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Optimization of Li-ion modelling for automotive application: comparison of optimization methods performances

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***Abstract*— the embedded storage system it is the main part in electric vehicle. The vehicle's autonomy and price influence depend to the chosen source technology. For that, we must optimize the sizing and the ageing of the storage system using heavy-duty models. These last ones must take in to account the battery behavior and the system cost. The development of an accurate multiphysical lithium battery model can be an extremely time consuming process due to the complexity of the battery electrochemical phenomena that could occurs during an automotive application. In this paper, we will start by introducing the proposed dynamic battery model, and submit the possibility of building an accurate dynamic design while highlighting the main objective of our study, which is the optimization algorithms performances comparison in terms of precision and computing time.**

I. Introduction

Threw the last years, the interest of research and automotive industries is focusing more and more on the vehicle powertrains electrification. One of the main reasons of this close interest is the fact that this kind of electrification can provide a convenient solution for the intense environmental pollution caused especially by the actual automotive industry based on the use of internal combustion engine (ICE). One of the best candidate to be the suitable alternative for this dominating Industrial technology is a pure transition toward the electric vehicle that can combine one or multiple energy storage devices.

The performances of electrical vehicle need to be optimized to match the actual market demands and to be able to compete with the ICE achievements. One important way to do that is to use the storage devices multiphysical models into the optimization process in order to be able predict the real components electrical, ageing and thermal behavior.

As explained the task of electrification encounter a main problem which consist of the conception of a suitable models for those chosen energy storage devices .Whereas the development of such complex models is extremely time consuming, since we need to consider all the relevant variables in the model, including the interaction between various parameters.

The process of making an accurate model lay on matching its outputs with high sampling frequency experimental results, in a way that the model should be able to predict the static and dynamic behaviors of the component.

Describing the complex behavior of the component, may implies using complex models, with parameters hard to define, especially when using the wrong optimization method, which can lead to a long computation time and can even converge to false results, with no convergent model output values comparing to the experimental results.

In this paper we will discuss and compare the results obtained by the optimization of the energy storage system models, the comparison will be in terms of compilation time, , sum of squared errors, relative error and initial point flexibility. We will aim this comparison by using the following list of optimization algorithms:

- Fmincon
- Pattern Search
- Genetic Algorithm
- PSO-Nelder_Mead
- Simulated Annealing

The compilation will be made using an I7-7700 CPU 3.60GHz with 16Go of Ram HP Computer.

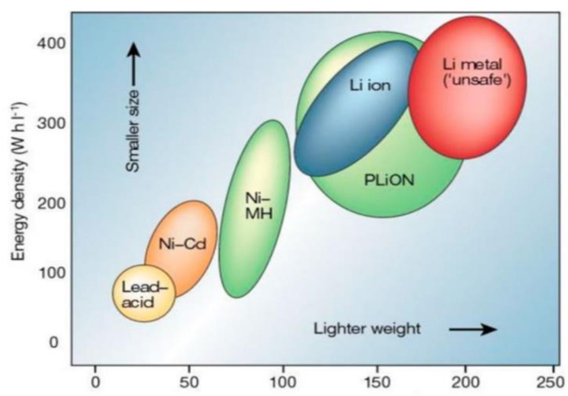

Figure 1. Ragone diagram of batteries technologies

In the first part of this paper, we will introduce the characteristics of the battery based storage system; afterwards we will discuss its electrical and aging models and the

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identification of these models parameters using different optimization algorithms quote above.

II. MODELING

A. Batteries Technologies

The batteries research field is very vast and constantly evolving. Today the most widely used rechargeable battery technologies are numerous, and they differs depending on the manufacturing process of their electrodes, electrolyte and separation corps.Figure 2 illustrates the batteries technological variety in terms of Energy and Power density.

