

Design assistance model of traction battery

SW for analysis of consumption of battery electric vehicles (BEV)

SW version 1.0, description from 10th December 2020

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1 Introduction

This document describes software, which is a result of the research and development project TN01000026 “Josef Bozek National Center of Competence for Surface Vehicles”. The software is called “Design assistance model of traction battery”. This assistance software tool for advanced traction battery modeling can be used as a part of comprehensive vehicle models within battery development process. It includes several constraints like SOC interval, voltage interval, maximum charge and discharge current or temperature. Assessment of traction battery design and economical parameters for expected traction battery operation for different drive cycles can be made using this SW.

2 Brief SW description

The main part of the SW is cell or battery model calibration. There are several common steps necessary for model calibration to be done within initial model setup described in section 4.1. Other parts of model calibration are optionally depending on expected application. There are model calibrations based on

- Capacity tests for different current rates and temperatures in section 4.2.
- SOC-OCV tests (pulse discharging and charging) for different temperatures in section 4.3.
- Determining internal impedance using EIS method in section 4.4.

All the calibrations are considered at the cell level, but they can be easily extended to the battery level. For Cell geometry, stacked electrode or cylindrical cell designs are considerable. In this SW, stacked electrode design was used.

As the traction battery model is once calibrated, it can be used within a comprehensive vehicle model. Such a model enables assessment of the main operational parameters (weight, acceleration, power, etc.) as well as economical parameters depending on price of components and consumption.

3 General

3.1 Environment

GT-Suite v2020 is used as a SW environment. The environment is developed by Gamma Technologies, LLC. It involves multi-physics system simulation and is used in the automotive industry for comprehensive vehicle models. GT-AutoLion used for modeling li-ion cells and batteries is an integrated part of GT-Suite v2020. The model used within GT-AutoLion is based on John Newman's pseudo 2D electrochemical model[3] as well as on several GT Company own experimental data sets for different cell chemistries under different conditions.

There are other battery models existing. The empirical lumped equivalent circuit models can be more accurate, but they are not that universal as P2D models. The 3D models are of highest accuracy for specific pieces, but they show low complexity and complicated usage not suited for the possibility of comparing different designs within traction battery and BEV development process.

3.2 Parameters considered

Several parameters considered within SW as factors or constraints are stated in the section below.

3.2.1 Geometry

Symbol	Unit	Name	Meaning
Out_W, Out_H, Out_T	mm	Outer dimensions	Outer Width, Height and Thickness of the cell
Wall_T	mm	Wall thickness	Wall thickness of the cell
JellyR_W, JellyR_T	mm	Jelly Roll dimensions	Jelly Roll Width and Thickness of the cell
Cat_part_size, Ano_part_size	μm	Particle size	Average diameter of cathode and anode active material
Thick_Cat, Thick_ano, Thick_Sep, Thick_CatFoil, Thick_AnoFoil	μm	Thickness	Thickness of cathode, anode, separator, cathode foil and anode foil respectively

3.2.2 Physical

Symbol	Unit	Name	Meaning
OCV_Full	V	Cell Open Circuit Voltage of Full Cell	The open circuit voltage of a full cell (100% SOC). This attribute is used to determine how much Lithium will be placed in the cathode and anode at 100% state of charge
CapLoading_Cat	mAh/cm^2	Cathode Capacity Loading	The loading (as defined by capacity over area) of the cathode. This attribute relates to energy vs. power balance of the cell.
Cat_Poros	-	Cathode Porosity	
NoverP or N/P Ratio	-	N/P Capacity Loading Ratio	Ratio of Capacity loading of negative electrode to Capacity loading of positive electrode.
Cat_FCC	mAh/g	Cathode first charge capacity	First charge capacity of the given cathode material.

Cat_FDC	mAh/g	Cathode first discharge capacity	First discharge capacity of the given cathode material.
Ano_FCC	mAh/g	Anode first charge capacity	First charge capacity of the given anode material.
Ano_FDC	mAh/g	Anode first discharge capacity	First discharge capacity of the given anode material.
Contact_res_Cat, Contact_res_Ano	$\Omega \cdot m^2$	Contact resistance of electrode	Contact resistance between cathode and positive current collector and between anode and negative current collector respectively.
DiffMult_Cat, DiffMult_Ano	-	Diffusivity multiplier of the electrode	Multiplier to the AutoLion database value of diffusivity of cathode and anode respectively.
HTC	$W/(m^2 \cdot K)$	Heat transfer coefficient	Convective heat transfer coefficient.
EntHeatMult	-	Entropic heat multiplier	Multiplier to the AutoLion database value of entropic heat.
Elyte_conc	mol/l	Electrolyte concentration	Concentration of electrolyte of the cell.
Cond_Cat, Cond_Ano	S/m	Electrode Conductivity	Conductivity of the cathode and anode respectively
Pol_Memb_Por	-	Polymeric Membrane Porosity	Porosity of separator (polymeric membrane)
DLC_Cat, DLC_Ano	F/m^2	Double Layer Capacitance	Double layer capacitance of cathode and anode respectively

3.2.3 Simulation

Symbol	Unit	Name	Meaning
SimDur	s	Simulation Duration	Duration of simulation given by duration of required current profile, which can be shortened when exceeding voltage interval limits.
ts or dt	s	Time step size	Time step size of the simulation

3.2.4 Design results

Symbol	Unit	Name	Meaning
Capacity	Ah	Cell capacity	Reversible capacity depends on the cell balance and whether the cell's capacity is limited by the cathode or anode [2]. The reversible capacity is the theoretical limit on the capacity of the cell for given design.

Note: the main results of simulations are voltage and temperature waveforms.

3.3 Cell chemistries

GT-AutoLion covers the main types of cathodes (NMC, LFP, LMO, NCA, LCO) and anodes (Graphite, LTO) of lithium ion cells. The following cells (accumulators) were used for demonstration of SW functionality:

- LFP 3.2 V/40 Ah
- LFP 3.2 V/90 Ah (used for pre-optimization of SOC-OCV test and EIS tests for LFP)
- LTO 2.3 V/10.4 Ah

4 Detailed SW description

4.1 Initial model setup

Initial model setup is based mostly on specification values of the cell or battery.

4.1.1 Experiments

No experiments are necessary for Cell geometry and Cell capacity adjustment. For Cell balancing, voltage and current waveforms of one full cycle with currents of roughly $C/40$ is needed¹.

