DEFACTO - battery DEsign and manuFACTuring Optimisation through multiphysic modelling

D.5.3

Date: 30.11.2022

This document is a description of the DEFACTO D5.3 deliverable (contract no. 875247 coordinated by CIDETEC). This document explains the details concerning the release of the efficient DEFACTO p4D cell model describing electrochemical and mechanical ageing ready for ROM, which constitutes the deliverable D5.3 itself. This deliverable provides an efficient yet accurate code for the numerical resolution of the p4D model with electrochemical and mechanical ageing, developed over an open-source platform. In the document, the present capabilities of this tool (called cideMOD v1.0.0) are described. 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

Project acronym	DEFACTO	**Start / Duration**	*01/01/2020 (42 months)*
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Website	**www.defacto-project.eu**		

Deliverable details

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Deliverable Contributors

	Name	Organization	Role / Title	*E-mail*
Deliverable leader	María Yáñez	CID	PhD Project Manager	myanez@cidetec.es
Contributing Author(s)	Raúl Ciria	CID	Partner	rciria@cidetec.es
	Clara Ganuza	CID	Partner	cganuza@cidetec.es
	Rubén Parra	CID	Partner	rparra@cidetec.es
	Diego del Olmo	CID	Partner	ddelolmo@cidetec.es
	Elixabete Ayerbe	CID	Partner	eayerbe@cidetec.es
Reviewer(s)	Jochen Zausch	FHG	WP5 leader	jochen.zausch@itwm.fraunhofer.de
Final review and quality approval	María Yáñez & Elixabete Ayerbe	CID	Project Coordinator	myanez@cidetec.es eayerbe@cidetec.es

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02.12.2022	3.0	FHG	Revision by WP leader
02.12.2022	4.0	CID	Final revision

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1 Acronyms and abbreviations

AGLP	Affero General Public License
DFN	Doyle-Fuller-Newman (model)
DMC	Dimethyl carbonate
EC	Ethylene carbonate
FOSS	Free Open-Source Software
GPL	General Public License
LAM	Loss of active material
p2D	Pseudo two-dimensional
p3D	Pseudo three-dimensional
p4D	Pseudo four-dimensional
pxD	Pseudo-X-dimensional
ROM	Reduced Order Model

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2 Executive Summary

In the framework of DEFACTO work package 5, an efficient DEFACTO p4D cell model describing electrochemical and mechanical ageing ready to integrate reduced order models (ROM) has been developed. As stated in DEFACTO grant agreement, deliverable D5.3 corresponds precisely to an updated release of the software cideMOD over an open-source platform (a first version of this tool was released in deliverable D6.1). These updated tool (called cideMOD v1.0.0 and developed in WP5) implements a continuum pseudo four-dimensional model (p4D) for a battery cell.

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. CIDETEC's open-source tool cideMOD documentation details the main aspects concerning the software organization.

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3 Introduction

The deliverable D5.3 corresponds to the release of an efficient DEFACTO p4D cell model describing electrochemical and mechanical ageing ready for reduced order models techniques implementation. This document contains a description of the software tool, which is now available at GitHub (https://github.com/cidetec-energy-storage/cideMOD), a provider of internet hosting for software development and version control.

This tool corresponds to a simulation software, called cideMOD v1.0.0, able to solve p2D, p3D and p4D continuum models. It is based on the FEniCS finite element library [1] and an extension of this library called multiphenics [2] . The meshing tool Gmsh [3] is also used. FEniCS library, multiphenics extension and Gmsh meshing tool are distributed under FOSS licenses.

cideMOD is copyright (C) 2022 of CIDETEC Energy Storage and is distributed under the terms of the Affero GNU General Public License (GPL) version 3 or later.