The pros and cons of the principal technologies are summarized in the table below (Tab.1)

TABLE I. PROS AND COND OF DIFFERENT BATTERIE TECHNOLOGIES

Technology	Pros	Cons
Lead-Acid	Solid Low Cost	Worst energy density(Heavy)
Ni-Cd	Fast charge Long Life expectancy	Cadmium is toxic
Ni-MH	Light weight Good energetic density	High Auto-discharge ratio
Li-ion	High energy density	highly flammable

Given their polyvalence in terms of energy and power deliverance, the Li-ion battery is the very suitable technology for automotive applications. However, even in the Li-ion technology, several sub-technologies exist.Theirs characteristics are illustrated in the kiviat diagram. [1][2]

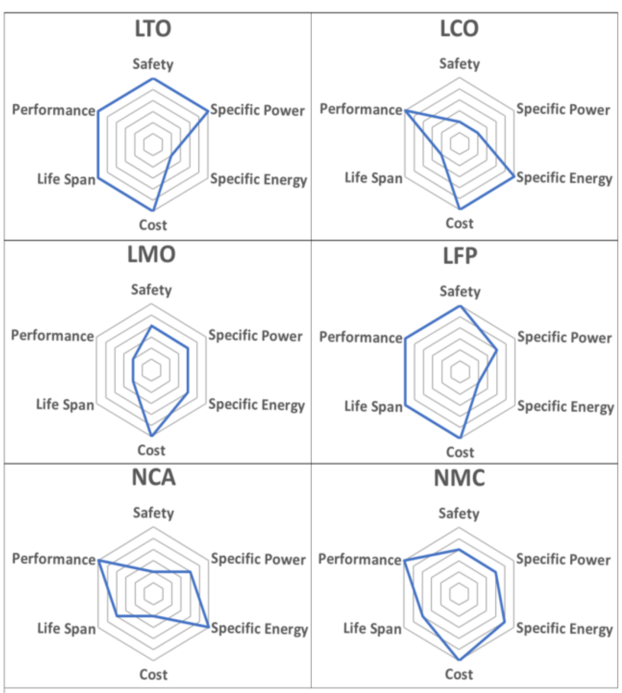

Figure 2. Kiviat diagram of the Li-ion batteries technologies

Figure 2 shows that the NMC technology have the best compromise between electrical performances (Specific power ans specific energy), safety and cost. For that, this technology, which is used actually in EV, is studied and characterized in ESTACA'LAB laboratory.

TABLE II. 1: KOKAM 40HED LI-ION BATTERY CARACTERESTICS

Battery	Value
Nominal Voltage (V)	3.7
Capacity (Ah)	40
Specific Energy (Wh)	133.8
Max current charge/discharge	40/40
Weights (Kg)	0.935
Volume (L)	0.42

B. Li-ion Battery Modeling

The battery is a complex electrochemical system, due to the non-linearity link between the different models (electrical, thermal and ageing) inputs and outputs.

Developing a reliable model of the Li-ion battery which can predict the behavior of a real component means taking in a count all the electrochemical reaction produced between each part inside the accumulator.

To achieve such a goal, a multiphysical model can be proposed, taking in consideration all of the electrical and ageing aspect of the Lithium battery

B.1 Electrical Li-ion Battery Model

The electrical model circuit is established using nonlinear equivalent electric circuit, composed of over circuit voltage (OCV), internal resistance and the RC circuit. The input and output of this model are respectively the battery current and voltage.

V_{OCV} depend directly to the Cell state of charge SoC, which in addition to the current load, influence on the R_{Ω} . This last parameter characterize the ohmic resistance of the cell electrodes and electrolyte. Furthermore, the double layer behavior and the diffusive behavior of the battery cell are respectively characterized by (R_{dll}, C_{dll}) and (R_{dif}, C_{dif})[3][4].