4.1.2 Cell geometry

For cell geometry, either disassembly or estimations with help of [2] is possible to obtain values of parameters stated within section 3.2.1.

4.1.3 Cell capacity

For Cell capacity adjusting, correct setup of Cathode porosity is needed. Either Cathode porosity or Cathode capacity loading had to be adjusted as both parameters are dependent on each other.

Several values of Cathode capacity loading were put in Case setup of the program to Cell capacity adjustment.

4.1.4 Cell balancing

Sensitivity analysis was performed for OCV_Full and NoverP within pre-optimization step to obtain correct values range for optimization. Optimization considered:

- OCV_Full, CapLoading_Cat, NoverP, Cat_FCC, Cat_FDC, Ano_FCC and Ano_FDC as factors.
- SimDur and Capacity as constraints.
- Objective function defined by the formula:

$$Obj = \min(RMSE_V)$$
$$RMSE_V = \sum_{i=1}^n (V_{iSim} - V_{iExper})^2$$

where V is Voltage, index i denotes data sample, Sim is for simulation, $Exper$ for experiment.

¹ Current $C/40$ means a current in Amperes of 1/40-multiple of nominal capacity of the cell in units of Ah.

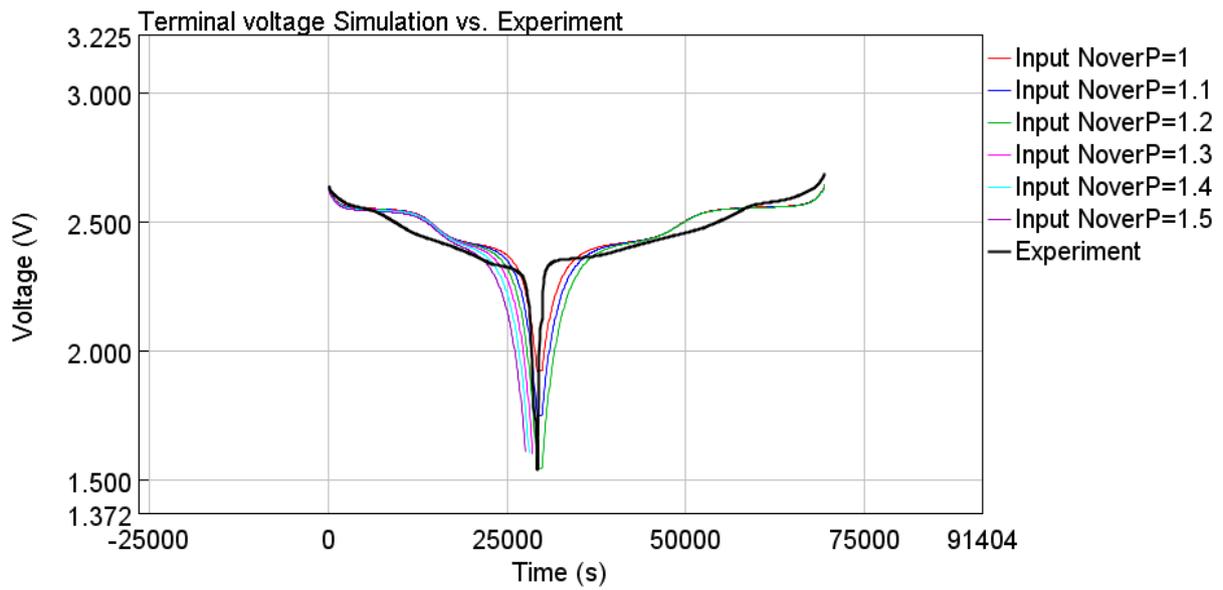


Fig. 1: NoverP sensitivity analysis illustration for LTO 10.4 Ah cell.

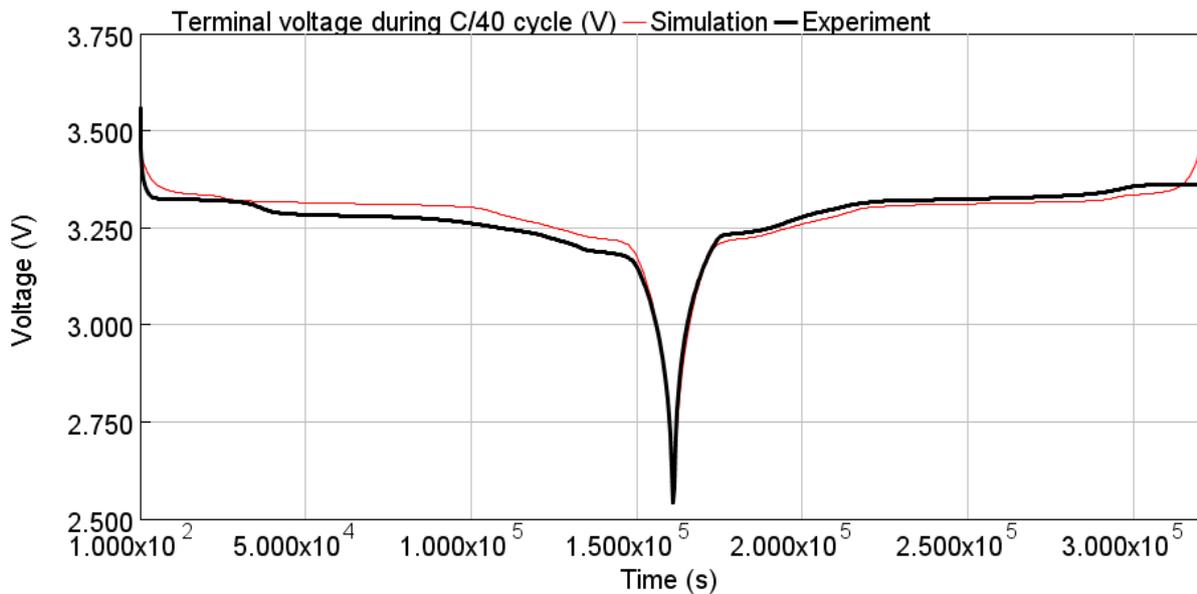


Fig. 2: Cell balancing optimization result illustration for LFP 40Ah cell, voltage RMSE = 0.025 V.

4.2 Model calibration based on capacity tests

The next step of model calibration is the calibration based on Capacity tests of different considerable current rates and temperatures.

