700 format cell). Multiple thermocouples were installed on the battery packs to measure brick-to-brick, module-to-module temperature for average data. Battery voltage, state-of-charge, and cooling data were recorded using OBD data. A total of 42 P2D cell parameters were reduced to 26 parameters using the Morris Method (aka Elementary Effect Method); then, the 26 parameters were optimized using the Genetic Algorithm optimization. Using the optimized 26 cell parameters, the cell and pack models could reasonably reproduce voltage, SOC, and temperature well under constant speed, WLTC, and FTP-HWFET cycles in winter and summer driving.

KEY WORDS: Electrochemistry, Parameter optimization, DFN model, WLTC, NCA/Gr.SiOx-C, 21700 cell

1. INTRODUCTION

Different battery electric vehicles (BEV) use different cell chemistries and material properties for the electrode and electrolyte [1]. In model-based development (MBD), the lithium-ion battery cell is modeled using Doyle Fuller Newman (DFN) theory based on the pseudo-2D (P2D) approach. Some researchers [2-3] reported that the DFN parameters range from 16-88 parameters. The numerous P2D parameters are a challenge regarding model identification and parameter optimization. The battery cell makers produce cells using different electrodes and electrolytes with different properties, the DFN parameters are also different for geometric, transport, and kinetic parameters [4]. Moreover, these cell parameters vary from cell to cell, depending on their manufacturers. Consequently, the P2D parameters cannot be transferred from cell to cell [1]. This proves to be a challenge for battery cell modeling before it can be scaled up to several thousand cells in a high-voltage pack.

While black-box models such as equivalent circuit models (ECM) and machine learning (ML) are promising models for vehicle simulation, the ECM relies on previous data to predict future cell responses (current, potential, and charge-discharge data). The ML models are fast but require large training data, and they do not provide insights into cell responses under different cell chemistry and operating conditions [5].

In addition, most of the previous studies have provided P2D parameter identification and optimizations using cell data from testing chambers. These experimental data do not account for the impact of actual vehicle thermal management systems (VTMS). Therefore, it is essential to consider the cell response (voltage, SOC, temperature) due to the influence of a cooling system of the VTMS. These limitations are investigated in this work. The present investigation utilizes experimental data from a mass-production BEV (Tesla Model Y, long-range, dual motors) equipped with a 75 kWh Li-ion battery (LIB) pack. The LIB pack consists of 4416 cells and is equipped with an octovalve VTMS. The vehicle experiments are performed at a constant speed, as well as WLTC driving tests. Experimental and Li-ion P2D cell modeling procedures are reported.

2. Research Methods

2.1. Battery electric vehicle experimental procedures

In this work, the Tesla Model Y, a long-range, dual-motor with a 75-kWh LIB pack, was used in the authors' experimental test facility, as shown in Figure 1 [6]. The vehicle is equipped with an octovalve VTMS using egl50 as a coolant. 80 thermocouples are installed on various modules and battery bricks for temperature distribution measurement. Battery pack inlet/outlet pressure and coolant flow rate are measured for a complete pack with cooling system model development. Figure 2 shows the complete pack model with battery thermal management system (BTMS) and modeled heat transfer characteristics from cell to coolant, coolant pipe wall, pack tray, air gap, and pack case. Table 1 lists baseline vehicle specifications. The 75-kWh LIB pack (96s46p) has 4416 cylindrical cells arranged into four modules.

Table 1. Base specification of the BEV and its battery [7]

Tesla Model Y, Year 2020, dual motors	
Vehicle weight	2000 kg
Coolant	EGL 50
Battery	75 kWh
Battery cell	Panasonic 21700 format
Cell specification	21 x 71 mm
Electrodes	NCA/Gr.SiOx-C

Table 2. Experimental condition for model validation

Case	Cycle	Tc, °C	Ta, °C	SOC, %
1	WLTC × 3	26	26	36 %
2	Constant 60 km/h	-9	-11	83.5
3	(FTP+HWFET) × 2	41	30	46.3

