DEFACTO - battery DEsign and manuFACTuring Optimisation through multiphysic modelling

D.2.1. Report on the definition of parameters required for modelling and description of the validation protocol

Date: 31/05/2020

This document is the Defacto D2.1 deliverable (contract no. 875247 leaded by CIDETEC). This document contains all relevant information regarding parameters required for modelling tasks of the project. It defines the nature and the sensitivity requirements for input parameters and the appropriate experiments and characterisation techniques. It provides first a list of usage scenarios, physical and chemistry characteristics and the associate experiments and characterisation techniques. Secondly, this report presents the list of samples for each experiment and the protocols of test associated, taking into account the three cell chemistries studied in the project (NMC622/G, NMC811/G-Si, LMNO/G-Si). Finally, the data type and format are defined.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 875247.

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Project details

Project acronym	DEFACTO	**Start / Duration**	*M1 / 42 months*
Topic	LC-BAT-6-2019	**Call identifier**	*H2020-LC-BAT-2019-2020*
Type of Action	RIA	**Coordinator**	*CIDETEC*
Contact persons	Elixabete Ayerbe		
Website	https://defacto-project.eu/		

Deliverable details

Number	*D2.1.*		
Title	*Report on the definition of parameters required for modelling and description of the validation protocol*		
Work Package	*WP2 - Testing, analytical tools and characterisation*		
Dissemination level	PU	**Nature**	*R*
Due date (M)	M3	**Submission date (M)**	*M3*
Deliverable responsible	**CEA**	**Contact person**	***Mathias GERARD***

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Document History

Date	Version	Name	Changes
05/06/2020	1	D2.1-v1	Initial document
XX/XX/XXXX	2	D2.1-v2	Contributions from XXX

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Content

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1 Executive Summary

The DEFACTO project objective is to develop a multiphysics and multiscale modelling integrated tool to better understand the material, cell and manufacturing process behaviour, therefore allowing accelerating cell development and the R&I process. The work is based on an iterative exchange process for model development, validation and optimisation using cell technologies for the automotive market.

D2.1. deliverable defines the parameters required for modelling and describes the associated validation protocols. It gathers contributions from all DEFACTO partners involved in modelling and characterization work namely **CEA, IRI, ABEE, CERTH, CID, DLR, TUBS, UPM, ESI, FHG** and contains:

- A list of physical and chemistry characteristics and the associate experiments and characterisation techniques,
- A list of samples for each experiment and the protocols of test, taking into account the three cell chemistries studied in the project (NMC622/G, NMC811/G-Si, LMNO/G-Si),
- The definition of the data type and format,
- Different usage scenarios.

It has been prepared in Task 2.1, started at M1 and ending at M3, through a dedicated workshop held on February 27th, 2020 and multiple cross-exchanges between partners.

2 Acronyms and abbreviations

NMC	$LiNi_xMn_yCo_zO_2$ with x+y+z=1
NMC622	$LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$
NMC811	$LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$
LMNO	$LiMn_{1.5}Ni_{0.5}O_4$
G	Graphite
Si	Silicon
PNM	Pore Network Model
P4D	Pseudo 4D
DEM	Discrete Elements Method
CFD	Computational Fluid Dynamics
LBM	Lattice Boltzmann Model

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3 Introduction

The DEFACTO project objective is to develop a multiphysics and multiscale modelling integrated tool to better understand the material, cell and manufacturing process behaviour, therefore allowing accelerating cell development and the R&I process. The work is based on an iterative exchange process for model development, validation and optimisation using two cell technologies for the automotive market: an industrial scale state of the art Layered Oxide $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ NMC622/Graphite cell (NMC622/G) and a competitive Nickel Rich Layered Oxide $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ NMC811/silicon-carbon composite prototype (NMC811/G-Si). Additionally, High-Voltage Spinel Oxide $LiNi_{0.5}Mn_{1.5}O_4$ /silicon-carbon composite (LMNO/G-Si) will be studied to explore the versatility of the built models.

Modelling work in DEFACTO WPs 3 to 6 requires input parameters and data for validation. Before starting the experimental work, it has been necessary to define precisely the nature, the sensitivity requirements for input parameters and the appropriate experiment and characterisation techniques. To achieve this goal, an internal workshop with IRI, modelling and experimental team from partners was organized in February 27th, 2020. The output of this workshop has been first a list of physical and chemical characteristics and the associate experiments and characterisation techniques. Secondly, the list of samples for each experiment and the protocols of test have been defined, taking into account the three cell chemistries studied in the project (NMC622/G, NMC811/G-Si, LMNO/G-Si). Finally, the last output of the task 2.1 has been the definition of the data type, format and a list of usage scenarios.