4.2.1 Experiments

Capacity tests are performed for different current rates within the scope of cell specification up to the maximum continuous discharge and charge current. Capacity test should be performed for more temperatures to cover expected operational temperature range.

4.2.2 Sensitivity analyses

Sensitivity analysis could be performed for EntHeatMult, Contact_res, DiffMult and HTC within pre-optimization step to obtain correct values range for optimization.

4.2.3 Optimization

Optimization considers:

- EntHeatMult, Contact_res², DiffMult and HTC as factors.
- SimDur and Capacity as constraints.
- Objective function defined by the formula:

$$Obj = \min(w_V \cdot RMSE_V + w_T \cdot RMSE_T)$$

$$RMSE_T = \sum_{i=1}^n (T_{iSim} - T_{iExper})^2$$

$$w_V + w_T = 1$$

where T is for temperature, w_V and w_T is for weights of voltage and temperature respectively, other symbols are analogical to section 4.1.4. More examples of weight sets are part of this SW, finally $w_V = 0.98$ and $w_T = 0.02$ are considered hereinafter.

Figures below show some of model calibration results.

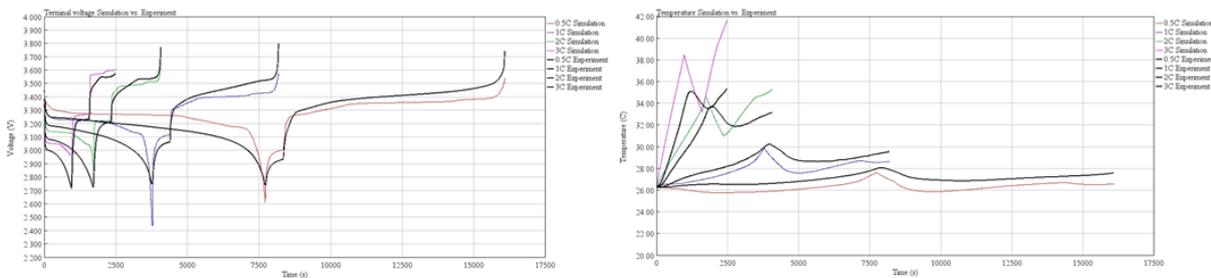


Fig. 3: Model calibration based on capacity tests with currents range from 0.5C to 3V - illustration of optimized voltage and temperature profiles for LFP 40Ah cell at 25 °C.

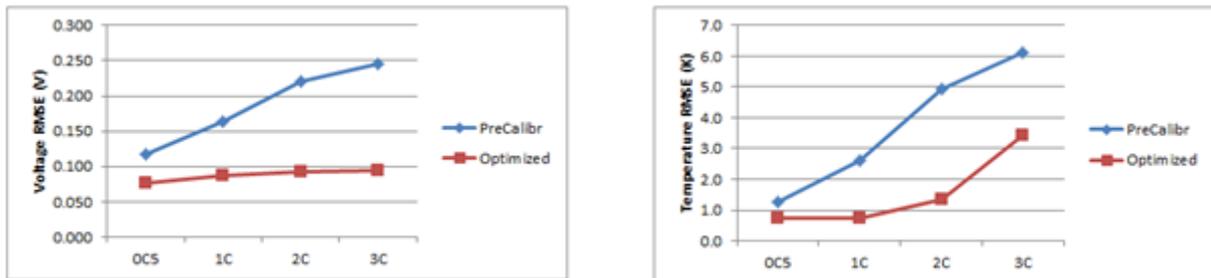


Fig. 4: Model calibration based on capacity tests with currents range from 0.5C to 3V at 25 °C – RMSE progress due to optimization

² equal to Contact_res_Cat and at the same time Contact_res_Ano

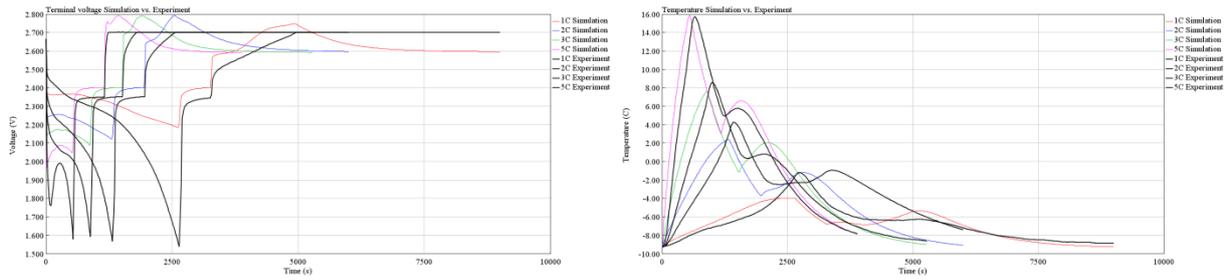


Fig. 5: Model calibration based on capacity tests - illustration of optimized voltage and temperature profiles for LTO 10.4Ah cell at -10 °C.

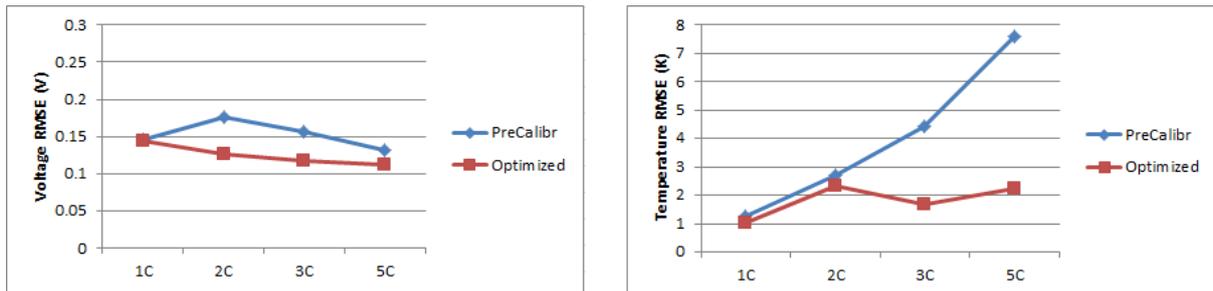


Fig. 6: Model calibration based on capacity tests at -10 °C – RMSE progress due to optimization

4.3 Model calibration based on SOC-OCV tests

The next option of model calibration is the calibration based on SOC-OCV tests, which covers dynamic voltage response on switched cell current.

