DEFACTO - battery DEsign and manuFACTuring Optimisation through multiphysic modelling

D6.6 Release of the DEFACTO fast prototyping tool based on time - adaptive DEFACTO reduced p4D model under FOSS

Date: 15.11.2023

This document is a description of the DEFACTO D6.6 deliverable (contract no. 875247 coordinated by CIDETEC). This document explains the details concerning the release of the DEFACTO fast prototyping tool based on time - adaptive DEFACTO reduced p4D model under a Free Open-Source Software (FOSS) license, which constitutes the deliverable D6.6 itself. In the document, the present capabilities of this tool and their extension in the planned updates are described. Some information concerning the used FOSS license and the distribution of the software using the project web page is included as well. Finally, a glimpse on the use of this software tool and some comments on the documentation provided are presented in the document.

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Project details

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Type of Action	RIA	**Coordinator**	*CIDETEC*
Contact persons	*Elixabete Ayerbe*		
Website	**www.defacto-project.eu**		

Deliverable details

Number	*D6.6*		
Title	*Release of the DEFACTO fast prototyping tool based on time - adaptive DEFACTO reduced p4D model under FOSS*		
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Dissemination level	Public	**Nature**	*Other (Software)*
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Deliverable responsible	CID	**Contact person**	*Elixabete Ayerbe*

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Final review and quality approval	Elixabete Ayerbe	CID	Project Coordinator	*eayerbe@cidetec.es*

Document History

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Content

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1 Executive Summary

In the framework of DEFACTO's work package 6, a fast-prototyping tool based on a time-adaptive reduced order model has been developed. As stated in DEFACTO's grant agreement, the software implementing this tool is being released under a Free Open-Source Software (FOSS) license. Deliverable D6.6 corresponds precisely to the first release of this software.

This software consists in one tool, which is based on a novel artificial intelligence algorithm known as physics-informed neural network (PINN). The tool is able to provide the evolution of lithium concentration in active material particles in both electrodes during a discharge process as well as the discharge curve of the full battery, based on the Single Particle Model [1].

The software is released using the GNU Affero General Public License version 3. This Free Open-Source Software (FOSS) license makes sure that any derivative work (including those related to cloud computing exploitation of the code) preserves the same freedoms offered now to any user of the released code.

The release of the tool is made through CIDETEC's GitHub. A repository with several files can be found there. The user just needs to download the repository and open the Jupyter notebook inside to use the tool.

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2 Introduction

Deliverable D6.6 corresponds to the release of a software tool able to prototype in a fast manner the design of a battery cell using an AI model. This document contains a description of the software tool which is available at the DEFACTO project website. According to DEFACTO's proposal this software tool is released under a Free Open-Source Software (FOSS) license.

In order to construct this software, an AI algorithm known as physics-informed neural network (PINN) has been used. This class of artificial neural network (ANN) techniques performs a regression analysis in order to identify the relationship between the solution of a differential equation and the independent variables (time and/or spatial variables) and, eventually, some model parameters. The (very) particular aspect of this AI technique is that it incorporates the differential equation itself (including initial and/or boundary conditions) in the training of the neural network (this is in sharp contrast to standard ANN where only the solution, obtained from experiments or numerical simulation, is used). This is done through the loss function, where residuals from the differential equation and error from initial and/or boundary conditions are incorporated. The loss function can also consider errors computed by comparison with stored solution data, but this is not essential. Thus, the PINN technique overcomes the need for large datasets since most of the information during the training (if not all) comes from the differential equation. This algorithm was developed in [2] and it is also reviewed in [3].

In the present case, a version of the PINN technique based exclusively on the differential equation and the initial and boundary conditions is considered (the ANN can then be trained without using any data). The inputs of the ANN will be the independent variables (time and the spatial point inside the particle), discharge C-rate and some cell parameters (100% initial SoC of the cell is assumed) while the ANN output will be (part of) the solution (lithium concentration in the active material particles). After training, the ANN will then be able to give (an approximation of) the solution of the initial value problem at any time.

