

CEN

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WORKSHOP

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AGREEMENT

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English version

Definition of parameters required for modelling of the material, cell and manufacturing process behaviour for battery cells for the automotive market - Part 1: Data required for modelling the material, cell and manufacturing process for cells for the automotive market

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European foreword

This CEN and CENELEC Workshop Agreement (CWA 18059-1:2023) has been developed in accordance with the CEN-CENELEC Guide 29 “CEN/CENELEC Workshop Agreements — A rapid prototyping to standardization” and with the relevant provisions of CEN/CENELEC Internal Regulations — Part 2. It was approved by a Workshop of representatives of interested parties on 2023-11-14, the constitution of which was supported by CEN and CENELEC following the public call for participation made on 2022-05-24. However, this CEN and CENELEC Workshop Agreement does not necessarily include all relevant stakeholders.

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Introduction

Modelling the material, cell and manufacturing process behaviour allows to accelerate cell development and the R&D process. The work can be done 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 $\text{LiNi}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$ NMC622/Graphite cell (NMC622/G) and a competitive Nickel Rich Layered Oxide $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$ NMC811/silicon-carbon composite prototype (NMC811/G-Si). Additionally, High-Voltage Spinel Oxide $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ /silicon-carbon composite (LMNO/G-Si) can be studied to explore the versatility of the built models.

Modelling work requires input parameters and data for validation. Before starting the experimental work, it is necessary to define precisely the nature, the sensitivity requirements for input parameters and the appropriate experiments and characterisation techniques for a list of physical and chemical characteristics.

This CWA is based on some of the results of the European Union's Horizon 2020 research and innovation programme [DEFACTO](#) (funded under grant agreement No 875247).

1 Scope

This document specifies the data required for modelling the material, cell and manufacturing process for cells for the automotive market, based on physical and chemical characteristics of cells of NMC622/G, NMC811/G-Si, LMNO/G-Si chemistry types.

This document shall be read in conjunction with the document CWA 18059-2:2023 “Definition of parameters required for modelling of the material, cell and manufacturing process behaviour for battery cells for the automotive market - Part 2: Experiments and characterisation techniques for data required for modelling cells”.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

CWA 18059-2:2023, *Definition of parameters required for modelling of the material, cell and manufacturing process behaviour for battery cells for the automotive market - Part 2: Experiments and characterisation techniques for data required for modelling cells*

3 Terms and definitions

No terms and definitions are listed in this document.

4 Acronyms and abbreviations

NMC	$\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ with $x + y + z = 1$
NMC622	$\text{LiNi}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$
NMC811	$\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$
LMNO	$\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$
G	Graphite
Si	Silicon
PNM	Pore Network Model
P4D	Pseudo 4D
DEM	Discrete Elements Method
CFD	Computational Fluid Dynamics
LBM	Lattice Boltzmann Method

5 List of models

The multiscale models follow a bottom-up approach: atomistic models’ parameters will be scaled up to homogenised parameters to be used in the continuum model. The scale range is extended 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 models, simulation methods, and software tools are used (see Table 1).