4 List of Models

In DEFACTO project, it is planned to build the multiscale models following a bottom-up approach: atomistic models parameters will be scaled up onto homogenised parameters to be used in the continuum model. DEFACTO will extend the scale range from atomistic to continuum and the physical domains covered (adding mechanical ageing mechanisms to the electrochemical ones) of the cell performance and ageing model built. To do so, different codes and models will be used (Table 1).

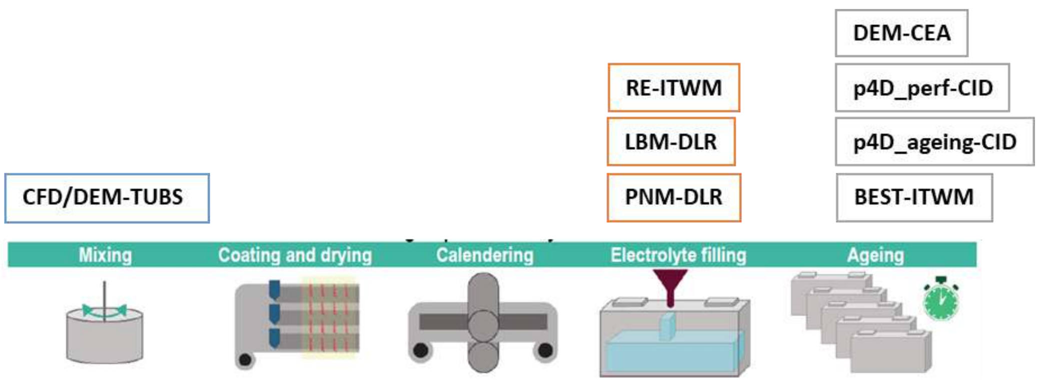

Figure 1 : models of DEFACTO project in the process worfflow

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Table 1 : List of models to developed in DEFACTO project

WP	Model codename	Method/Software	Scale	Output from model and characterization	Output for battery optimisation
WP3	CFD/DEM-TUBS	Discrete Elements Method with LIGGGHTS coupled with Computational Fluid Dynamics (OpenFOAM)	Electrode/ Slurry	Slurry composition after dispersing and microstructure after drying and calendering	Optimisation of carbon black structure for maximum electric conductivity. Optimisation of the mixing process. Efficient electrode structure prediction, optimisation structure regarding ionic and electric conductivity. Mechanical integrity. Systematic electrode design.
WP4	LBM-DLR	Lattice Boltzmann using in-house code	Electrode	Wetting behaviour and electrolyte distribution	Optimised electrode materials and structures. Optimal electrolyte filling process conditions
WP4	PNM-DLR	Pore Network Models with openPNM	Electrode/ Cell	Wetting behaviour and electrolyte distribution	
WP4	RE-ITWM	Richards-Equation using in-house code	Cell	Simulation of filling process	
WP5	DEM-CEA	Discrete Elements Method with LIGGGTHS	Electrode	Mechanical behaviour of electrode (performances and ageing)	Deformation (evolution of microstructure) and change of material properties due to mechanical ageing. Efficient continuum model (p4D cell model) including mechanical and electrochemical ageing (addressing inhomogeneous and homogeneous ageing). Optimum conditions for using and battery pack design.
WP5	p4D_perf-CID	Finite Element platform FENICS	Cell	Electrochemical and mechanical behaviour of the cell	
WP5	p4D_ageing-CID	Finite Element platform FENICS	Cell	Electrochemical and mechanical degradation of the cell	
WP5	BEST-ITWM	Continuum model	Electrode	Mechanical behaviour of electrode (performances and ageing)	

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5 List of Model requests

During the internal workshop with all DEFACTO partners, all the data required to build and validate each model have been listed. The following tables list all these data and detail the data usage (input parameters, model calibration[1] or model validation[2]) and expected delivery date. Some methods for data determination have been proposed and experimental techniques available in DEFACTO partners' facilities have been identified.