Using two PINNs with Single Particle Model (SPM) equations as physics knowledge, the tool provides the evolution of lithium concentration in the active material particles in both electrodes during a discharge process and calculates the discharge curve of the full battery. It is trained using DEFACTO G/Si-NMC811 cell parameters and in wide ranges of geometrical parameters (thickness and porosity) and C-rates, in particular:

- Negative electrode thickness in [5e-5, 2e-4] m
- Positive electrode thickness in [5e-5, 2e-4] m
- Negative electrode porosity in [0.2, 0.6]
- Positive electrode porosity in [0.2, 0.6]
- C-rate from 1C to 3C

However, due to the training process, it can provide results even further. The tool will indicate to the user when its limits have been exceeded.

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3 How to use the released tool

The deliverable consists of a repository in CIDEMOD webpage where the user can find:

- DEFACTO G/Si-NMC811 default data ("data_DEFACTO").
- PINN model for negative electrode ("SPM NE").
- PINN model for positive electrode ("SPM PE").
- Jupyter notebook where the tool can be used ("PINN notebook").
- Script with required functions for the model to work ("PINN_utils")

Firstly, users need to download this repository in their personal computer. Then, in the notebook, the user can easily read how to proceed. Simply by running the indicated cells, all the required packages will be installed and the functions from "PINN_utils" imported. The tool is then ready to run simulations. As written in the notebook, users can use the existing example cells or create their own to request simulations. They just have to fill the desired values for the inputs and run the cell, the simulation will be given instantly. The inputs for the tool are:

- Negative electrode thickness (thickness_n) in meters.
- Positive electrode thickness (thickness_n) in meters.
- Negative electrode porosity (porosity_n).
- Positive electrode porosity (porosity_p).
- C-rate.

The values for these inputs will be written in `plot_Battery()` as follows:

```
plot_Battery(thickness_n= , thickness_p= , porosity_n= , porosity_p= , C_rate=1)
```

Three plots appear immediately after running the cell:

- Lithium concentration in negative electrode ($c_{s,NE}$ in mol/m^3) along the radius in the negative particle (r_{NE} in meters) for an instant of time (t in seconds).
- Lithium concentration in positive electrode ($c_{s,NE}$ in mol/m^3) along the radius in the positive particle (r_{PE} in meters) for an instant of time (t in seconds).
- Battery voltage (V in volts) for an instant of time (t in seconds).

Notice that the model is solved mathematically by the neural network, which may lead to situations that are possible mathematically but not physically in the electrode plots, such as extremely high (or low) lithium concentration in an electrode. In any case the full discharge curve is realistic, since it stops when one of the electrodes reaches its physical limit.

Example of the tool:

Inputs: `plot_Battery(thickness_n=1e-4, thickness_p=7e-5, porosity_n=0.5, porosity_p=0.3, C_rate=1)`

Output: shown in figure 1.