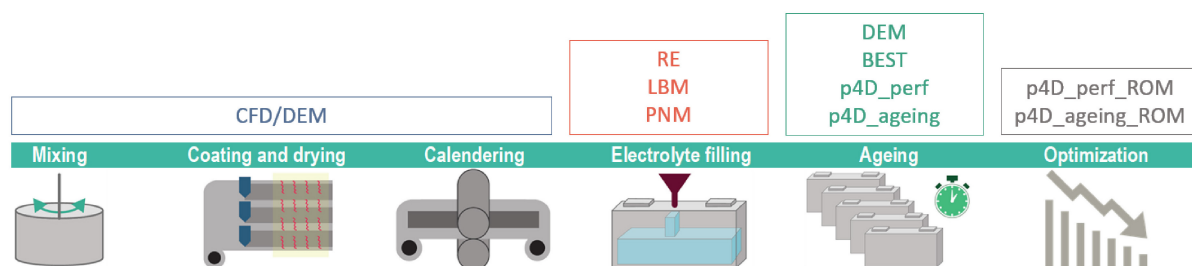


Figure 1 — Models in the process workflow

Table 1 — List of models

Model codename	Method/Software	Scale	Output from model and characterization	Output for battery optimisation
CFD/DEM	Discrete Elements Method with LIGGGHTS coupled with Computational Fluid Dynamics (OpenFOAM)	Electrode/ Slurry	Slurry composition after dispersing and microstructure after drying and calendaring.	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.
LBM	Lattice Boltzmann Models using in-Palabos	Electrode	Wetting behaviour and electrolyte distribution for a selected range of influencing factors at high level of detail.	Optimised electrode materials and structures. Optimal electrolyte filling process conditions.
PNM	Pore Network Models using OpenPNM and PoreSpy	Electrode/ Cell	Wetting behaviour and electrolyte distribution for a broad range of influencing factors at medium level of detail.	
RE	Richards-Equation using in-house code FLUID	Cell	Simulation of filling process.	
DEM	Discrete Elements Method with LIGGGHTS	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
p4D_perf	Finite Element platform FENICS	Cell	Electrochemical and mechanical	

Model codename	Method/Software	Scale	Output from model and characterization	Output for battery optimisation
			behaviour of the cell.	electrochemical ageing (addressing inhomogeneous and homogeneous ageing). Optimum conditions for using and battery pack design.
p4D_ageing	Finite Element platform FENICS	Cell	Electrochemical and mechanical degradation of the cell.	
p4D_perf_ROM	Finite Element platform FENICS and Model Order Reduction tool EchROM	Cell	Electrochemical and mechanical degradation of the cell.	
p4D_ageing_ROM	Finite Element platform FENICS and Model Order Reduction tool EchROM	Cell	Electrochemical and mechanical degradation of the cell.	
BEST	Continuum model	Electrode	Mechanical behaviour of electrode (performances and ageing).	

6 List of model requests

The following tables list all the data and detail the data usage (input parameters, model calibration¹⁾ or model validation²⁾). Some methods for data determination and experimental techniques have been proposed. The descriptions of the experiments and the data types are contained in CWA 18059-2.

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 obtain by numerical simulation and experimental data.

Table 2 — List of requested data for models' construction and validation on electrode processing

Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments
CFD/DEM	Model input parameter	Solvent viscosity (solvent for slurry preparation)	Rheological Measurements	Rheology electrode
CFD/DEM	Model input parameter	Solvent surface tension	Tensiometer	Tensiometer
CFD/DEM	Model input parameter	Solvent density	Mass/Volume; literature for water and NMP solvent	Solvent density
CFD/DEM	Model input parameter	Particle Shape	μ CT (T3.5)	μCT
CFD/DEM	Model input parameter	Particle size distribution (Active Material + Additive)	Laser diffraction analysis	Laser diffraction
CFD/DEM	Model input parameter	AM and Additive density	Literature pycnometer	Pycnometry
CFD/DEM	Model input parameter	Poisson's ratio of AM and additive particles	Literature	Literature
CFD/DEM	Model input parameter	Coefficient of restitution of particles	Literature	Microcompression/ Nanoindentation
CFD/DEM	Model input parameter	Young's modulus of AM and additives	Nanoindentation Literature	Microcompression/ Nanoindentation
CFD/DEM	Model calibration	Friction coefficients	Angle of repose	Angle of repose
CFD/DEM	Model calibration/validation	CB agglomerate strength	Microcompression	Microcompression/ Nanoindentation
CFD/DEM	Model calibration	VdW-Attraction/ Electrostatic repulsion	Zeta Potential Measurement, Agglomeration Kinetics	Zeta potential
CFD/DEM	Model input parameter	Slurry viscosity	Rheological Measurement	Rheology electrode
CFD/DEM	Model input parameter	Shear rate during dispersing	Simulation/Calcul. based on stirrer tip speed/planetary motion, viscosity	Simulation
CFD/DEM	Model calibration/validation	Electrode 3D structure before and after calendaring	SEM, μ CT in T2.2 and T3.5	FIB-SEM and μ-CT
CFD/DEM	Model calibration/validation	Pore size distribution of electrodes	Mercury intrusion	Mercury intrusion

Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments
CFD/DEM	Model calibration/validation	Binder distribution	SEM, EDX on cathode, Later Induced Breakdown Spectroscopy on anode with CMC	SEM-EDX
CFD/DEM	Model input parameter	Mass related slurry component concentrations	Simple calculations based on formulations used in WP7	Simulation & Slurry density
CFD/DEM	Model input parameter	Coating thickness right before drying	In-line measurement	Coating thickness
CFD/DEM	Model input parameter	Coating temperature during drying	Infrared, T° sensor	Coating_T_drying
CFD/DEM	Model input parameter	Convection	Volumetric flow measurement	Flow_T_drying
CFD/DEM	Model input parameter	Air temperature	T° sensor	Flow_T_drying
CFD/DEM	Model input parameter	Drying rate	Solvent content during drying/coating mass during drying/coating thickness during drying	Electrode thickness drying
CFD/DEM	Model calibration/validation	Adhesion strength	Material Testing Machine	Electrode adhesion strength
CFD/DEM	Model calibration/validation	Micromechanical properties of electrode	Nanoindentation	Microcompression/Nanoindentation
CFD/DEM	Model calibration/validation	Electrode thickness before and after calendering	Laser triangulation for contact-free measurement (or tactile measurement if not available)	Electrode thickness
CFD/DEM	Model calibration/validation	Electrode elastic recovery thickness during calendering (depending on gap between rolls)	Force-Sensors, Displacement Sensors, in line measurement	Electrode thickness calendering
CFD/DEM	Model calibration/validation	Temperature of calender rolls		T-calendering
CFD/DEM	Model calibration/validation	Lab scale drying behavior for model development	Tabletop coater + heating + laser triangulation	Electrode thickness drying

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

Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments
LBM/PNM	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
LBM/PNM	Model input parameter	Electrolyte surface tension	Tensiometer	Tensiometer
LBM/PNM	Model input parameter	Electrolyte contact angles with active materials, separator	Optical measurements on model materials	Angle of repose
LBM/PNM/RE	Model input parameter	Electrolyte density	Balance	Electrolyte density
LBM/PNM/RE	Model input parameter	Electrolyte viscosity	Rheometer	Rheology electrolyte
LBM/PNM/RE	Model calibration/validation	Pressure Saturation curves of electrodes and separator	Measurements in special setup	p-s-curves
RE	Model calibration/validation	Relative permeabilities of electrodes and separator	calculation; empirical approximation	Angle of repose
LBM/PNM/RE	Model calibration/validation	Electrolyte distribution pore scale	Ultrasonic acoustic wave or operando tomography/radiography with extra-collaboration with Large Instruments?	Acoustic and Chronoamperometry
RE	Model validation	Electrolyte distribution cell scale	Impedance measurements on segmented cell	Segmented cell
RE	Model validation	Pressure profiles of filling process over time	Pressure sensors in production process	Pressure electrolyte