Table 2 : List of requested data for WP3 models construction and validation on electrode processing

WP	Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments	When is data needed
WP3	CFD/DEM-TUBS	model input parameter	Solvent viscosity (solvent for slurry preparation)	Rheological Measurements	Rheology electrode	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Solvent surface tension	Tensiometer	Tensiometer	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Solvent density	Mass/Volume ; literature for water and NMP solvent	Solvent density	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Particle Shape	µCT (T3.5)	µCT	M20 to M32
WP3	CFD/DEM-TUBS	model input parameter	Particle size distribution (Active Material + Additive)	Laser diffraction analysis	Laser diffraction	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	AM and Additive density	Literature pycnometer	Pycnometry	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Poisson's ratio of AM and additive particles	Literature	Literature	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Coefficient of restitution of particles	Literature	Microcompression/ Nanoindentation	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Young's modulus of AM and additives	Nanoindentation Literature	Microcompression/ Nanoindentation	M12 to M32
WP3	CFD/DEM-TUBS	model calibration	Friction coefficients	Angle of repose	Angle of repose	M12 to M32
WP3	CFD/DEM-TUBS	model calibration/ validation	CB agglomerate strength	Microcompression	Microcompression/ Nanoindentation	M12 to M32
WP3	CFD/DEM-TUBS	model calibration	VdW-Attraction/Electrostatic repulsion	Zeta Potential Measurement, Agglomeration Kinetics	Zeta potential	M12 to M32

[1] Model calibration also called analytical validation, refers to the identification of individual parameter
[2] Model validation refers to the comparison and quantification of the results obtained by numerical simulation and experimental data.

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WP3	CFD/DEM-TUBS	model input parameter	Slurry viscosity	Rheological Measurement	Rheology electrode	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Shear rate during dispersing	Simulation/Calcul. based on stirrer tip speed/planetary motion, viscosity	Simulation	M12 to M33
WP3	CFD/DEM-TUBS	model calibration/ validation	Electrode 3D structure before and after calendering	SEM, µCT in T2.2 and T3.5	FIB-SEM and µ-CT	M16 to M32
WP3	CFD/DEM-TUBS	model calibration/ validation	Pore size distribution of electrodes	Mercury intrusion	Mercury intrusion	M16 to M32
WP3	CFD/DEM-TUBS	model calibration/ validation	Binder distribution	SEM, EDX on cathode, Later Induced Breakdown Spectroscopy on anode with CMC	SEM-EDX	M16 to M32
WP3	CFD/DEM-TUBS	model input parameter	Mass related slurry component concentrations	simple calculations based on formulations used in WP7	Simulation & Slurry density	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Coating thickness right before drying	in line measurement	Coating thickness	M12 to M33
WP3	CFD/DEM-TUBS	model input parameter	Coating temperature during drying	Infrared, T° sensor	Coating_T_drying	M12 to M32
WP3	CFD/DEM-TUBS	model input parameter	Convection	Volumetric flow measurement	Flow_T_drying	M12 to M33
WP3	CFD/DEM-TUBS	model input parameter	Air temperature	T° sensor	Flow_T_drying	M12 to M34
WP3	CFD/DEM-TUBS	model input parameter	Drying rate	Solvent content during drying/coating mass during drying/ coating thickness during drying	Electrode thickness drying	M12 to M33
WP3	CFD/DEM-TUBS	model calibration/ validation	Adhesion strength	Material Testing Machine	Electrode adhesion strength	M16 to M32
WP3	CFD/DEM-TUBS	model calibration/ validation	Micromechanical properties of electrode	Nanoindentation	Microcompression/ Nanoindentation	M16 to M32
WP3	CFD/DEM-TUBS	model calibration/ validation	Electrode thickness before and after calendering	laser triangulation for contact-free measurement (or tactile measurement if not available)	Electrode thickness	M20 to M32
WP3	CFD/DEM-TUBS	model calibration/ validation	Electrode elastic reconvery thickness during calendering (depending on gap between rolls)	Force-Sensors, Displacement Sensors, in line measurement	Electrode thickness calendering	M20 to M32
WP3	CFD/DEM-	model	Temperature of		T-calendering	M20 to

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	TUBS	calibration/ validation	calender rolls			M33
WP3	CFD/DEM-TUBS	model calibration/ validation	Lab scale drying behavior for model development	Tabletop coater + heating + laser triangulation	Electrode thickness drying	M12 to M32

Table 3 : List of requested data for WP4 models construction and validation on electrolyte filling process