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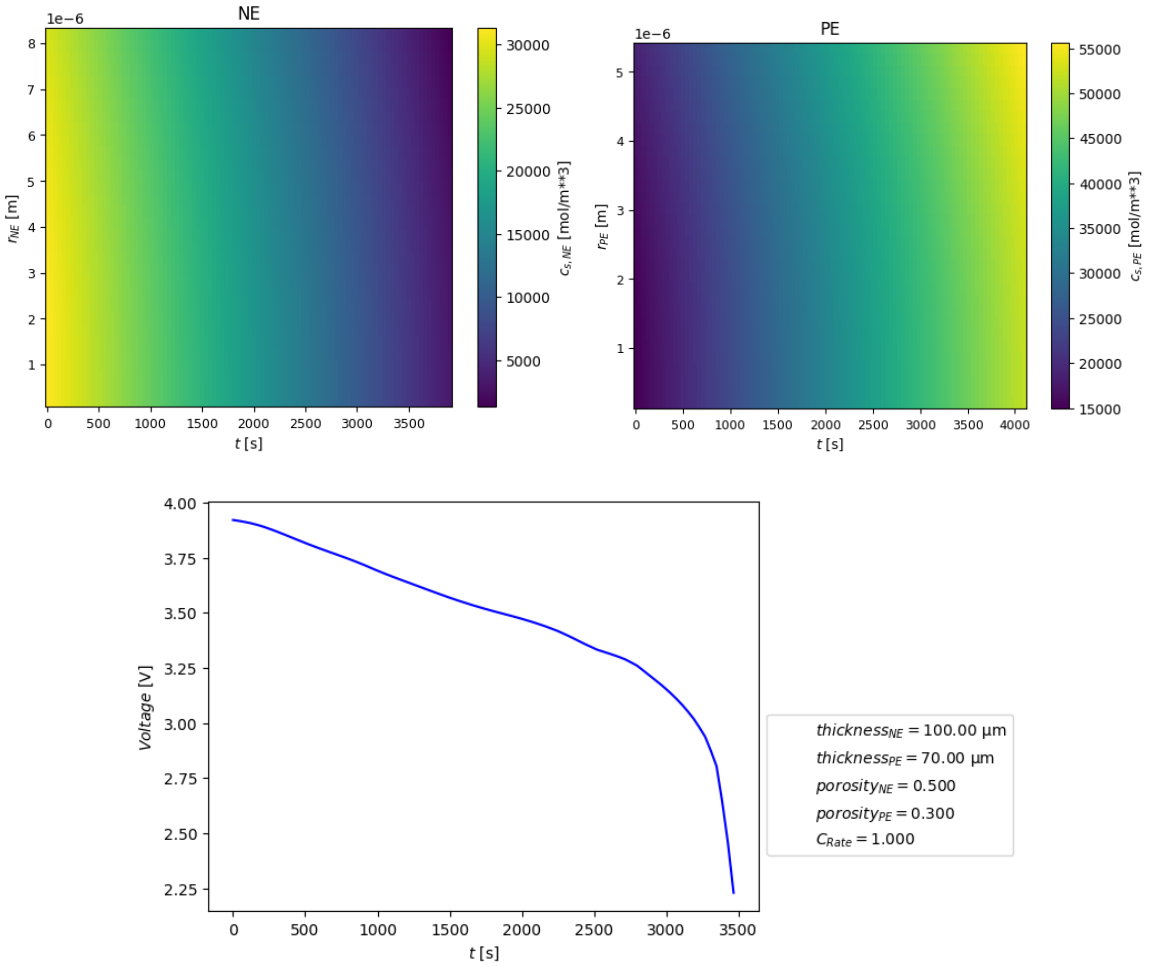

Figure 1. Tool output. Upper left: lithium concentration in negative electrode, upper-right: lithium concentration in positive electrode, down: discharge voltage curve.

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4 Free Open-Source Software license

The DEFACTO project established the release of the developed software using a Free Open-Source Software (FOSS) license. GNU Affero General Public License version 3 (AGPLv3 in short), and endorsed by the Free Software Foundation (https://fsf.org) was selected.

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5 Conclusions

A tool for fast prototyping based on an AI algorithm known as physics-informed neural network has been developed and released. It is an open and free tool that users can utilize to simulate lithium concentration in particle electrodes and discharge voltage curve for a wide range of parameters.

The tool is available at GitHub: https://github.com/cidetec-energy-storage/PINN-SPM-fast-prototyping

References

[1] G. Ning y B. Popov, «Cycle Life Modeling of Lithium-Ion Batteries,» *Journal of The Electrochemical Society,* vol. 151, 2004.

[2] M. Raissi, P. Perdikaris y G. Karniadakis, «Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations,,» *Journal of Computational Physics,* vol. Volume 378, pp. Pages 686-707, 2019.

[3] G. Karniadakis, . I. Kevrekidis, L. Lu, P. Perdikaris, S. Wang y L. Yang, «Physics-informed machine learning,» *Nature Reviews Physics,* vol. 3, p. 422–440, 2021.

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