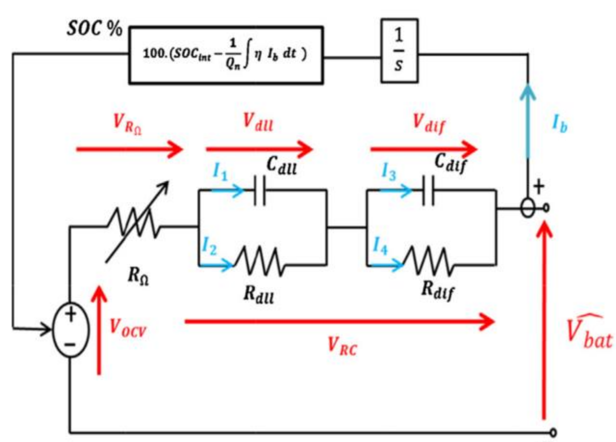

Figure 3. Electrical equivalent circuit of the li-ion battery model

The relation bellow (1) describing the evolution of VOCV with relation to the SoC is the results of multiple tests and averaging techniques

$$V_{OCV}(SoC) = x_1 + x_2 e^{(c_1(1-SoC))} + x_2 e^{c_2(SoC)} + x_3 e^{(c_3(1-SoC)^2)} + x_4 e^{(c_4(SoC)^2)} + x_5 e^{(c_5(1-SoC)^3)} + x_6 e^{(c_7(SoC)^3)} \quad (1)$$

The evolution of internal electrical resistance R_Ω and the values of the two RC branches parameters (R_{dl}, C_{dl}) and $\left(R_{dif}, C_{dif}\right)$ can be described by the following relations:

$$R_\Omega = \frac{x_8}{SoC\left(1 + c_7 Sign(I)\right)} \quad (2)$$

$$R_{dll} = c_8 \quad (3)$$

$$C_{dll} = \frac{c_9}{c_8} \quad (4)$$

$$R_{dif} = c_{10} \quad (5)$$

$$C_{dif} = \frac{c_{11}}{c_{10}} \quad (6)$$

B.2 Ageing Li-ion Battery Model

The battery ageing aspect is very important factor in the automotive industry. The ageing model must allow the estimation of the capacity and the resistance over time.

The model described by the equation (3) proposed by M. Ecker AND AL. [5] is chosen.

$$\frac{C_{bat\_act}}{C_{bat\_nom}} = \left[1 + c_a.\sqrt{t}\left(c_T{}^{\frac{T-T_0}{\Delta T}}.c_V{}^{\frac{V-V_0}{\Delta V}}\right]\right. \quad (7)$$

- C_{bat_act} : Actual Capacity Value
- C_{bat_nom} :Nominal Capacity Value
- c_a, c_T, c_V : Optimization coefficients
- T : Temperature
- V : Voltage

III. OPTIMIZATION ALGORITHMS

The optimization algorithm panoply form two major family, gradient based like Fmincon and Pattern Search, and gradient free ones as PSO, Genetic algorithm.

The general characteristics of those algorithms can be summed up in the table (Table.II) below. [6]

Table III. COMPARAISON BETWEEN GRADIENT FREE AND GRADIENT BASED OPTIMIZATION

Gradient Based	Gradient Free
Widely used	Easy to implement
Fast performances	No derivatives required
Scales well	
Requires smooth gradient	No guarantee of optimal solution
Local minima	

In the following, we will introduce each optimization algorithm used

Fmincon: (Find a minimum of a constrained nonlinear multivariable function) It’s a large/Medium scale algorithm used to finds a constrained minimum of a scalar function with several variables starting at an initial estimate.

For large Scale optimization the gradient must be supplied, that way, the algorithm will apply the interior-reflective Newton method [7] and for each iteration, the algorithm will approximate the solution for a large linear system using precondition conjugate gradient.

In the case of Medium scale optimization, the algorithm uses the sequential quadratic programming method at each iteration.

Genetic Algorithm: GA is gradient free algorithm, instead of proposing just a single solution for the optimization problem, it generates many possible solutions that form a population, and every solution is scored using the objective function [8].

These candidate solutions , are then recombined so that the best of them reproduce to form a new best generation of solution with the finest traits of the previous ones, and this continues until the improvement stops or the max iteration number is reached.