WP	Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments	When is data needed
WP4	LBM/PNM -DLR	model input parameter	Electrode and separator morphology	3D-FIB-SEM in T2.3 and DEM Simulations in WP3	FIB-SEM and µ-CT and tortuosity separator	M12 to M24
WP4	LBM/PNM -DLR	model input parameter	Electrolyte surface tension	Tensiometer	Tensiometer	M12 to M24
WP4	LBM/PNM -DLR	model input parameter	Electrolyte contact angles with active materials, separator	Optical measurements on model materials	Angle of repose	M12 to M24
WP4	LBM/PNM -DLR/RE-ITWM	model input parameter	Electrolyte density	Balance	Electrolyte density	M12 to M24
WP4	LBM/PNM -DLR/RE-ITWM	model input parameter	Electrolyte viscosity	Rheometer	Rheology electrolyte	M12 to M24
WP4	LBM/PNM -DLR/RE-ITWM	model calibration/validation	Pressure Saturation curves of electrodes and separator	Measurements in special setup	p-s-curves	M12 to M24
WP4	RE-ITWM	model calibration/validation	Relative permeabilities of electrodes and separator	calculation; empirical approximation	Angle of repose	M12 to M24
WP4	LBM/PNM -DLR/RE-ITWM	model calibration/validation	Electrolyte distribution pore scale	Ultrasonic acoustic wave or operando tomography/radiography with extra-collaboration with Large Instruments?	Acoustic and Chronoamperometry	M18 to M30
WP4	RE-ITWM	model validation	Electrolyte distribution cell scale	Impedance measurements on segmented cell	Segmented cell	M12 to M24
WP4	RE-ITWM	model validation	Pressure profiles of filling process over time	Pressure sensors in production process	Pressure electrolyte	M6 to M18

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Table 4 : List of requested data for WP5 models construction and validation on cell performances and ageing

WP	Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments	When is data needed
WP5	DEM-CEA	model input parameter	Young modulus of bulk active materials	DFT calculation in T5.1	Simulation	M12 to M24
WP5	DEM-CEA	model input parameter	Binder rheological behavior	nanoindentation	Microcompression/Nanoindentation	M12 to M24
WP5	DEM-CEA	model calibration /validation	SEI thickness evolution	2D imaging, XPS, thickness measurement upon aging	XPS and EQCM	M12 to M24
WP5	DEM-CEA	model input parameter	Electrode morphology	3D-FIB-SEM in T2.3	FIB-SEM and µ-CT	M12 to M24
WP5	DEM-CEA	model input parameter	Volume change of active materials in negative electrode	Literature or µ-CT? Or tomography with extra-collaboration with Large Instruments?	µCT	M12 to M24
WP5	DEM-CEA	model input parameter	Positive electrode swelling	Swelling measurement on monolayer pouch cell upon cycling with dedicated test bed	DFORM	M12 to M24
WP5	DEM-CEA	model input parameter	OCV profile	Literature and half cell or 3-electrodes measurements in T2.4	GITT	M12
WP5	DEM-CEA	model validation	Electrode thickness evolution	Swelling measurement on monolayer pouch cell upon cycling with dedicated test bed	DFORM	M24
WP5	BEST-ITWM	model input parameter	Young modulus of bulk active materials, binder and separator	calculation/experimental	DFORM for separator ; literature	M12 to M24
WP5	BEST-ITWM	model input parameter	Poisson ratio of bulk active materials, binder and separator	calculation/experimental	DFORM for separator ; literature	M12 to M24
WP5	BEST-ITWM	model input parameter	volumetric expansion coefficient of bulk active materials	calculation/ experimental	XRD?	M12 to M24
WP5	BEST-ITWM	model input parameter	electrode morphologies (3d)	calculation (WP3)	FIB-SEM and µ-CT	M12 to M24