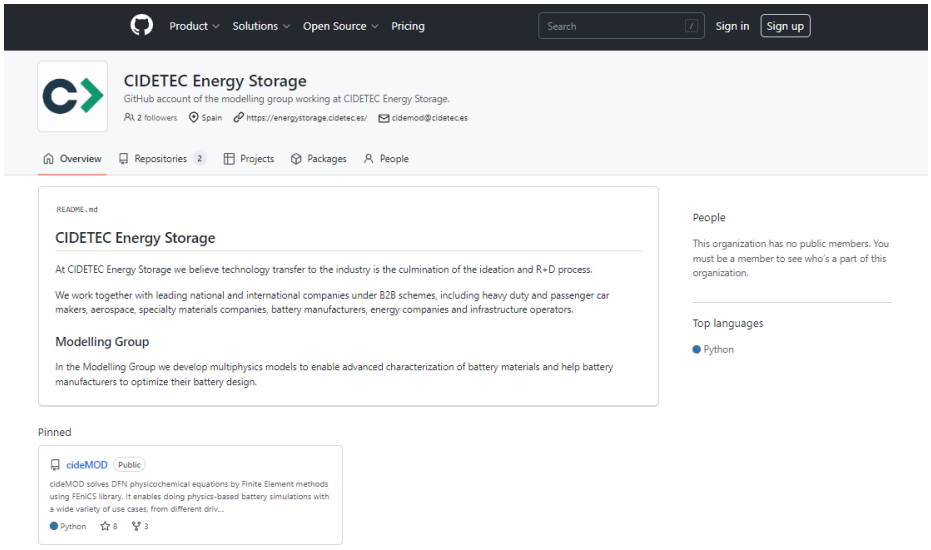

Figure 1. Screenshot of CIDETEC Energy Storage's GitHub platform

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4 Software documentation

Programming documentation includes a document detailing the main aspects concerning the software organization. Documentation on Python subprograms has been collected using the Sphinx tool (https://www.sphinx-doc.org) thus providing a very convenient interface to access software documentation, that it is available in the following here (https://cidemod.readthedocs.io/en/latest/). Figure 2 shows an example of this interface.