The battery cell is Panasonic 21700 (cell diameter 21 mm, cell height 70 mm) cylindrical format with NCA cathode and Graphite-SiOx anode. Table 2 lists the vehicle test conditions for model development and validation. Case 1 is test under repeated WTLC x 3 for an initial SOC = 36%. The test was conducted at the ambient air temperature Ta equal to the cell temperature Tc at 26 °C. Pack performance data (voltage and current) are scaled to a cell level for cell model development and parameter identification to speed up the simulation time. Once the cell parameters are identified and optimized, they are used in the pack model. Case 2 presents the test and validating conditions under a fixed 60 km/h driving under extreme weather (Tc = - 9 degC, Ta = -11 degC, SOC = 83.5%) [7]. Case 2 is considered as cell heating since Ta < Tc. Case 3 (2 times repeated FTP+HWFET cycle) is assumed as the battery cooling since Ta = 30 degC < Tc = 41 degC. Hotter Tc than Ta is assumed to be the condition in which the 2nd vehicle trip starts after the 1st trip at a certain stop time. Cases 1-3 are chosen to ensure the cell model parameterizations can be used at the pack level without modifications, and the cell and pack modeling methods are valid for constant and transient vehicle speeds under winter and summer driving.

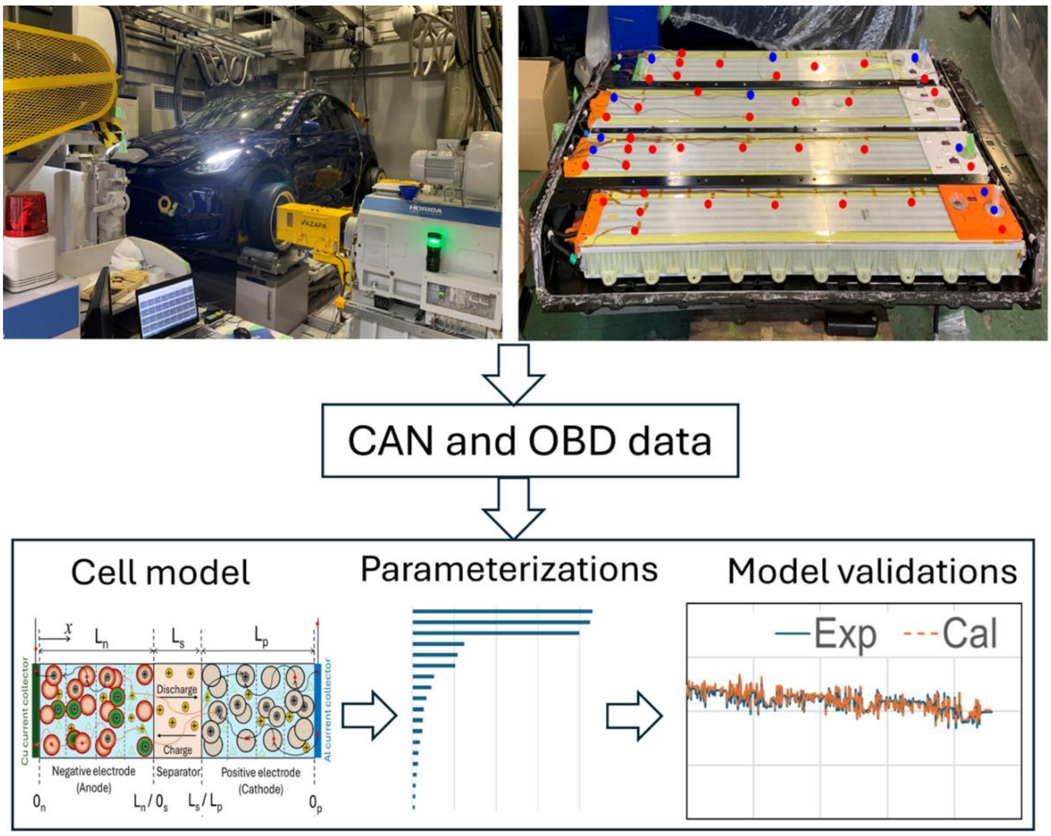

Figure 1. Vehicle testbench at Waseda University, and thermocouple setup for temperature measurement

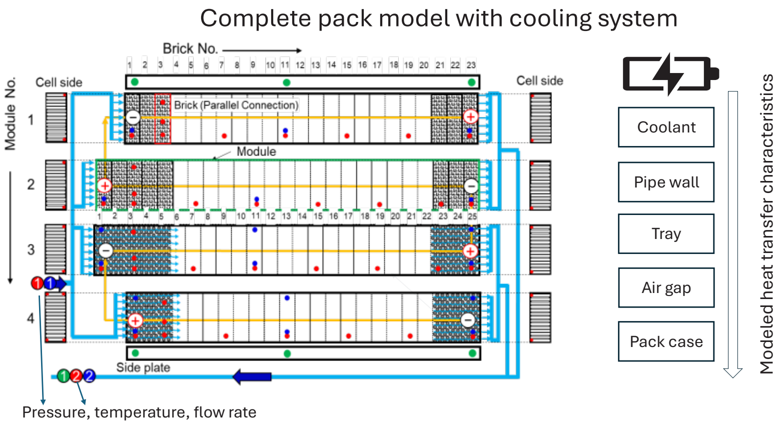

Figure 2. Overview of pack model with cooling system (left) and modeled heat transfer characteristics from cell to ambient (right)