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

Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments
DEM	Model input parameter	Young modulus of bulk active materials	DFT calculation in T5.1	Simulation
DEM	Model input parameter	Binder rheological behaviour	Nanoindentation	Microcompression/ Nanoindentation
DEM	Model calibration/ validation	SEI thickness evolution	2D imaging, XPS, thickness measurement upon aging	XPS and EQCM
DEM	Model input parameter	Electrode morphology	3D-FIB-SEM in T2.3	FIB-SEM and μ-CT
DEM	Model input parameter	Volume change of active materials in negative electrode	Literature or μ -CT? Or tomography with extra-collaboration with Large Instruments?	μCT
DEM	Model input parameter	Positive electrode swelling	Swelling measurement on monolayer pouch cell upon cycling with dedicated test bed	DFORM
DEM	Model input parameter	OCV profile	Literature and half-cell or 3-electrodes measurements in T2.4	GITT
DEM	Model validation	Electrode thickness evolution	Swelling measurement on monolayer pouch cell upon cycling with dedicated test bed	DFORM
BEST	Model input parameter	Young modulus of bulk active materials, binder and separator	Calculation/experimental	DFORM for separator; literature
BEST	Model input parameter	Poisson ratio of bulk active materials, binder and separator	Calculation/experimental	DFORM for separator; literature
BEST	Model input parameter	volumetric expansion coefficient of bulk active materials	Calculation/experimental	XRD
BEST	Model input parameter	electrode morphologies (3d)	Calculation (WP3)	FIB-SEM and μ-CT
BEST	Model input parameter	Which other parameters might be relevant for mechanical aging? e.g. yield strength of active materials	Experimental	NA

Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments
BEST	Model input parameter	Max. Li Concentration of active materials	Experimental/literature	GITT
BEST	Model input parameter	Electronic conductivity of active materials	Experimental/literature	EIS
BEST	Model input parameter	Li Diffusivity of active material	Experimental/literature	GITT
BEST	Model input parameter	Butler-Volmer reaction rate of active materials	Experimental/literature	Electrochemical tests
BEST	Model input parameter	OCV of active materials	Experimental/literature	GITT
BEST	Model input parameter	Ionic conductivity of electrolyte, and Carbon Binder	Experimental/literature	EIS
BEST	Model input parameter	Li+ Diffusivity of electrolyte and Carbon Binder	Galvanostatic pulse-relaxation (Li-Li)	GITT
BEST	Model input parameter	Li+ transference number of electrolyte	Experimental EIS (Li-Li)/literature	EIS
BEST	Model input parameter	Effective electronic conductivity of Carbon Binder (optional)	Literature	Literature
BEST	Model input parameter	Porosity of Carbon binder (optional)	Literature	Literature
BEST	Model validation	Cell voltage	Experimental	Electrochemical tests
BEST	Model validation	Quantification of mechanical aging	Experimental	Electrode adhesion strength
BEST	Model validation	Electrode thickness evolution	Experimental	DFORM
p4D_perf & p4D_perf_ROM	Model input parameter electrolyte	Ionic conductivity	EIS (Electrode - Electrode)	EIS
p4D_perf & p4D_perf_ROM	Model input parameter electrolyte	Diffusion coefficient in electrolyte	Galvanostatic pulse-relaxation (Li-Li)	GITT
p4D_perf & p4D_perf_ROM	Model input parameter electrolyte	Transference number	EIS (Li-Li)	EIS
p4D_perf & p4D_perf_ROM	Model input parameter - electrolyte	Initial concentration	Material provider	Input of electrolyte manufacturer

Model codename	Data usage	Description of requested data	Method for data determination	Name of experiments
p4D_perf & p4D_perf_ROM	Model input parameter	Mechanical parameters/ properties	Model upscaling from DEM and Cont-ITWM	Simulation
p4D_perf & p4D_perf_ROM	Model input parameter	Specific heat capacity (Cp), thermal conductivity	Thermal characterization	ARC, TGA-GC
p4D_perfy & p4D_perf_ROM	Model validation	Cell performance tests	C-rate tests, cell thermal inhomogeneities, electrode swelling with lithiation procedure	Electrochemical tests
p4D_ageing & p4D_ageing_ROM	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
p4D_ageing & p4D_ageing_ROM	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
p4D_ageing & p4D_ageing_ROM	Model validation	Aging test results of finished cells, characterisation of finished electrodes, etc)	Ageing tests with deformation gauges? With tomography?	Test campaign