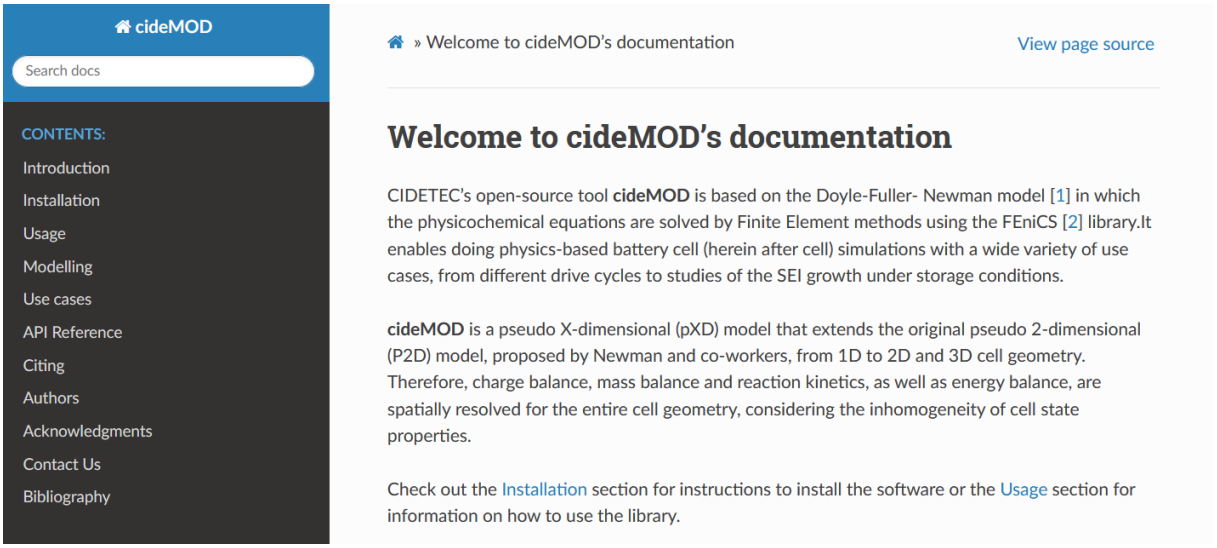

Figure 2. Corresponding cideMOD's documentation interface

4.1 Introduction

The cideMOD tool v1.0.0, released within deliverable D5.3, is a pseudo-X-dimensional (pXD) model that extends the original pseudo-2-dimensional (P2D) model, proposed by Newman and co-workers [4] for the modelling of lithium-ion battery cells to work with 1D, 2D or 3D cell geometries coupled to the mechanical ageing model. In the DEFACTO project the focus is put on the 3D geometry and therefore in the p4D model. Therefore, charge balance, mass balance and reaction kinetics, as well as energy balance, are spatially resolved for the entire cell geometry, considering the inhomogeneity of cell state properties. The current version of cideMOD (detailed in this deliverable) couples the version of the tool in which apart from the electrochemical model, thermal model as well as SEI growth was included, includes the loss of active material due to concentration gradients in the active particles. In addition, the tool also supports several active materials in the electrodes, and, nonlinear and temperature dependent electrode and electrolyte transport properties.

The library is built on top of FEniCS, using it as the underlying finite element and automatic differentiation engine. The cideMOD library allows the simulation of different battery configurations with arbitrary materials in a single interface. Making use of Gmsh meshing software, different battery shapes can be created and simulated including the tab position for optimal configuration, as well as highly customizable simulation conditions. It also comes with a simplified interface to run automatically arbitrary testing conditions, cycling protocols and usage profiles.

Read the Introduction Section in the documentation for more information.

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4.2 Software Installation

The preferred way to install and use cideMOD is using the Docker image of multiphenics. Optionally, one can install cideMOD in a FEniCS working environment (with multiphenics) by downloading everything from source and installing it with the Python package manager.

Read the Installation Section in the documentation for more information and installation options.

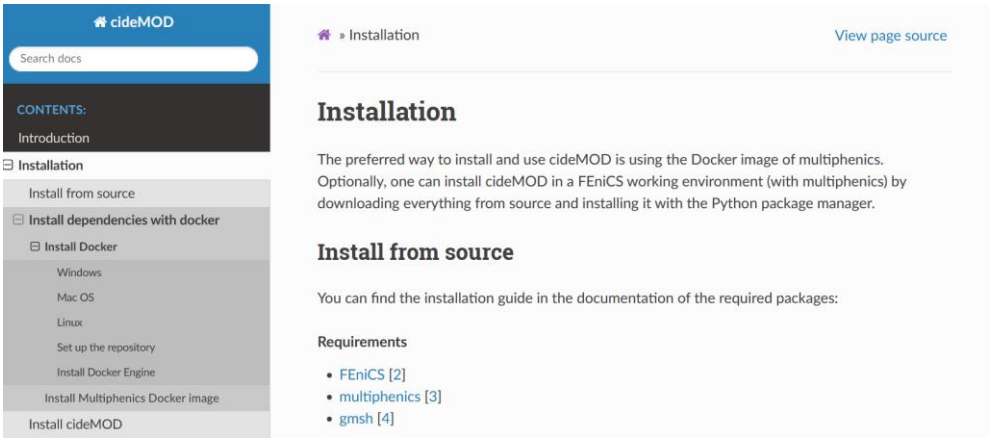

Figure 3. cideMOD software Installation

4.3 Usage section

Within this usage section, it is described in depth which are the different mandatory INPUTS and OUTPUTS of cideMOD. Cell properties and material parameters are specified in a single json file or optionally a Python dictionary can be used as well. Several examples of different cell datasets are given under the data folder. The json file must contain different mandatory objects:

- Structure: The "structure" entry determines the configuration of the cell. It is a list containing the tags of the different subdomains in order. The easiest configuration would be ["a","s","c"] corresponding to a cell composed of an anode, separator and cathode. A cell composed of two units could have this other structure ["ncc","a","s","c","pcc","c","s","a","ncc"]. All the subdomains specified in the “structure” entry must have its own entry defined in the following points.
- Current collectors: There is a distinction between the "positiveCurrentCollector" and "negativeCurrentCollector", as they often have different properties. These keywords must contain geometry properties and conductivity. If the thermal model is used, thermal properties should be specified as well.
- Electrodes: There is a distinction between the "positiveElectrode" and "negativeElectrode", as they have different properties. These keywords must contain information about geometry, porosity, and conductivity. If the thermal model is used, thermal properties should be specified as well. Additionally, electrodes should contain a list of the active materials that it contains.

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- **Active materials:** Each electrode can have one or more active materials. These are specified as dictionaries with the electrochemical properties that they have.
- **Separator:** The "separator" keyword must contain geometry and porosity properties. If the thermal model is used, thermal properties should be specified as well.
- **Electrolyte:** The "electrolyte" keyword must contain the electrochemical properties such as diffusivity, conductivity, transference number and activity parameter. If the thermal model is used, thermal properties should be specified as well.

There are two kinds of outputs available. For each simulation, the library saves results to a folder on the fly in case of internal variables, and at the end of the time-loop in the case of global variables.

- **Internal variables:** These are the problem variables, or any derived value that has different values for each point in the cell geometry. These are automatically defined in the code and written in the XDMF Format. The parameter store_delay can be modified to a negative value to suppress this output, or to a positive value to specify the frequency (in timesteps) at which the results are saved to the disk.
- **Global variables:** These are overall cell figures (for example, cell voltage, current, maximum temperature, etc.), that are calculated and saved as a list of values over time internally in the memory. When the time iterations are finished, they are saved to disk as text files.

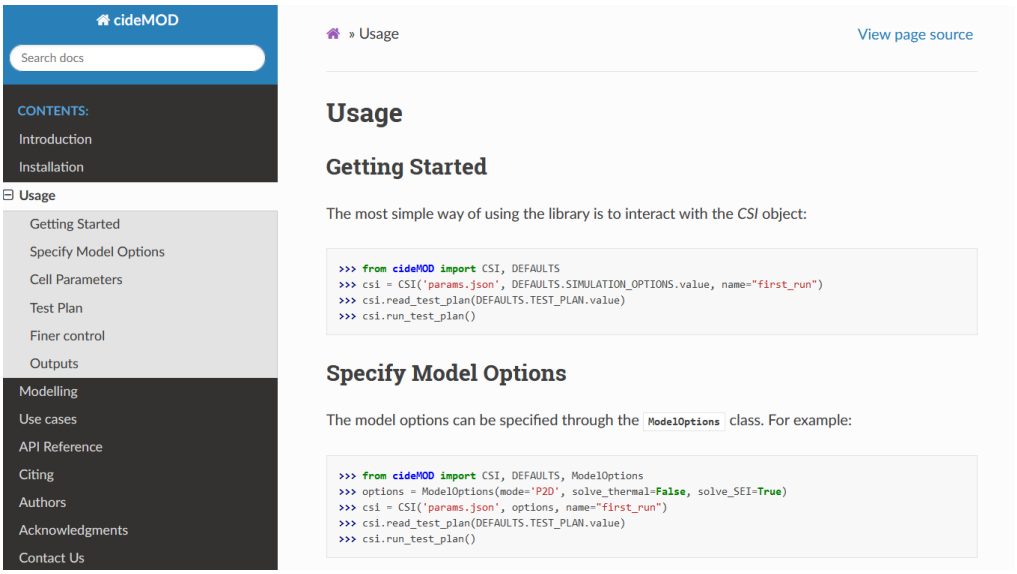

Figure 4. cideMOD usage section

Read the Usage Section in the documentation for more information and specify model options.

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4.4 Modelling

Depending on the physics of the mechanisms taking place in each domain, a different set of variables is taken into account on each domain. Here we define the models included in cideMOD and the domains that they involve. Some of the features of the p4D model are summarized here:

General features: The dimensions of these domains can be customized in the cell parameter JSON file. The structure of the cell can be customized up to certain level.