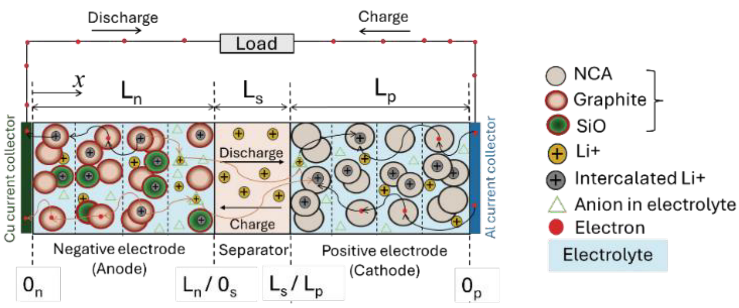

Figure 3. P2D electrochemical cell model overview [8]

2.2. P2D cell model, global sensitivity analysis using Morris Method and cell parameterization using Genetic Algorithm

Figure 3 shows an overview of the P2D cell model. The details of the modeling theory and its derivations can be found in [4]. For the sake of brevity, detailed cell modeling is not included in this paper. An expanded modeling theory for the P2D cell model can be found in a previous work of the authors [8]. The Elementary Effect (EE) or Morris Method [9] is utilized to rank the most and least essential parameters out of 42 P2D cell parameters, as listed in Table 3. These parameters are classified as cathode, anode, electrolyte, and other categories. The parameter boundaries are taken from literature studies and initial guesses [1, 10-13]. Once the most and least essential parameters are identified, 16 parameters are left out due to their low standard deviations. Parameters with high standard deviations are 26 parameters and are further optimized using a Genetic Algorithm. An overview of the GA parameter optimization is shown in Figure 4.

Figure 5 overviews the experimental results of Case 1 (Ta = Tc = 26 degC, initial SOC = 36%, WLTCx3). The pack current and voltage are scaled to a cell level for the model validation. The cell operating conditions are 4.24 V (open circuit voltage at 100% SOC) and 2.319 V (open circuit voltage at 0% SOC). Initial SOC and scaled cell current requests are initialized as model inputs. Once the model is well calibrated in Case 1 using the cell model parameterization in Section 2.2, the same P2D parameters are used to validate Cases 2-3 at the pack level. This method ensures model consistency at the cell and pack under steady and transient driving cycles at hot and cold temperatures.

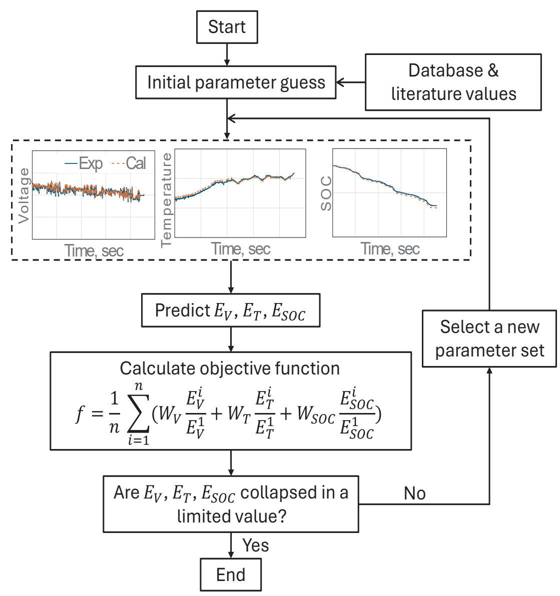

Figure 4. Genetic algorithm optimization for 26 parameters.