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WP5	BEST-ITWM	model input parameter	Which other parameters might be relevant for mechanical aging? eg. yield strength of active materials	experimental	NA	M12 to M24
WP5	BEST-ITWM	model input parameter	max. Li Concentration of active materials	experimental/ literature	GITT	M12 to M24
WP5	BEST-ITWM	model input parameter	electronic conductivity of active materials	experimental/ literature	EIS	M12 to M24
WP5	BEST-ITWM	model input parameter	Li Diffusivity of active material	experimental/ literature	GITT	M12 to M24
WP5	BEST-ITWM	model input parameter	Butler-Volmer reaction rate of active materials	experimental/ literature	Electrochemical tests	M12 to M24
WP5	BEST-ITWM	model input parameter	OCV of active materials	experimental/ literature	GITT	M12 to M24
WP5	BEST-ITWM	model input parameter	ionic conductivity of electrolyte, and Carbon Binder	experimental/ literature	EIS	M12 to M24
WP5	BEST-ITWM	model input parameter	Li+ Diffusivity of electrolyte and Carbon Binder	Galvanostatic pulse-relaxation (Li-Li)	GITT	M12 to M24
WP5	BEST-ITWM	model input parameter	Li+ transference number of electrolyte	experimental EIS (Li-Li)/literature	EIS	M12 to M24
WP5	BEST-ITWM	model input parameter	effective electronic conductivity of Carbon Binder (optional)	literature	Literature	M12 to M24
WP5	BEST-ITWM	model input parameter	porosity of Carbon binder (optional)	literature	Literature	M12 to M24
WP5	BEST-ITWM	model validation	cell voltage	experimental	Electrochemical tests	M24
WP5	BEST-ITWM	model validation	Quantification of mechanical aging	experimental	Electrode adhesion strength	M24
WP5	BEST-ITWM	model validation	Electrode thickness evolution	experimental	DFORM	M24
WP5	p4D_perf-CID	model input parameter - electrolyte	Ionic conductivity	EIS (Electrode - Electrode)	EIS	M12 to M24
WP5	p4D_perf-CID	model input parameter - electrolyte	Diffusion coefficient in electrolyte	Galvanostatic pulse-relaxation (Li-Li)	GITT	M12 to M24
WP5	p4D_perf-CID	model input	Transference number	EIS (Li-Li)	EIS	M12 to M24

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		parameter - electrolyte				
WP5	p4D_perf-CID	model input parameter - electrolyte	Initial concentration	Material provider	Input of electrolyte manufacturer	M12 to M24
WP5	p4D_perf-CID	model input parameter	mechanical parameters/properties	Model upscaling from DEM-CEA and Cont-ITWM	Simulation	M12 to M24
WP5	p4D_perf-CID	model input parameter	Specific heat capacity (Cp), thermal conductivity	Thermal caracterization	ARC, TGA-GC	M12 to M24
WP5	p4D_perf-CID	model validation	Cell performance tests	C-rate tests, cell thermal inhomogeneities, electrode swelling with lithiation procedure.	Electrochemical tests	M12 to M24
WP5	p4D_ageing-CID	model input parameter	mechanism identification (SEI growth, Li plating), physicochemical equations, parameters estimation	Ageing tests with post-mortem analyses (NMR, TEM, dQ/dV, reference electrode measurement, ...)	Test campaign	M12 to M24
WP5	p4D_ageing-CID	model input parameter	mechanism identification (active material cracking, active material loss), physicochemical equations, parameters estimation	Ageing tests with DFORM at small pouch cell level	Test campaign	M12 to M24
WP5	p4D_ageing-CID	model validation	aging test results of finished cells, characterisation of finished electrodes, etc)	Ageing tests with deformation gauges? With tomography?	Test campaign	M12 to M24

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6 List of Experiments

The experimental characterisation and cell prototyping activities within the project will allow to build validate and optimise multiscale and multiphysics models which will improve the understanding of the mechanical and electrochemical processes occurring during cell manufacturing and performance: from the atomistic to the cell level, from the slurry mixing to the cell assembly and finishing steps. The following table list all the experiments which are needed to determine the model parameters defined previously. A short description and the data type are also defined for each experiment.