4.3.1 Experiments

SOC-OCV test starts with fully charged cell. The first part of SOC-OCV discharging consists of repeating discharge pulses of 2% of nominal cell capacity followed by pause of 10 min duration until the terminal voltage reaches the lower cut-off voltage. Before the second part the cell is fully discharged. The second part of SOC-OCV charging consists of repeating charge pulses of 2% of nominal cell capacity followed by pause of 10 min duration until the terminal voltage reaches the lower cut-off voltage.

Experiment should be performed for more temperatures to cover expected operational temperature range.

4.3.2 Sensitivity analyses

Sensitivity analysis could be performed within pre-optimization step to determine significant factors and to obtain correct values range for optimization for these factors: Cat_part_size, Ano_part_size, Thick_Cat, Thick_ano, OCV_Full, Cat_Poros, N/P Ratio, Cat_FCC, Cat_FDC, Ano_FCC, Ano_FDC, Contact_res_Cat, Contact_res_Ano, DiffMult_Cat, DiffMult_Ano, Elyte_conc, Cond_Cat, Cond_Ano, Pol_Memb_Por, DLC_Cat and DLC_Ano.

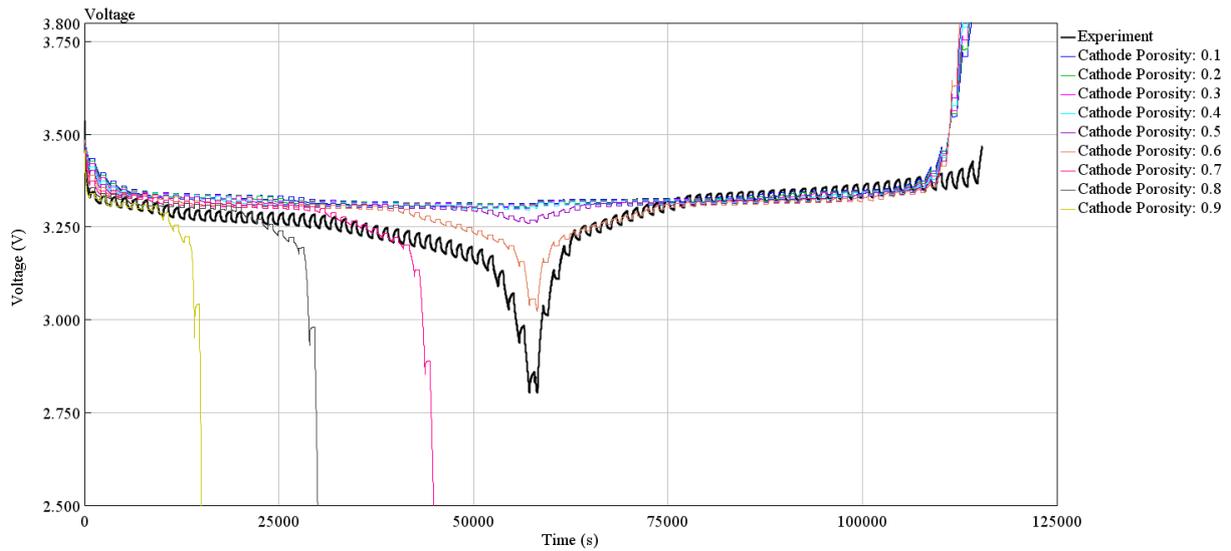


Fig. 7: Experiment vs. simulation for different values of Cathode porosity for LFP 40Ah cell.

4.3.3 Optimization

Optimization considered:

- OCV_Full, CapLoading_Cat, NoverP, Contact_res³, Cath_part_size, Elyte_conc as factors.
- SimDur and Capacity as constraints.
- Objective function of the same formula as in the section 4.2.3.

Figures below show some of model calibration results.

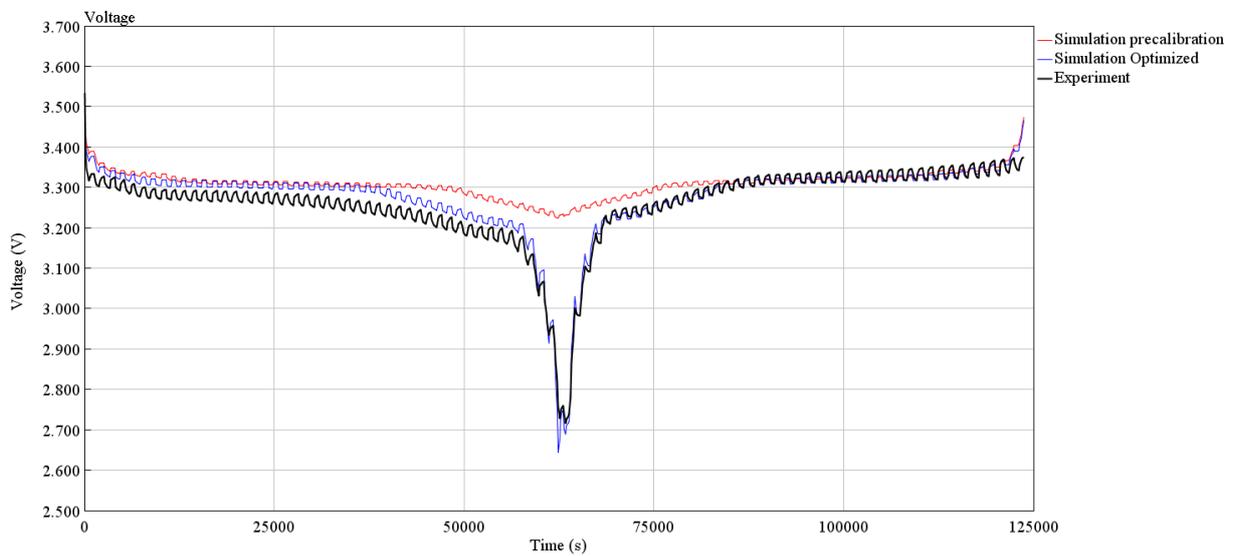


Fig. 8: Model calibration based on SOC-OCV tests – pre-calibration simulation and optimized simulation vs. experiment for ambient temperature 25 °C, voltage profiles for LFP 40Ah cell. Voltage RMSE had dropped from 0.092 V to 0.027 V.

