Swappable Container Waterborne Transport Battery

Call Identifier: H2020-LC-BAT-2020

Topic: LC-BAT-11-2020

Reducing the Cost of Large Batteries for Waterborne Transport

D3.2
Cell Design Modelling

1 April 2021

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No. 963603.

TABLE OF CONTENTS

GLOSSARY OF TERMS

Term	Definition
BOL	Beginning of Life
CD	Current Direct
Co	Cobalt
DOD	Depth of Discharge
Mn	Manganese
Ni	Nickel
NMC	Nickel Manganese Cobalt Oxide
SOC	State of Charge
SOH	State of Health

DOCUMENT PROPERTIES

Project Information	
Program	Reducing the Cost of Large Batteries for Waterborne Transport
Project Acronym	Current Direct
Grant Agreement Number	963603
Deliverable Number	D3.2
Work Package/Task Related	WP3 / T3.2

Document Information	
Document Name	CD_D3.2_Cell Design Modelling_v1.0
Date of Delivery	1 April 2021
Status and Revision	Initial Public Release, Version 1.0
Number of Pages	14

Responsibility	
Work Package Lead	Blackstone
Work Package Partners	Blackstone, Lloyd's Register, Vito, Aviloo, University of Hasselt, Spear Power Systems, Umicore
Reviewer(s)	Umicore, Blackstone, Spear Power Systems
Approver	Spear Power Systems

Dissemination Level	
Type (Distribution Level)	☒PU, Public
	☐CO, Confidential, only for members of the consortium (including the Commission Services)
	☐EU-RES, Restricted, Classified Information
	☐EU-CON, Confidential, Classified Information
	☐EU-SEC, Secret, Classified Information

REVISION HISTORY

Version	Issue Date	Changes Made / Reason for Issue
1.0	1-Apr-21	Initial Version Submitted

"This document reflects only the author's view and the Agency is not responsible for any use that may be made of the information it contains".

PROJECT SUMMARY

Current Direct, a new research and innovation project funded by the European Commission's Horizon 2020 program, will revolutionize the way we move goods and people by water. The vast majority of water transport in Europe is propelled by dirty, noisy diesel engines. By cutting the cost of today's marine battery electric drivetrains in half and relieving ship owners of the burden of capital expense, Current Direct will enable rapid adoption to reduce greenhouse emissions.

Current Direct's innovative Energy as a Service platform will enable ship owners to accelerate their participation in the shift to clean energy while creating new business opportunities for shipyards and local entrepreneurs. By changing the model for acquiring and storing energy aboard vessels, Current Direct will create a new energy economy, adding thousands of new jobs. Current Direct provides a vehicle for energy companies, institutional investors, and government stakeholders to participate in the green transformation of Europe's merchant and passenger fleet.

Current Direct brings together thirteen dynamic partners from across Europe's marine electrification value chain. The project is led by Spear Power Systems, makers of the world's lightest, most flexible marine batteries certified to the most stringent international safety standards. Blackstone Technology is lowering the cost of manufacturing tomorrow's 3D printed lithium-ion cells using state of the art active materials from Umicore. The University of Hasselt will use its electrochemical expertise to develop physics-based models of the Current Direct cells that will help optimize the life and return on investment of battery systems deployed across Europe as part of the Current Direct Energy as a Service platform developed by the accomplished engineers and data scientists at Rhoé Urban Technologies and Aviloo. Naval architecture and marine engineering company Foreship will lend its expertise to EDP CNET's in-depth knowledge of electrical markets to ensure the Current Direct platform targets optimal vessels and locations maximizing reductions in emissions. VUB's material science experts are creating low-cost composites to improve the safety of battery packs that are designed for recyclability and feature VITO's smart cell monitoring electronics. Wärtsilä will develop modular battery containers and charging infrastructure that will be certified to innovative standards developed together with Lloyd's Register. The project will culminate in a demonstration of the Current Direct battery, shore charging, and asset management platform by Kotug in Rotterdam.

The Current Direct EcoSystem is shown in Figure 1.