Pattern Search: it is a free gradient optimization algorithm, which is even usable with discontinuous and differentiable functions.

This algorithm finds a string of points that approach the optimal solution, at each iteration the value of the objective function either decreases or remains the same using the convergence method, based on the theory of positive bases [9].

PSO-Nelder_Mead: it is a hybridation between two optimization algorithms. First, the Nelder-Mead algorithm, which is an unconstrained optimization tool that searches the optimal solution using a Simplex, shape solution.

This simplex converge to the optimal solution by growing it size, shrinking it according a set of rules, however the major drawback of this algorithm is the importance of initial points choice which is not easy to define, and depending on those initials points the algorithm may guarantee or not finding a global optimum. In the other hand, the particle swarm optimization where the swarm is a possible iteration created at each iteration, each particle has its own direction, velocity [2]

Simulated Annealing: It is a probabilistic method to approximate the global optimum of an unconstrained bounded optimization problem.

With this algorithm, an initial guess is taken followed by another randomly guessed solution near the previous one; the new solution is evaluated to see if it is better than the first one.

Initially some bad solutions are accepted to allow the algorithm to explore and maybe getting out of a local optimum.As iterations goes on, less and less bad results are accepted and at the end only better solution than the previous one are accepted until it converges to the global optimum.[10]

A. Optimization Results

The objective function of the battery model in general is given by

$$J(X) = \left(\sum_{i=1}^{n} \left(\hat{R} - R\right)^2 + \sum_{i=1}^{n} \left|\hat{R} - R\right| \right) \Big/ Length(R) \qquad (8)$$

- $\hat{R}$: Model output(Battery terminal voltage for the electric model and Capacity in the ageing one)
- R: Real component outputs

After doing multiple tests in order analyze the solution convergence area, we set the initial point and boundary conditions showed in the appendix to assure the convergence of all algorithms with the minimal computing time possible

The optimization results of the electrical and ageing model showed down below are obtained by using the following current cycling profile.