³ equal to Contact_res_Cat and at the same time Contact_res_Ano

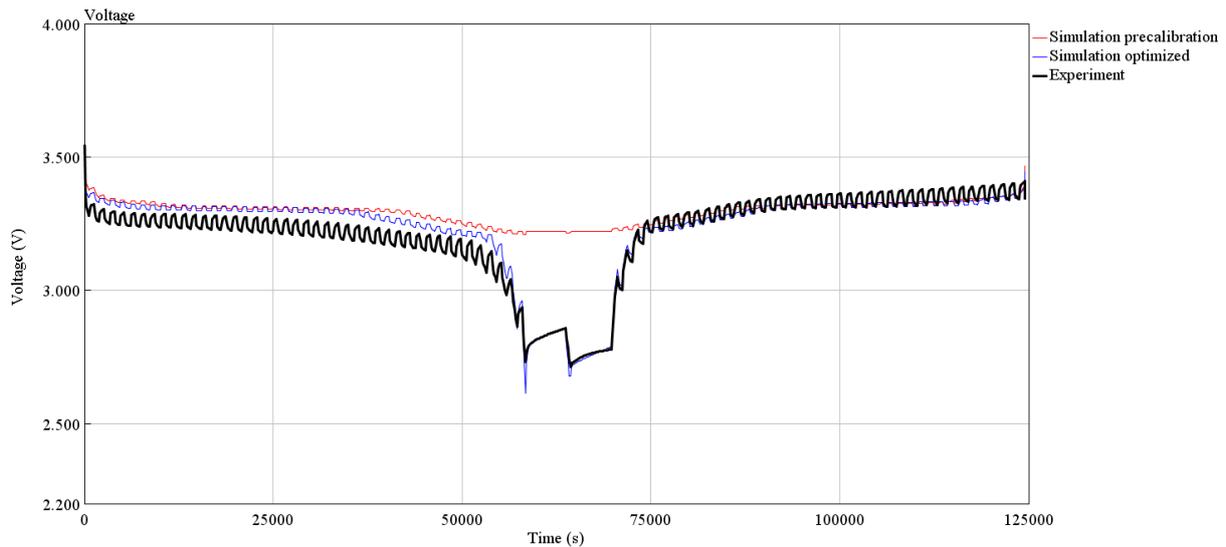


Fig. 9: Model calibration based on SOC-OCV tests – pre-calibration simulation and optimized simulation vs. experiment for ambient temperature 10 °C, voltage profiles for LFP 40Ah cell. Voltage RMSE had dropped from 0.075 V to 0.024 V.

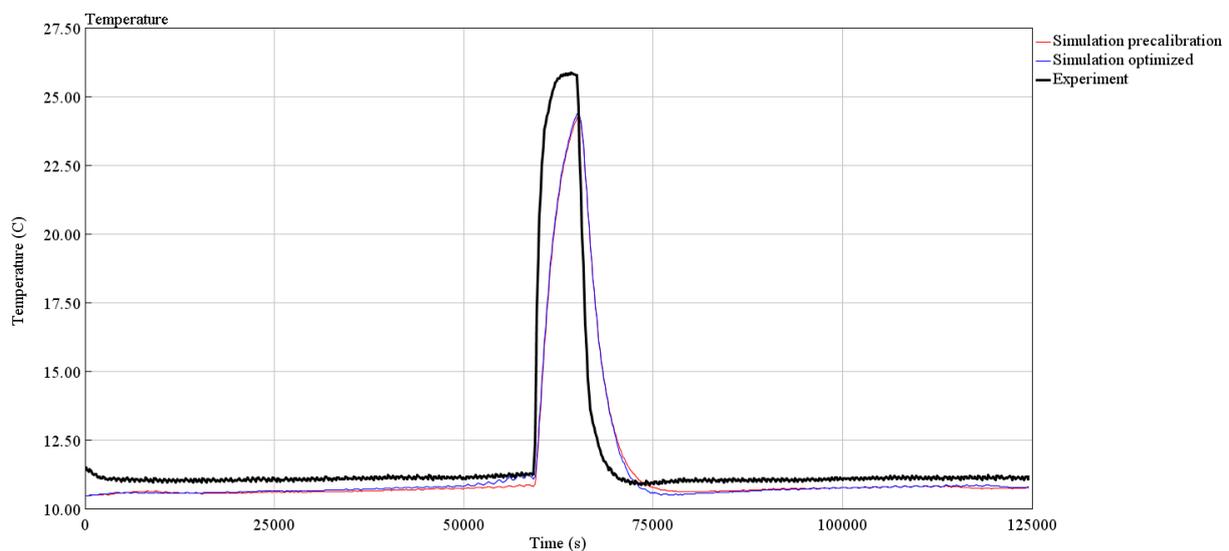


Fig. 10: Model calibration based on SOC-OCV tests – pre-calibration simulation and optimized simulation vs. experiment for ambient temperature 10 °C, temperature profiles for LFP 40Ah cell. Voltage RMSE had remained at 0.7 K.

4.4 Model calibration based on EIS tests

The next option of model calibration is the calibration based on Electrochemical impedance spectroscopy (EIS) tests, which covers frequency dependence of internal impedance of the cell on state quantities (SOC and temperature).

4.4.1 Experiments

Capacity of the cell has to be known prior to the EIS test, which are performed for more temperatures to cover expected operational temperature range. The test starts with fully charged cell and continues with reaching chosen SOC levels, e.g. 100, 98, 96, 94, 90, 85, 80, 70, 60, 50, 40, 30, 20, 15, 10, 6, 4, 2 and 0 %. Two sets of Galvanostatic EIS results for chosen SOC levels are obtained. The first set is subsequently after cell discharging, the second one is subsequently after charging. It is recommended to perform EIS for frequencies range from approximately 3 mHz up to 3 kHz with 4 values per decade.