Table 3. A total of 42 P2D cell parameters for global sensitivity analysis and GA-optimization

No.		Parameters	Unit	Definition	Boundaries
1	Cathode	L_p	micron	Cathode thickness	60 – 95
2		r_p	micron	Cathode particle Size	3 – 12
3		$t_{foil,p}$	micron	Cathode foil thickness	10 – 20
4		$D_{s,p}$	-	Cathode solid diffusion multiplier	0.7 – 1.2
5		$i_{0,p}$	-	Cathode ECD multiplier	0.7 – 1.2
6		$mult_{dU/dT,p}$	-	Cathode OCP entropic heat multiplier	0.7 – 1.2
7		σ_p	S/m	Cathode conductivity	90 – 120
8		q_{fcc}^{cat}	mAh/g	Cathode first charge capacity	150 – 200
9		$U_{max,p}$	V	Open circuit potential of cathode	3.9 – 4.2
10		$t_{film,p}$	nm	Cathode's initial film thickness	1.0 – 2.5
11		ρ_p	g/cm^3	Conductive agent density of cathode	1.8 – 2.1
12		$\rho_{b,p}$	g/cm^3	Cathode binder density	1.5 – 2.0
13		$k_{ref,p}$	$m^{2.5}/mol^{0.5}s$	User kinetic rate constant of cathode	9.6e-11 – 9.6e-10
14		$D_{s,p}$	m^2/s	Solid diffusivity of cathode	2e-14 – 2e-13
15	Anode	L_n	micron	Anode thickness	60 – 95
16		$r_{Gr.,n}$	micron	Particle size of Gr.-anode	15 – 20
17		$r_{SiOx,n}$	micron	Particle size of SiO_x anode	8 – 12
18		σ_n	S/m	Anode conductivity	90 – 110
19		$i_{0,n}$	-	Anode ECD multiplier	0.7 – 1.2
20		$D_{s,n}$	-	Anode solid diffusion multiplier	0.7 – 1.5
21		$mult_{dU/dT,n}$		Anode OCP entropic heat multiplier	0.7 – 1.2
22		$U_{max,n}$	V	Anode OCP	1.8 – 2.1
23		$q_{fcc}^{Gr.}$	mAh/g	First charge capacity of Gr. anode	1600 – 1760
24		$t_{film,n}$	nm	Initial film thickness of anode	2 – 5
25		q_{fcc}^{SiOx}	mAh/g	First charge capacity of anode SiO_x	1600 – 1760
26		q_{fdc}^{SiOx}	mAh/g	First discharge capacity of anode SiO_x	1400 – 1600
27		m_{SiO}	fraction	Active material #1 Mass Fraction of SiO_x	0.005 – 0.04
28		$E_{D,SiO}$	kJ/mol	Activation energy of SiO anode, , D: solid diffusivity	5.0 – 16.55
29		$E_{a,SiO}$	kJ/mol	Activation energy_ECD for SiO_x anode	5.0 – 12.85
30		$D_{s,Gr.}$	m^2/s	Solid diffusivity of Gr. anode	1e-14 – 1e-13
31		$D_{s,SiO}$	m^2/s	Solid diffusivity of SiO_x anode	8.09e-15 – 8.09e-14
32	electrolyte	$mult_{k_e}$	-	Electrolyte ionic conductivity multiplier	0.7 – 1.2
33		$mult_{D_e}$	-	Electrolyte diffusional conductivity multiplier	0.7 – 1.2
34		k_D^{eff}	-	Electrolyte ionic diffusivity multiplier	0.7 – 1.2
35		c_e	mol/m^3	Electrolyte concentration	1100 – 1300
36		ρ_e	g/cm^3	Electrolyte density	1.1 – 1.3
37		ε_e	-	Electrolyte volume fraction	0.5 – 0.8
38		$mult_{t_+^0}$	-	Transference number multiplier of electrolyte	0.2 – 0.4
39	Other	L_s	micron	Separator thickness	10 – 20
40		ε_m	-	Membrane porosity	0.2 – 0.6
41		R_c	$Ohm\text{-}m^2$	Contact resistance (@ SEI film and anode/foil and cathode/foil interfaces)	1.0e-5 – 8.58e-4
42		h	$W/(m^2\text{-}K)$	Convective heat transfer coefficient	1 – 10