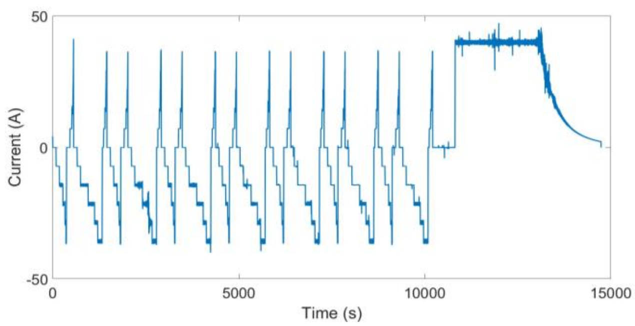

Figure 4. Cycling current profile

- **Fmincon Optimization**

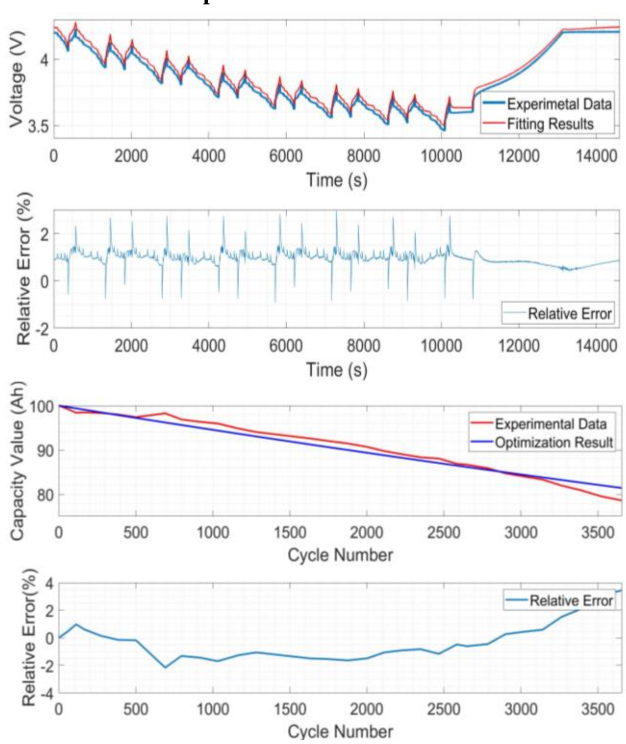

Figure 5. Fmincon electrical and ageing model optimization results

- **Pattern Search**

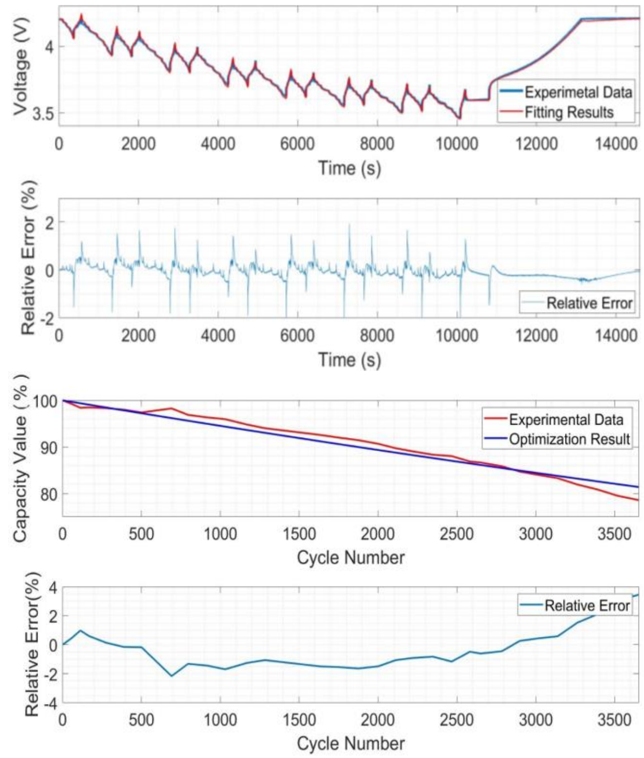

Figure 6. Pattern Search electrical and ageing model optimization results

- **PSO-NM**

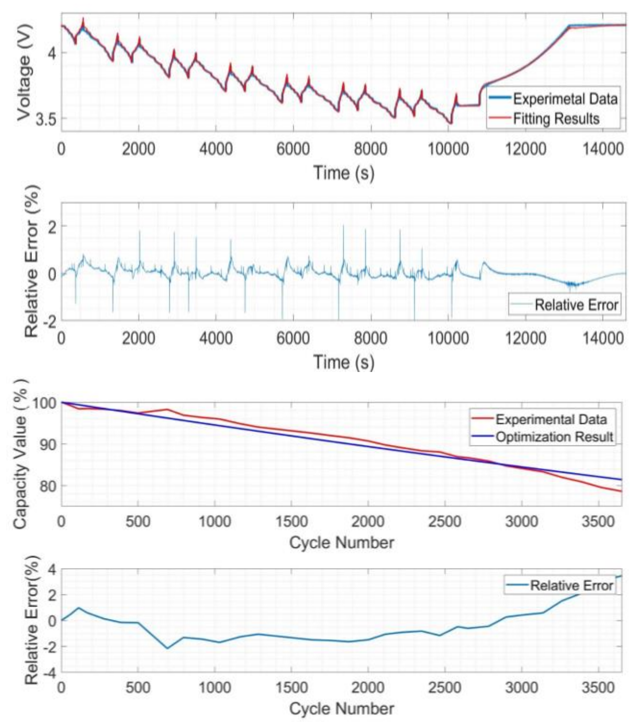

Figure 7. PSO-NM electrical and ageing model optimization results

- **Genetic Algorithm**

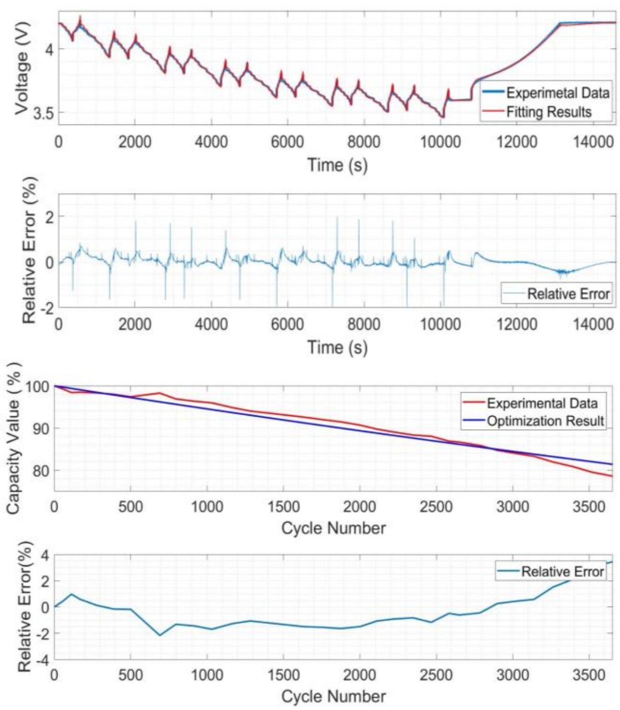

Figure 8. GA electrical and ageing model optimization results

- **Simulated Annealing**

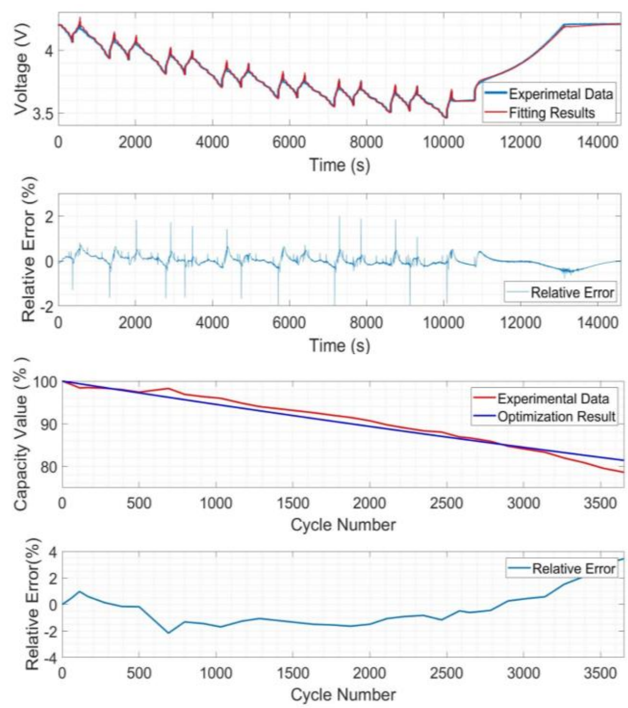

Figure 9. Simulated Annealing electrical and ageing model optimization results

The table below illustrate the optimization algorithm performances comparison in terms of Computing Time and objective function final value.

B. *Results Discussion*

For the electrical model optimization case, the results showed in the figures and the table highlights the comparison between the global voltage evolution obtained by the electrical model and the real component experimental data.

Compared to the gradient free algorithms, the gradient based ones; take much less computing time however, the given results are relatively worst with a maximum of 3% relative error value compared with the 2% obtained with the gradient free algorithms.

This is due to the fact that algorithm based on the calculation of derivatives can easily and rapidly be trapped in a local minima, contrary to the gradient free algorithms which compute random solution to explore all the possible results in between the boundary constraint in order to get the optimum value.

In the other hand, for the ageing model optimization, there is not much difference in the objective function final value; all algorithms converged to the same optimum minima inside the boundary conditions.