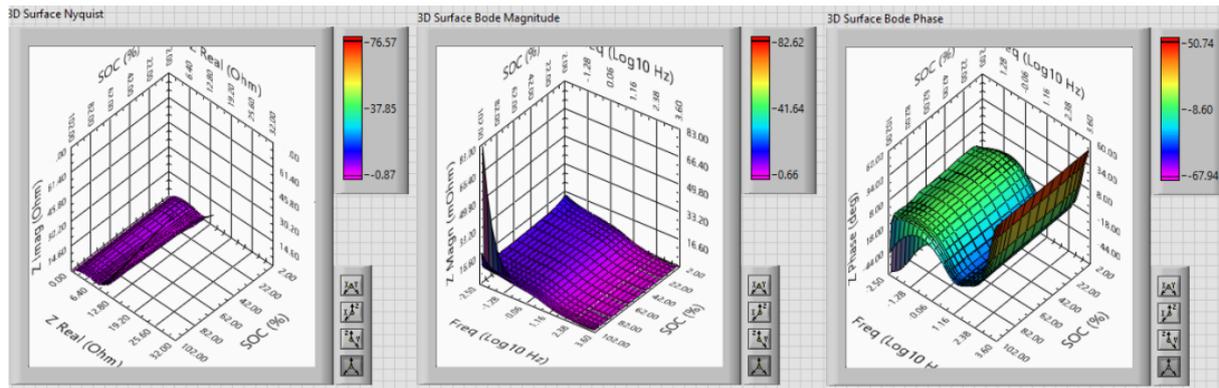


Fig. 11: Experimental results of EIS test following both discharging and charging for ambient temperature 10 °C for LFP 40Ah cell.

4.4.2 Sensitivity analyses

Sensitivity analysis could be performed within pre-optimization step to determine significant factors and to obtain correct values range for optimization for these factors: Cat_part_size, Ano_part_size, Thick_Cat, Thick_ano, OCV_Full, Cat_Poros, N/P Ratio, Cat_FCC, Cat_FDC, Ano_FCC, Ano_FDC, Contact_res_Cat, Contact_res_Ano, DiffMult_Cat, DiffMult_Ano, Elyte_conc, Cond_Cat, Cond_Ano, Pol_Memb_Por, DLC_Cat and DLC_Ano.

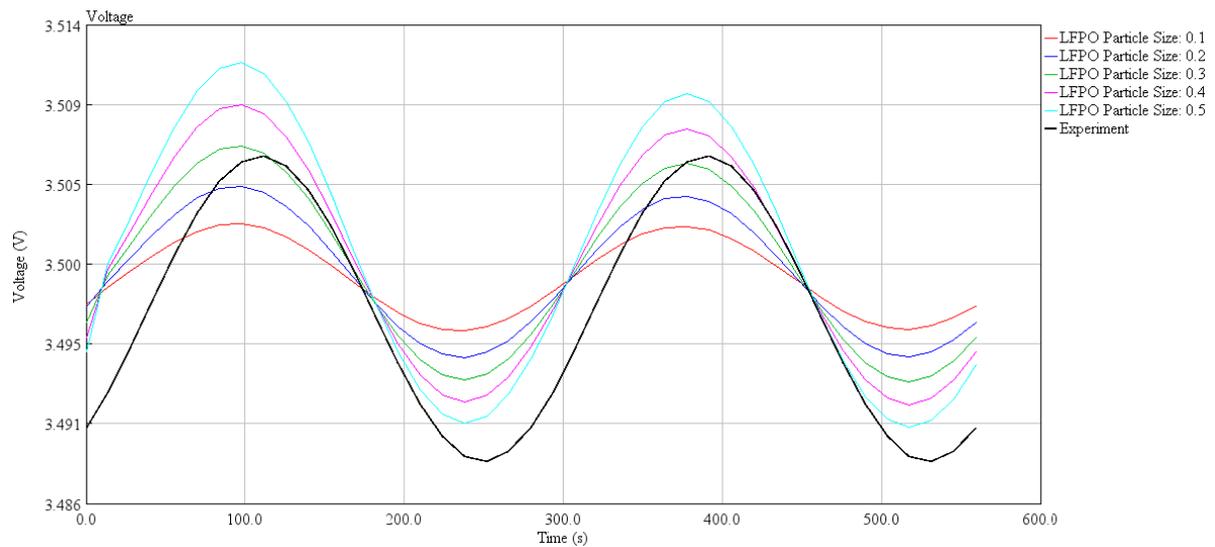


Fig. 12: Experiment vs. simulation for different values of Cathode particle size for LFP 40Ah cell.

4.4.3 Optimization

Optimization considers:

- OCV_Full, CapLoading_Cat, N/P Ratio, Contact_res_Cat, Cath_part_size, Elyte_conc as factors
- SimDur and Capacity as constraints,
- Objective function identical to the one in section 4.1.4, defined by the formula:

$$Obj = \min(RMSE_V)$$

$$RMSE_V = \sum_{i=1}^n (V_{iSim} - V_{iExper})^2$$

Figure below shows model calibration result example⁴.

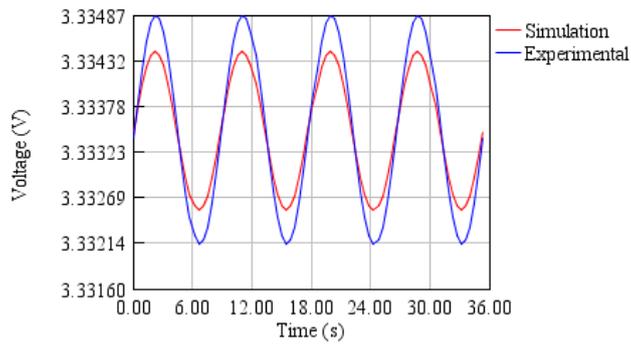


Fig. 13: LFP accumulator 3.2V/40Ah – Voltage comparison example of optimized model at SOC=90%, $\mu=25^{\circ}\text{C}$, $f=0.113\text{Hz}$.

Figures below show model calibration results in terms of RMSE minimization.

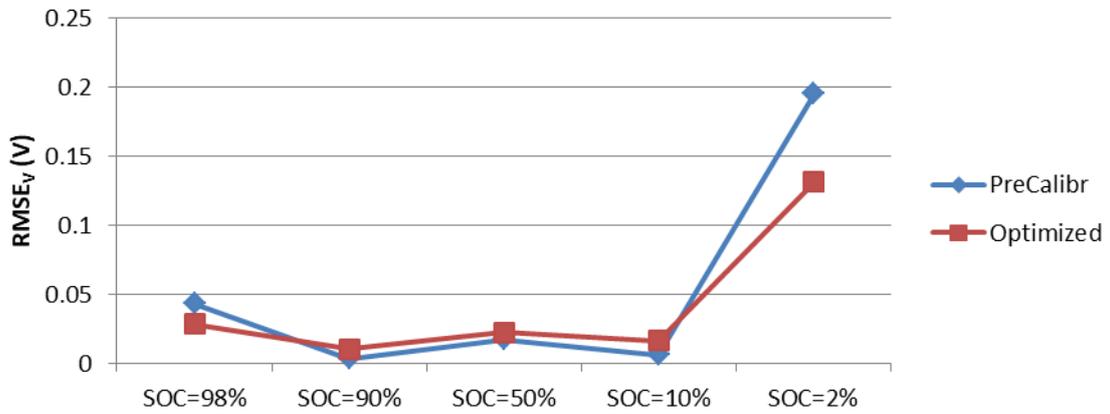


Fig. 14: Model calibration based on EIS tests performed subsequently after discharging – RMSE progress due to optimization.