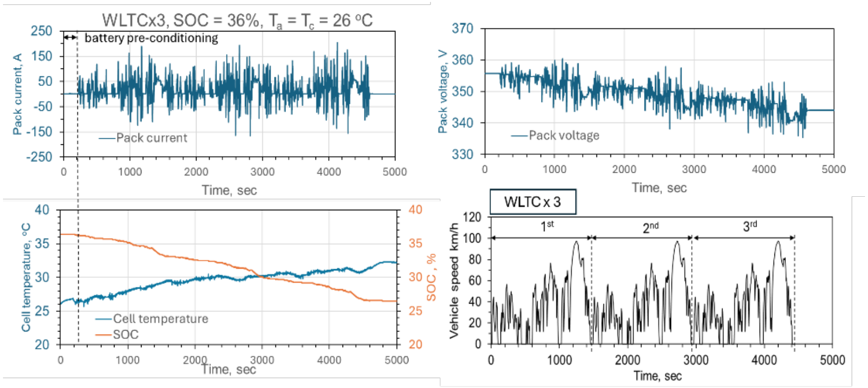

Figure 5. Voltage, temperature, SOC under WLTCx3, ambient temperature Ta = cell temperature Tc = 26 ºC, SOC_i = 36%

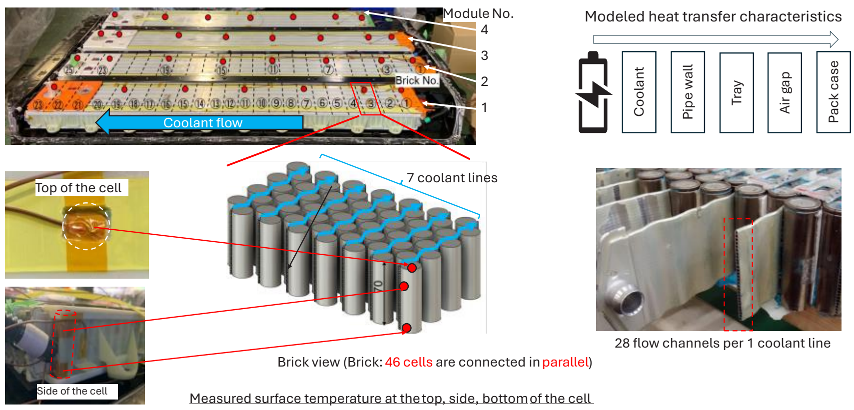

Figure 6. Overview of the complete pack with cooling system model.

2.3. Pack model with cooling system model overview

Figure 6 presents an overview of the total pack model with its cooling system. Modules 1 and 4 have 23 bricks, while Modules 2-3 have 25 bricks. Each brick has 46 cells connected in parallel. The model consists of 4416 Li-ion cells with multiple thousands of flow channels and pipe bends. As shown in Figure 6, each pack contains 7 coolant lines, each with 28 flow channels. Heat transfer characteristics are modeled from cell to coolant, pipe wall, tray, air gap, and pack case to capture the dynamic temperature of the coolant outlet from the LIB pack.

4. Results and discussion

4.1 Cell response validation

Figure 7 shows the validations of the cell model responses, such as terminal voltage, temperature, and SOC. Using the Morris Method to identify the most and least important P2D parameters before GA optimization is suitable for validating the battery model using the electrochemical approach (P2D or DFN model). The result shows that the cell voltage, temperature, and SOC are sufficiently validated with over 90% accuracy.

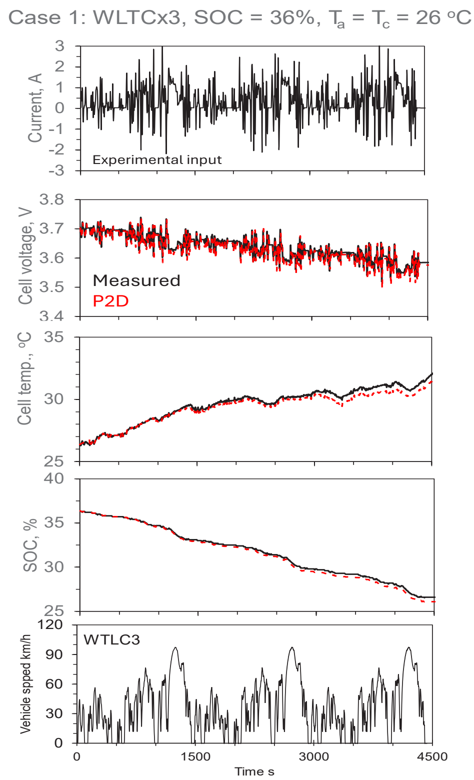

Figure 7. Cell response validation for Case 1 (Ta = Tc = 26 degC, 36% SOC, WLTC x 3)