The high relative error value (a +3.8% maximum) is due to the fact that the ageing equation does not well describe the evolution of the capacity during the cycling. This equation will be improved in the future work.

In term of computing time, contrary to the electrical model, the ageing model shows that the gradient based optimization algorithms are taking more time to converge toward the optimum result, this could be explained by the fact that this

Table IV. FINAL OBJECTIVE FUNCTION VALUE AND COMPUTING TIME RESULTS

		FMINCON	PATTERN_SEARCH	PSO-NM	GA	SIM_ANNEALING
ELECTRICAL MODEL	Computing Time	10	21	112.72	163.15	350.10
	J Final Value	0.0368	0.008666	0.00631	0.00625	0.006685
AGEING MODEL	Computing Time (s)	353.6031	618.423	162.1	249.24	473,1
	J Final Value	1.444	1.444	1.444	1.444	1.444

- **J Final Value: The final value of the objective function equal to:** $\boldsymbol{J}(\boldsymbol{X}) = \left(\sum_{i=1}^{n}(\hat{\boldsymbol{R}}-\boldsymbol{R})^2 + \sum_{i=1}^{n}|\hat{\boldsymbol{R}}-\boldsymbol{R}|\right)/\boldsymbol{Length}(\boldsymbol{R})$

optimizers type are as their type indicate, designed for smooth functions which is apparently not the case of the ageing model objective function.

it worth to be mentioned that the gradient free algorithms don't need the initial points configuration which could be a huge time gain, because in the other hand gradient based algorithms require to configure the initial points, which is not evident since the objective function need to be defined at those delicately chosen points to allow the convergence of the function.

IV. CONCLUSION

In this paper, a comparison of the optimization algorithm performances has been discussed.

The algorithm benchmarking used, constitute of the optimization of a multiphysical model which can faithfully describe the electrical and ageing behavior that can occur in the chosen battery cell during an automotive application.

The realized benchmarking highlights the importance of choosing the adequate optimization algorithm by taking in consideration the nature of the objective function, this was well demonstrated in the ageing modeling part, where all the algorithms converged to the same results however between the best and worst algorithm choice, we noticed a ¼ ratio for the computing time.

The electrical modeling part shows that event if the gradient based algorithm converged to an acceptable results (±3% relative error) in our case, they can easily be trapped in a local minima especially if the initial point and the boundary conditions are not suitably configured.

APPENDIX

- Ageing Model

Initial Points: ones (1, 3)
Lower Bounds: -10*ones (1, 3)
Upper Bounds: 10*ones (1, 3)

- Electrical Model

Initial Points: [1e-7 0.1 1e-7 1e-7 1e-7 1e-7 0.5 0.5 23 1 25]
Lower Bounds: [0 0 0 0 0 0 0 0 20 0 20]
Upper Bounds: [1e-3 1 1e-2 1e-3 1e-4 1e-4 1 1 60 1 60]

Table V. OPTIMAL ELECTRICAL MODEL PARAMETERS

Parameter	Value	Parameter	Value
C_1	$6.33e^{-4}$	X_1	333.32
C_2	0.6105	X_2	-278.96
C_3	0.0086	X_3	$-1.8102e^{17}$
C_4	$1.938e^{-4}$	X_4	$-2.55e^{17}$
C_5	$3.444e^{-5}$	X_5	$-8.792e^{-85}$
C_6	$8.114e^{-5}$	X_6	-45.28
C_7	0.005	X_7	$5.249e^{11}$
		X_8	0.0187

Table VI. OPTIMAL AGEING MODEL PARAMETERS

Prameter	Value	Unit
R_{dll}	0.109081	Ω
C_{dll}	531.5757	F
R_{dif}	0.7032	Ω
C_{dif}	82.4712	F

Table VII. OPTIMAL AGEING MODEL PARAMETERS

Prameter	Value
C_a	-9.21785286882035E-12
C_T	0.18960713229746537
C_v	0.8269171370507831

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