- Customizable pouch cell geometry and tab position.
- Highly customizable simulation conditions.
- Portable input/output format (json/[xdmf-txt]).

Electrochemical model: Electrolyte potential and concentration (and) are defined in the electrodes as well as in the separator. Solid phase potential () is defined only at the electrodes. At the current collectors there is also a solid phase potential but due to the disparity of conductivity scales, another variable is created , and continuity is imposed at the interface between electrode and current collectors with a Lagrange multiplier. Particle concentration () and intercalation current density () are also defined as variables but only at their corresponding electrode. This means that each electrode has many of these variables as active materials.

Thermal model: Temperature (T) is a scalar function defined in all of the domains. Heat sources considered are ohmic, polarization and reaction heat sources. In isothermal simulations (solve_thermal=False) the temperature is set as a constant value over the domain.

Electrochemical ageing models:

- SEI growth model: The anode SEI model implemented is based on Safari et al. (2009) [5] and it assumes that the electrolyte solvent concentration (primarily EC and DMC) is the limiting factor for SEI growth. Therefore, solvent species (cEC) transport across the SEI is solved with an spectral method using Laplace polynomials. Additionally, the side reaction current density and SEI thickness are defined in the anode (jSEI and δSEI).

Mechanical ageing model

- LAM model: The LAM model estimates the loss of active material due to particle cracking driven by stresses. Therefore, the decrease of the volume fraction of active material (εs) is computed as described on O'Kane et al. [6] and implemented following an explicit Euler time integration scheme. Hydrostatic stresses (σh) are computed following the stress model described on Zhang et al. [7]

Read the Modelling Section in the documentation for more information and installation options.

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4.5 Application example cases

In the repository or docker image, several use cases are included together with corresponding literature datasets used in the examples. [5], [8], [9]

- **Single Discharge:** This is one of the most basic use cases to simulate a single discharge using the low-level Problem interface.
- **Storage:** In this case, using the CSI interface, we can simulate the degradation under rest conditions.
- **Cycling:** Using a different test plan, we can simulate a cycling protocol.