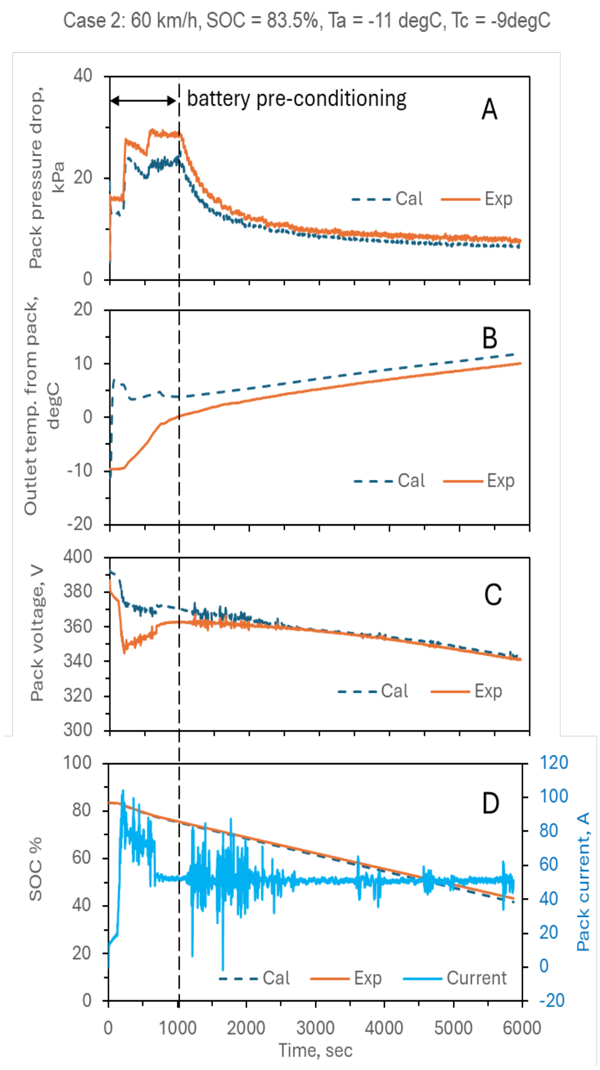

Figure 8. Pack + cooling system model validations (pressure drop, outlet temperature, voltage, SOC) for Case 2 (60 km/h, Ta = -11 degC, Tc = -9 degC, SOC = 83.5%)

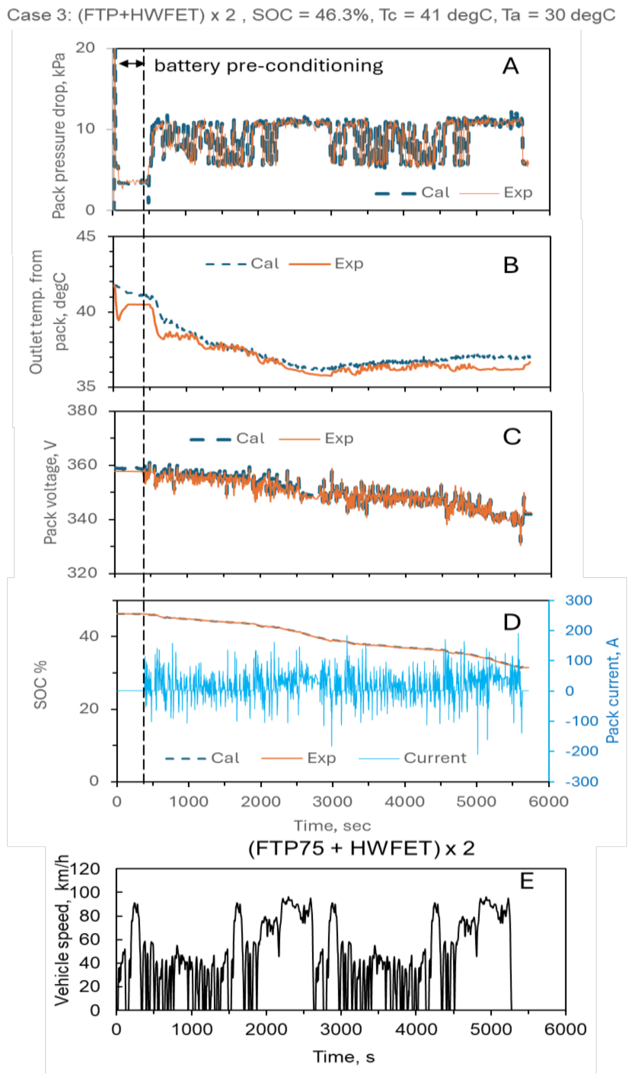

Figure 9. Pack + cooling system model validations (pressure drop, outlet temperature, voltage, SOC) for Case 3 (FTP + HWFET x 2, Tc = 41 degC, Ta = 30 degC, SOC = 83.5%)