Table 5 : List of experiments to determine data for modeling

Name	Code Name	Type	Description	Data type
Micro Computed Tomography	µCT	Imaging	Electrode structure determination	Picture
Ultrasonic acoustic wave	Acoustic	Process	Ultrasonic acoustic wave transportation through batteries to study the filling kinetics of the porous structures by electrolyte and detect possible defects	Float functional
Angle of repose	Angle of repose	Process	Rotating drum/heap measurement	Point
Accelerated Rate Calorimeter	ARC	Thermal	Netzsch ARC 254 for cylindrical cells & Netzsch MMC 274 Nexus for button cells	Float functional
Chronoamperometry	Chronoamperometry	Electrochemical	Determination of time dependancy of filling process	Float functional
Coating thickness	Coating thickness	Process	Wet thickness: ultrasonic absorption Dry thickness: beta gauge and micrometer caliper Ultrasonic Absorption and Beta Gauge: Thickness as a function of the loading in g/m^2; for the double-side coated anode it is only possible to determine the loading of both sides simultaneously. Each side individually is not possible	Point
Coating temperature during drying	Coating_T_drying	Process	Single point measurement by infrared sensor	Point
DFORM	DFORM	Mechanics	In-house test bed to measure the swelling pouch cell upon cycling	Float functional
Incremental capacity	dQ/dV	Electrochemical	The dQ/dV analysis takes a refined step to estimate the capacity displaced in each incremental change of voltage in the reaction	Float functional
Electrochemical Impedance Spectroscopy	EIS	Electrochemical	Electrochemical impedance spectroscopy to determine ionic resistances, charge transfer resistance, transport numbers, and post-mortem analysis, using coin cells (half, symetric or full) configurations	Float functional
Electrochemical characterization of	Electrochemical tests	Electrochemical	C-rate and galvanostatic tests in coin cell and pouch cell at different	Float functional

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the cells			temperatures	
Electrode adhesion strength	Electrode adhesion strength	Mechanics	Adhesive strength of the electrode determined with pull-off adhesive test or simple in-house designed method	Float functional
Electrode thickness	Electrode thickness	Process	Micrometer caliper	Point
Electrode thickness during calandering	Electrode thickness calendering	Process	Measurement by the gap between calander rolls	Point
Electrode thickness during drying	Electrode thickness drying	Process	Tabletop coater + heating + laser triangulation. Specific measurement for lab scale kinetics of thickness during drying for model development	Float functional
Electrolyte density	Electrolyte density	Process	Precision balance	Point
Electrochemical quartz crystal micro balance	EQCM	Electrochemical	Measurement of layer deposition and stripping during operation of electrode (ex : growth of SEI layer during formation). Balance swings in a certain frequency and shows changes in electrode weight through changes in frequency	Float functional
Focus Ion Beam - Scanning Electron Microscopy	FIB-SEM	Imaging	Images 2D & 3D of the electrode microstructure	Picture
Air convection and temperature during drying	Flow_T_drying	Process	Hand unit to measure air flow	Float functional
Galvanostatic Intermittent Titration Technique	GITT	Electrochemical	Determination of OCV and diffusion coefficients in coin cells configuration	Float functional
Laser diffraction	Laser diffraction	Process	Particle size distributions of powders	Float functional
Mercury intrusion	Mercury intrusion	Process	Pore size distribution	Float functional
Microcompression/ Nanoindentation	Microcompression/ Nanoindentation	Mechanics	Mechanical behavior of particles and electrodes	Float functional
Nuclear Magnetic Resonance	NMR	Chemistry	Lithium metal detection	Float functional
Pressure during electrolyte filling	Pressure electrolyte	Process	Pressure sensors during electrolyte filling	Float functional
Capilary pressure saturation	p-s-curves	Process	Measurement of saturation of porous system for given capillary pressure	Float functional
Pycnometry	Pycnometry	Process	Density measurement of solids	Point
Reference electrode	Reference electrode	Electrochemical	Measurement of each electrode potential	Float functional
Rheology for electrode	Rheology electrode	Process	Measurement of solvent and slurry	Float functional
Rheology for electrolyte	Rheology electrolyte	Process	Measure viscosity of electrolye	Float functional
Segmented cell	Segmented cell	Process	Determination of time dependency of filling process with better accuracy than chronoamperometry. Can also be used to determine inhomogeneities of porous system, current distribution etc.	Float functional

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Scanning Electron Microscopy - Energy Dispersive X-ray spectrometry	SEM-EDX	Imaging	Image microstructure coupled with elemental analysis for material distribution in electrodes	Picture
Slurry density	Slurry density	Process	Precision balance; Coriolis mass flowmeter	Point
Solvent density	Solvent density	Process	Precision balance	Point
Transmission Electron Microscopy	TEM	Imaging	Image of crystal structure	Picture
Temperature of calendaring rolls	T-calendering	Thermal	The temperature of the rolls is measured externally with a hand-held equipment. It is also possible to measure and control the temperature of the flowing oil that is used to heat up the rolls.	Point
Tensiometer	Tensiometer	Process	Surface tension for solvent, electrode suspension	Point
Thermogravimetric analysis connected with gas chromatograph	TGA-GC	Process	TGA shows at which temperatures material decomposes into gas phase. Gas chromatograph is used to analyse evaporated species to determine which componed decomposes at which temperature.	Float functional
Estimation of separator tortuosity	Tortuosity separator	Process	Technique based on work of Landesfeind and uses two copper contacts in an electrolyte bath	Point
Xray Photoelectron Spectroscopy	XPS	Chemistry	Electrode surface analysis	Float functional
X-Ray Diffraction	XRD	Chemistry	Lithiation stage, identification of the phase	Float functional
Zeta potential	Zeta potential	Process	Electrostatic interactions between particles	Point