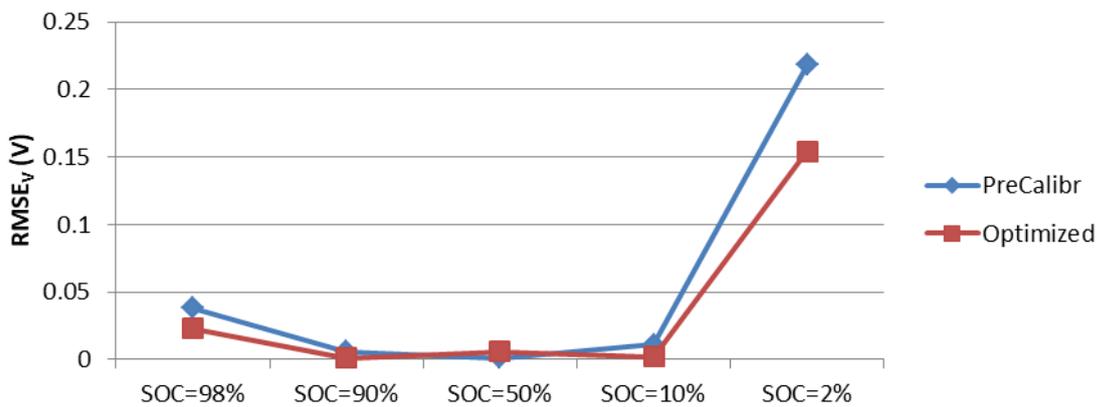


Fig. 15: Model calibration based on EIS tests performed subsequently after charging – RMSE progress due to optimization.

⁴ There are together 1350 waveforms for 18 SOC levels, 3 temperatures and 25 frequencies

The results are slightly better for EIS tests performed subsequently after charging. But it could be observed in general, that there are most inaccuracies of the model for lowest and highest SOC. This is mainly caused by inaccuracy of OCV(SOC) dependency, as the harmonic cell voltage is superimposed on the OCV, the mean value of the voltage.

4.5 Using calibrated model

As the model of the cell is calibrated, it can be simply adapted to the model of the traction battery by assigning the number of series cells and parallel cells. Such a model can be then used in comprehensive vehicle model. Example of vehicle model under driving test cycles is available as part of the SW described in this document. NEDC and WLTC Class 3 driving cycles are used within the example.

The figures below show example of using calibrated model of traction battery LFP 33.8 kWh, 192V/176Ah. Model of one cell was calibrated as per sections 4.1, 4.2 and 4.3 of this document.

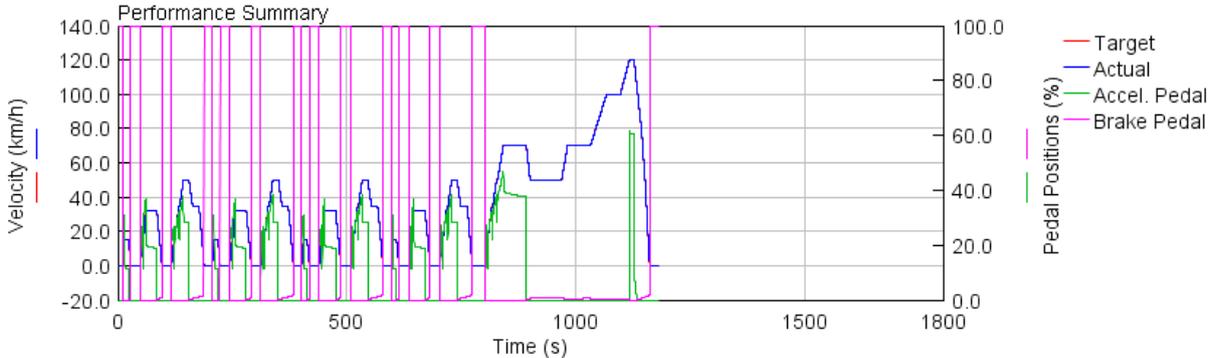


Fig. 16: NEDC drive cycle test with traction battery LFP 33.8 kWh, 192V/176Ah, vehicle speed and pedal position.

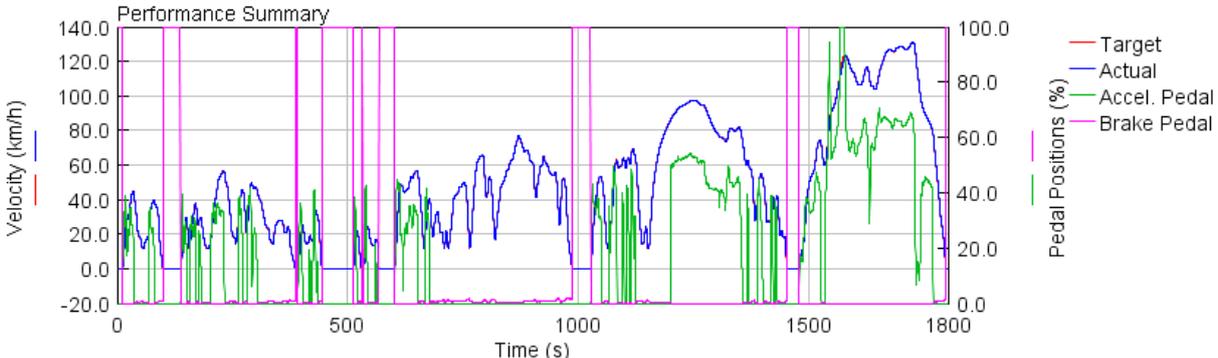


Fig. 17: WLTC Class 3 drive cycle test with traction battery LFP 33.8 kWh, 192V/176Ah, vehicle speed and pedal position.