4.2 Pack response validations in winter and summer tests

Optimized P2D cell parameters from Case 1 are utilized in the pack model validations in Cases 2-3. It is noted that the pack model includes all cells with their cooling system, pipe bend, and heat transfer characteristics from cell-ambient (via coolant, coolant pipe wall, tray, air gap, and pack case). Each model has 7 coolant flow channels, allowing egl50 to pass through 23-25 battery bricks, as depicted in Figure 2. The battery pack benchmark data were taken from a third-party cost analysis report [14], while detailed specifications of the battery pack with its battery thermal management system were based on previous works of the authors [6-8]. It can be seen in Figure 8 that the pack model with optimized P2D parameters is valid for sub-negative temperatures driving at 60 km/h. Reasonable LIB pack pressure drop, coolant temperature at pack outlet, pack voltage, and SOC are reasonably reproduced. At t = 0 – 1000 sec, predicted thermal and electrical performances of the battery pack are underestimated because this time is used for battery pre-conditioning to reach a desired temperature by changing the current request or vehicle speed. This vehicle test is considered a cell heating mode. The measurement started once the Tc reaches -9 °C (from Ta = -11 °C). Overall, the thermal, electrical, and pressure drop performances of the complete pack model with its BMTS are well captured even under negative temperature driving. The following section shows a model validated under repeated transient driving to prove that the pack + BTMS model is valid under transient conditions.

Figure 9 shows the pack model validation for Case 3, in which the test is repeated 2 times under the combined Federal Test Procedure (FTP) and EPA Highway Fuel Economy Test Cycle

(HWFET) at Tc = 41 °C, Ta = 30 °C, and SOC = 83.5%. This test condition is assumed to be a cell cooling mode since Tc > Ta, considering the 2nd vehicle trip starts after the 1st trip while the battery pack is still hot. Pack pressure drop, outlet coolant temperature, pack terminal voltage, and SOC are well reproduced.

The results in Cases 1-3 conclude that the cell parameter identification using the Morris Method (aka Elementary Effect Method) combined with the GA-optimization are valid for hot (26 degC and 30 degC) and cold (-11 degC) driving conditions. Considering pipe bends, friction losses, and heat transfer characteristics from cell to ambient, the complete pack model could capture the thermal and electrical performance of the 75-kWh battery pack. This complete pack model can be a benchmark model for a vehicle-level simulation to develop an advanced thermal management system.

5. Conclusion

An accurate prediction of cell responses (voltage, temperature, SOC) was obtained using a systematic optimization approach under constant speed, WLTC, and FTP+HWFET driving cycles. The cell model can be scaled to a LIB pack using the same P2D parameters. The cell model parameterization based on the Morris Method (aka Elementary Effect Method) combined with the genetic algorithm optimization is effective in predicting cell response (SOC, voltage, temperature) under a transient driving cycle.

The cell parameters are used in a pack model considering pipe friction due to pipe bends, detailed geometric specifications, coolant properties, and heat transfer between cells and the ambient. The developed pack model with a complete battery cooling system is reasonably validated under winter (-11 °C) and summer (26 – 30 °C) test data. This pack model can be used as a benchmark platform for vehicle-level simulation. The model can be used to test various cooling strategies and advanced thermal management systems.

One shortcoming of this work is the CPU time since the model has several thousand cells and pipe bends, which could be a challenge when the model is integrated with a vehicle model. A data-driven or neural network model will soon be developed to speed up the simulation time. A digital twin simulation model can be developed by combining a data-driven pack model and driving-aware vehicle speed and road conditions data from GPS.

ACKNOWLEDGMENT

This work received financial and technical support from an undisclosed OEM partner. We thank our former graduate students for their modeling and experimental help - Mr. Kentaro Kishida and Kamaleshwar Nandagopal, both now in Toyota Motor Corporation, Mr. Yunkui Ma (now in Mercedez Benz Group China), and Mr. Enbo Cui (now in AESC).