Global overview of the experiments and tests

Figure 2 and Figure 3 gives the global view of the different experiments and type of model parameters. In DEFACTO project, two work packages are dedicated to process modelling. Therefore, 55% of experiments proposed are linked to the process. Around 30% of experiments are electrochemical, thermal and chemical measurements directly linked to full cell behaviour. Such experiments will bring data for WP5 model development. Finally, some mechanical experiments and imaging are required at different scales and step of cell manufacturing process (WP3, 4) and tests in WP5.

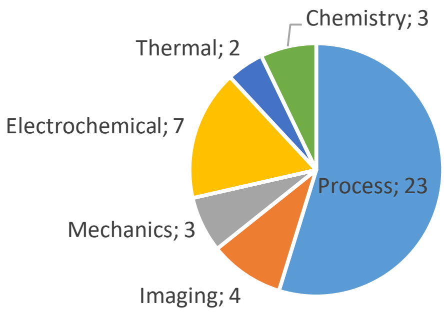

Figure 2 : Number of possible experiments in DEFACTO project

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Among all the parameters needed, 30 are process-type with on-line measurements (thickness, temperature, pressure) or physical parameters determination (viscosity, zeta potential, pore and particle size distribution…).

Process-type as well as electrochemical and mechanical experiments will be necessary both for model calibration and validation. Thermal and chemical analyses will be mainly used for model calibration in order to assess the full cell stability behaviour and identify main degradation reactions upon aging. Imaging experiments are required for all WP3-4-5 models as microscopy and tomography can bring useful information on microstructure.

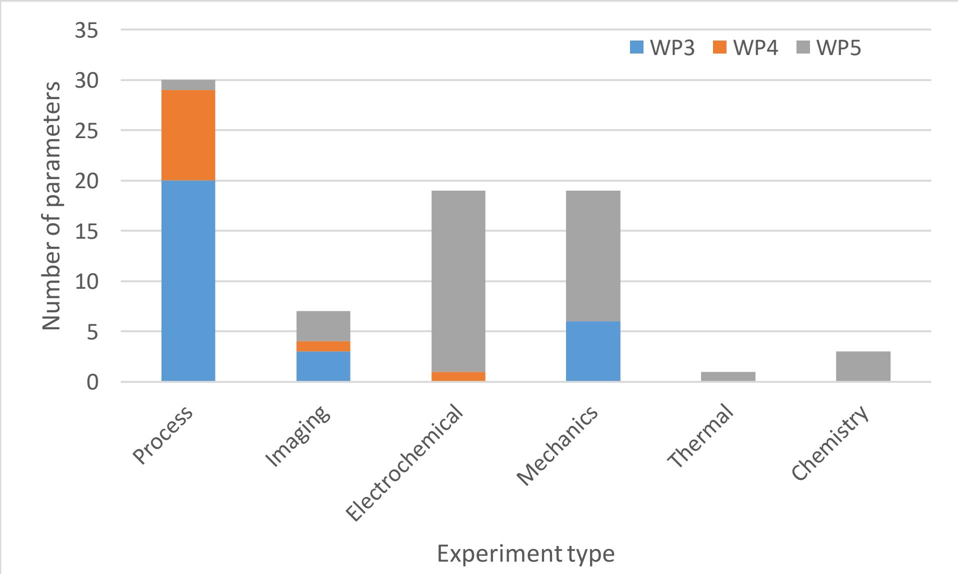

Figure 3 : Number of parameters required for WP3-4-5 models and type of experiment associated

7 List of usage scenarios

A typical profile from IRIZAR uses, corresponding to 273 kWh energy in their vehicle (12 m length) is shown below. The cycle is composed of 20 series of pulses, each series with 10-20 min duration, each pulse with 5-6 sec duration and maximum C-rate 1.3C in charge and 1C in discharge. Around 25% of time, the vehicle is in charge or discharge.