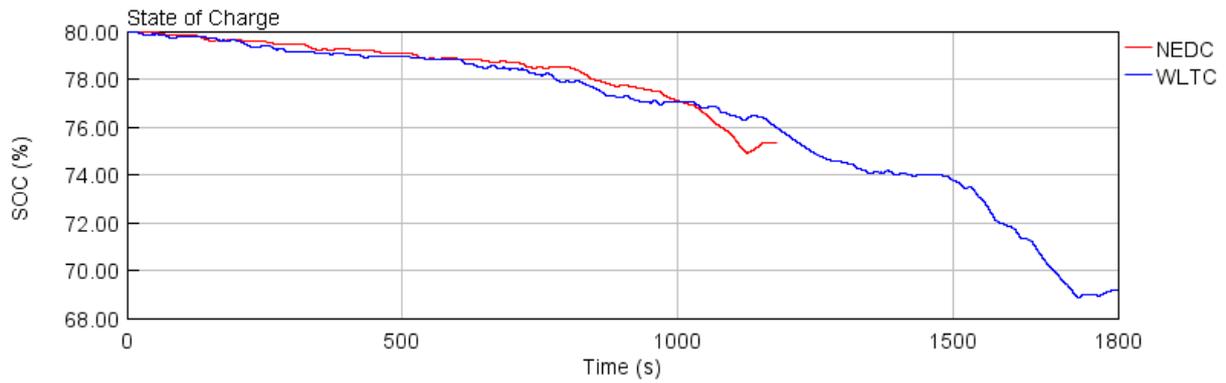


Fig. 18: NEDC and WLTC Class 3 drive cycle test with traction battery LFP 33.8 kWh, 192V/176Ah, state of charge.

4.6 Economical assessment

As the consumption of intended vehicle operation is known for given traction battery and vehicle design, economical analysis of vehicle consumption can be made to assess the overall BEV design.

Another economical issue of traction batteries is their capacity fade. GT-AutoLion has means to estimate both cycle and calendar life of the battery using simulated number of cycles of given parameters. With help of that feature, total cycle life or total vehicle distance range until battery end of life can be estimated with respective impact on economical assessment of the vehicle.

5 SW package

5.1 License

The SW consists of several files with extensions .autolion, .gdx, and .gu, these files are referred to as partial files hereinafter. There is no license needed for downloading partial files. GT-Suite and GT-AutoLion licence is necessary for launching partial files, however. Information could be found at <https://www.gtisoft.com/>

For commercial usage of partial files please contact the representative of the authors of the SW sadil@fd.cvut.cz.

5.2 Download

The SW is available at the website

<http://www.lss.fdvut.cz/Members/sadil/hlavni-stranka/design-assistance-model-of-traction-battery>

5.3 Files extensions

There are several types of files distinguishable by the file extension:

- .autolion: GT-AutoLion file in GT-ISE environment, model assignment
- .gdx: GT-Post file in GT-Postprocess environment, model results
- .gu: GT-Post file in GT-Postprocess environment, reports, usually exported waveforms as results of simulations

5.4 Files structure

The file structure is as follows:

- **LFP**: folder of model calibrations using LFP cells
- **LTO**: folder of model calibrations using LTO cell
- **Vehicle**: folder of using calibrated model

For **LFP** and **LTO**, subfolders have the following meaning:

- **1_Cell Geometry** as per section 4.1.2
- **2_Cell Capacity** as per section 4.1.3
- **3_Cell Balancing** as per section 4.1.4
- **4_Capacity tests_T=XXdegC** as per section 4.2, where XX is temperature in °C.
- **5_SOC-OCV tests_T=XXdegC** as per section 4.3, where XX is temperature in °C.
- **6_EIS tests_discharge** as per section 4.4, EIS tests performed subsequently after discharging
- **6_EIS tests_charge** as per section 4.4, EIS tests performed subsequently after charging

Each subfolder mentioned above usually contains an overall report .gu file and detailed GT-AutoLion and GT-Post files for the following steps:

- **Step0**: precalibration with the necessary experimental data
- **Step1**: pre-optimization sensitivity analyses performed, which can be done for all newly calibrated battery, but often not in such an extent as in presented examples. The more comprehensive pre-optimizations are saved in extra subfolders.
- **Step2**: optimization: optimization setup

- **Step2_Optimized**: optimization result

5.5 Fit for user data

The SW can be user adapted to fit his/her own measured data, when prescribed experiments are performed and respective experimental data (in GT-Suite represented through Transient profiles) are replaced within respective model calibration phase. As mentioned above, some sensitivity analyses are to be recommended, but not all of them performed within examples are necessary. The relevance of individual factors is apparent from optimization reports with extensions .gu, which are part of the SW described in this document.

6 References

6.1 Shortcuts

BEV	Battery Electric Vehicle
DLC	Double Layer Capacity
GT	Gamma Technologies, LLC
HTC	Heat Transfer Coefficient
ISE	Integrated Simulation Environment
LFP	Lithium Iron Phosphate (LiFePO_4)
LMO	Lithium Manganese Oxide (LiMn_2O_4)
LCO	Lithium Cobalt Oxide (LiCoO_2)
LTO	Lithium Titanate Oxide
NCA	Lithium Nickel Cobalt Aluminium Oxide (LiNiCoAlO_2)
NCM	Lithium Nickel Cobalt Manganese Oxide (LiNiCoMnO_2), often found as NMC
OCV	Open Circuit Voltage
P2D	Pseudo 2-Dimensional
RMSE	Root mean square error
SOC	State of Charge

6.2 Bibliography

- [1] AutoLion - Electrochemical Lithium-ion Battery Model, GTISE Help version 2020, Gamma Technologies LLC
- [2] AutoLion Application Manual and Calibration Procedure, version V2020, GT-SUITE, Gamma Technologies LLC
- [3] Jokar A., Rajabloo B., Désilets M., Lacroix M.: Review of simplified Pseudo-two-Dimensional models of lithium-ion batteries, Journal of Power Sources, Volume 327, 2016, Pages 44-55, ISSN 0378-7753,

6.3 Acknowledgement

This research has been realized using the support of Technological Agency, Czech Republic, programme National Competence Centres, project # TN01000026 Josef Bozek National Center of Competence for Surface Vehicles.

This support is gratefully acknowledged.