REFERENCES

(1) Chen C. H., Planella F.B, O'Regan K., Gastol D., Widanag W. D., Kendrick E. Development of Experimental Techniques for Parameterization of Multi-scale Lithium-ion Battery Models. J. Electrochem. Soc. 167 080534. https://doi.org/10.1149/1945-7111/ab9050

(2) Forman, J. C., Moura, S. J., Stein, J. L., & Fathy, H. K. (2012). Genetic identification and fisher identifiability analysis of the Doyle–Fuller–Newman model from experimental cycling of a LiFePO4 cell. Journal of Power Sources, 210, 263-275. https://doi.org/10.1016/j.jpowsour.2012.03.009

(3) Fan, G. (2020). Systematic parameter identification of a control-oriented electrochemical battery model and its application for state of charge estimation at various operating conditions. Journal of Power Sources, 470, 228153. https://doi.org/10.1016/j.jpowsour.2020.228153

(4) Newman J., Thomas-Alyea K. E. Electrochemical Systems, 3rd Edition. Wiley 2004.

(5) Li, W., Demir, I., Cao, D., Jöst, D., Ringbeck, F., Junker, M., & Sauer, D. U. (2021). Data-driven systematic parameter identification of an electrochemical model for lithium-ion batteries with artificial intelligence. Energy Storage Materials, 44, 557-570. https://doi.org/10.1016/j.ensm.2021.10.023

(6) Sok, R., Kishida, K., Otake, T., Nandagopal, K. et al., "A Methodology to Develop and Validate a 75-kWh Battery Pack Model with Its Cooling System under a Real Driving Cycle," SAE Technical Paper 2024-37-0012, 2024, https://doi.org/10.4271/2024-37-0012.

(7) Ma, Y., Sok, R., Cui, E., Kishida, K. et al., "Development and Validation of a Battery Thermal Management Model for Electric Vehicles under Cold Driving," SAE Technical Paper 2023-01-1610, 2023, https://doi.org/10.4271/2023-01-1610

(7) Kishida, K. and Sok, R. et al. A Digital-Twin Simulation on Battery Eco-Cooling to Improve the Energy Consumption

of Electric Vehicles Under Transient Driving Cycle and GPS Mission Profiles. Preprint: http://dx.doi.org/10.2139/ssrn.4902996

(8) Sok, R and Kusaka, J, Global Sensitivity Analysis on Parameter Identifications of Electrochemical Li-Ion Cell Model Using Transient Test Data Scaled from Battery Electric Vehicle Experiments. Preprint at http://dx.doi.org/10.2139/ssrn.5027287

(9) Morris, M. D. (1991). "Factorial Sampling Plans for Preliminary Computational Experiments". Technometrics. 33 (2). Taylor & Francis: 161–174. https://doi.org/doi:10.2307/1269043

(10) Pan, K., Zou, F., Canova, M., Zhu, Y., & Kim, J. (2019). Systematic electrochemical characterizations of Si and SiO anodes for high-capacity Li-Ion batteries. Journal of Power Sources, 413, 20-28. https://doi.org/10.1016/j.jpowsour.2018.12.010

(11) O'Regan, K., Brosa Planella, F., Widanage, W. D., & Kendrick, E. (2022). Thermal-electrochemical parameters of a high energy lithium-ion cylindrical battery. Electrochimica Acta, 425, 140700. https://doi.org/10.1016/j.electacta.2022.140700

(12) Zulke A., Korotkin I., Foster J M., Nagarathinam M., Hoster H., Richardson G. (2021). Parametrisation and Use of a Predictive DFN Model for a High-Energy NCA/Gr-SiOx Battery. J. Electrochem. Soc. 168 120522. https://doi.org/10.1149/1945-7111/ac3e4a

(13) Landesfeind J, Gasteiger H A. Temperature and Concentration Dependence of the Ionic Transport Properties of Lithium-Ion Battery Electrolytes. J. Electrochem. Soc. 166 A3079. https://doi.org/10.1149/2.0571912jes

(14) Munro & Associates, Inc., “2020 Tesla Model Y Cost Analysis Zone 4: Powertrain & Battery Pack”, 2020

Nomenclatures

BTMS: Battery thermal management system
EPA: Environmental Protection Agency
VTMS: Vehicle thermal management system
Ta: ambient temperature
Tc: Cell temperature
P2D: Pseudo 2-dimensional
DFN: Doyle-Fuller-Newman
NCA: Nickel Cobalt Aluminum
Gr-SiOx: Graphite – Silicon Oxide
GA: Genetic algorithm
SOC: State of charge
WLTC: Worldwide Harmonized Light vehicles Test Cycle
FTP: Federal Test Procedure
HWFET: Highway Fuel Economy Test Cycle