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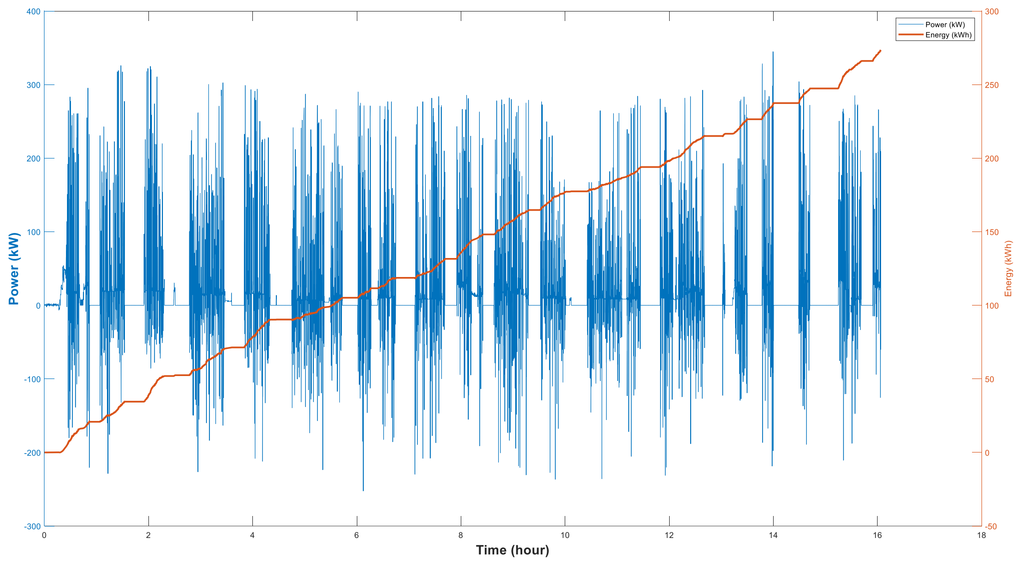

Figure 4 : Irizar power profile

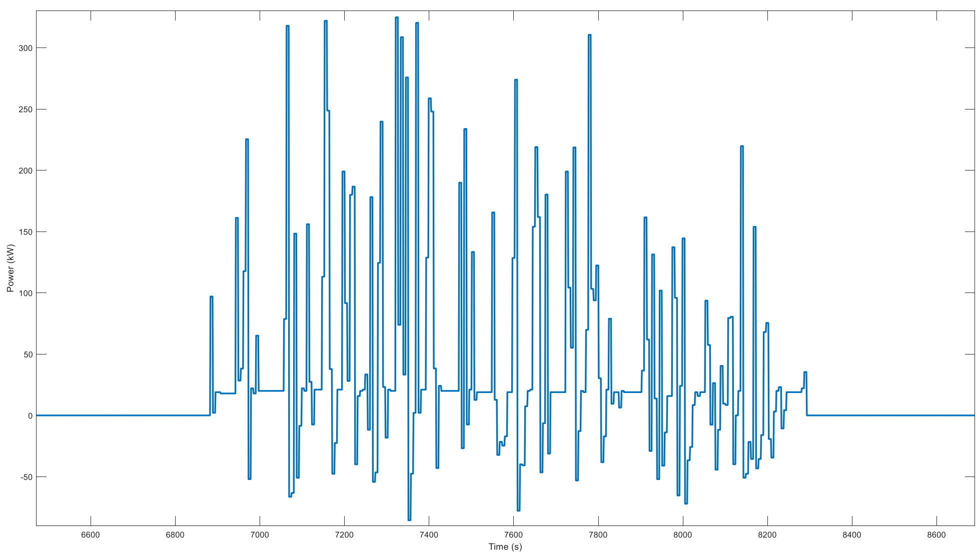

Figure 5 : zoom on the power profile peaks

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8 Conclusions

76 data and 42 possible experiments needed to build and validate models have been listed in this report. It takes into account all the manufacturing process steps and cell performances and ageing. DEFACTO modelling and experimental teams have exchange about their respective requirements and agreed on delivery time. Some experiments could be performed by several partners. It could be useful as backup or for cross-checking. At that time, 95% of input data required can be determined with experiments; the few remaining will be estimated from literature or calculation. The experimental work will now start in WP2-T2.2 to bring first input data for WP3-4-5 models. In parallel, a workshop will be organized in WP7 by LECLANCHE in order to specify more precisely the strategic parameters and boundary conditions for modelling of P and A cells manufacturing processes.

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