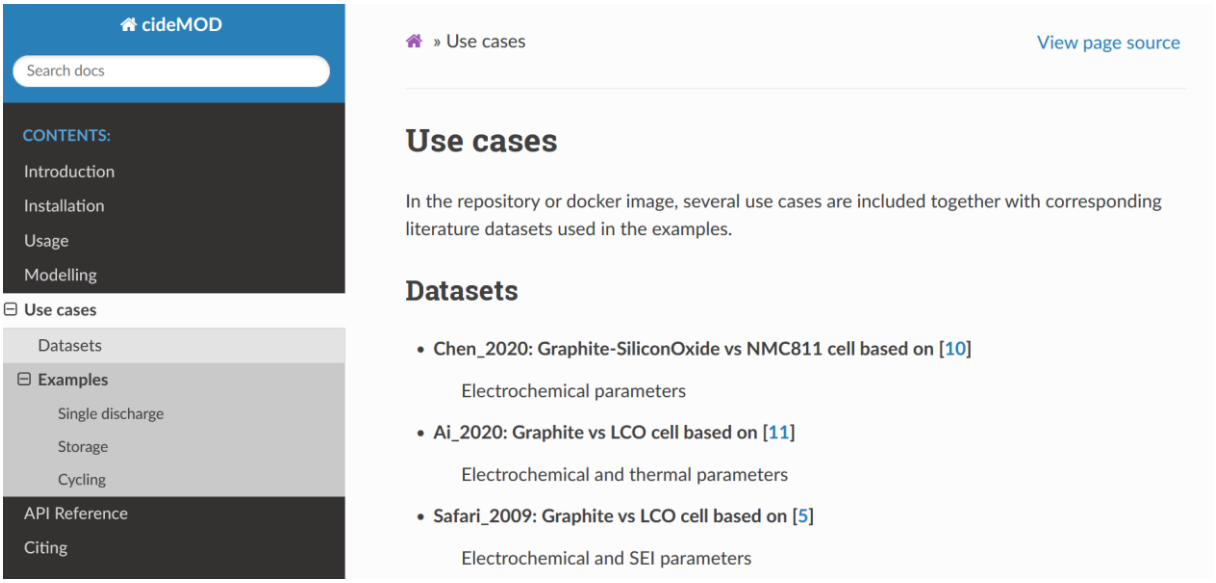

Figure 5. cideMOD use case section

Read the Examples Section in the documentation for more information.

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4.6 Acknowledgments

This software code cideMOD v1.0.0 has been developed within the framework of the project DEFACTO funded by the European Union's Horizon 2020 research and innovation programme, grant agreement no. 875247.

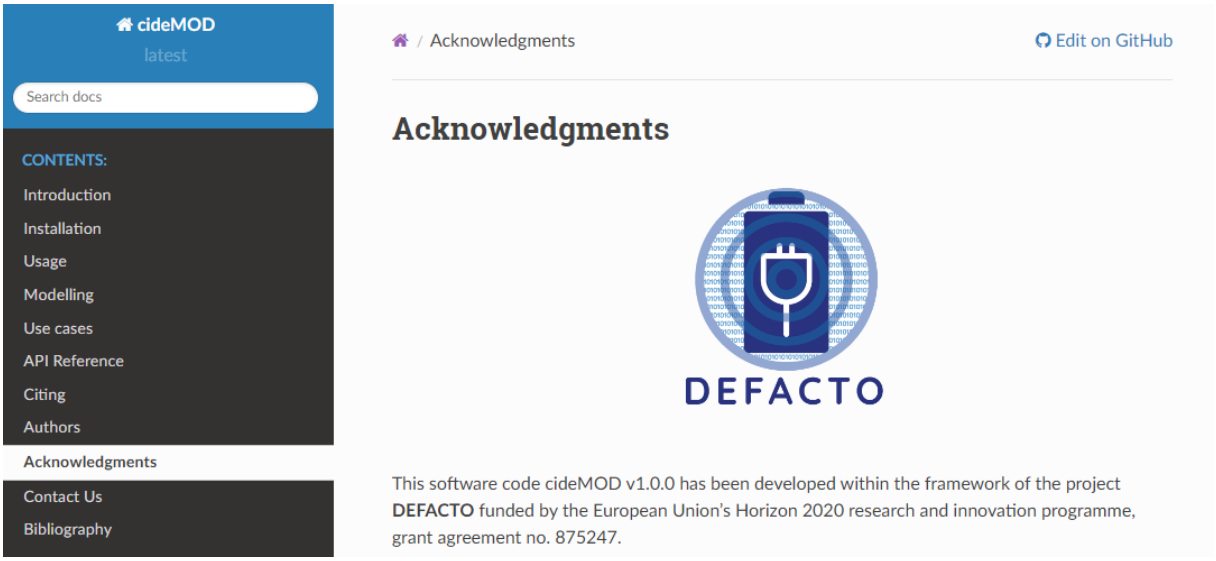

Figure 6. cideMOD acknowledgments

For issues and bug reports visit: https://github.com/cidetec-energy-storage/cideMOD

For other questions about cideMOD, you are welcome to contact us via email: cidemod@cidetec.es

5 Conclusions

As explained in the current D5.3, the release of the efficient DEFACTO p4D cell model describing electrochemical and mechanical ageing ready for ROM (developed in WP5 task T5.5) under a Free Open-Source Software (FOSS) license has been accomplished.

In this document, an explanation of the most important aspects of this software release (which constitutes the D5.3 deliverable itself) has been presented. In particular, (1) the main features of the software tool have been described, (2) software distribution and installation has been briefly described, (3) a short overview of software use through examples has been presented, and (4) distributed documentation has been discussed.

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