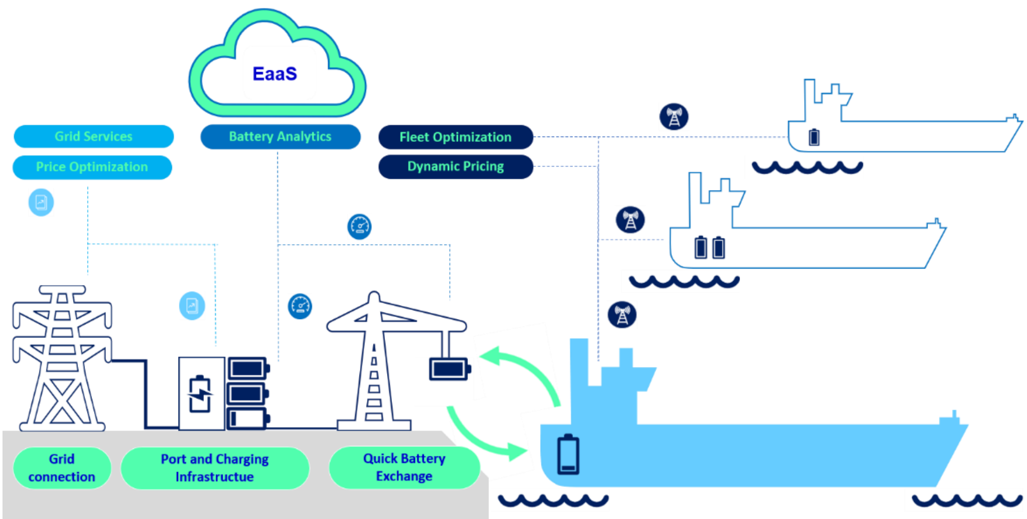

Figure 1. Current Direct EcoSystem

1. SPECIFIC OJECTIVES FOR WORK PACKAGE 3

This WP develops a lithium-ion cell optimized for the Current Direct Waterborne Transport Battery applications of inland and short sea shipping. It leverages state of the art commercial active materials and the unique disruptive electrode printing process capabilities. The cells will be tested, and a physics-based model developed to provide accurate SOC and SOH estimates.

Specific Objectives:

- Model and specify state of the art NMC cathode with a focus on cost, safety, cycle life, and energy density specific for the Waterborne Transport Battery application
- Design of a safe, low cost, long life, energy dense cell for the Current Direct Waterborne Transport Battery
- Produce prototype of the Current Direct cell
- Test Current Direct cell for performance and lifetime characterization
- Develop and verify a physics-based model for SOC and SOH estimation
- Produce Current Direct cell in small, pilot quantities

2. SUMMARY

Several simulations were executed on the Umicore's cathode material to model its performance against Current Direct's cell requirements. According to the simulations, to fulfill the minimum requirement of energy, NMC333 or higher Ni cathode material is required. However, NMC811 material or higher Ni NMC material come with the sacrifice of cycle life making it difficult to meet the cell design requirements. Although difficult to precisely predict the cycle life using only the cathode material, a commercially optimized cell with Umicore's NMC 622 cathode material is expected to best fulfill all design requirements according to the study conducted as it provides the most balanced performance.

2.1. Introduction

The cell performance specifications according to the application needs of the Current Direct Waterborne Container detailed in the Cell Requirements section of the deliverable D2.1 provided the basis for the cathode material requirements. Positive active material, or cathode, is one of the major components of a cell responsible for its performance specifications such specific energy and energy density. In Current Direct the most suitable cathode material was selected based on simulation performed on a model, developed in Umicore. This model is often used to simulate major electrochemical performance of a cell equipped with different cathode materials. This deliverable presents simulation results to justify and support the selection of cathode material to meet the Current Direct application requirements.

3. TECHNICAL REQUIREMENTS OF THE CELL

The major cell requirements contained in D2.1 which have significant dependence on the cathode material are listed below in Table 1.

Table 1. Major Cell Requirements

Description	Type	Target
Energy Density	Shall	≥ 500 Wh/L
	Should	≥ 580 Wh/L
Specific Energy	Shall	≥ 242 Wh/kg
	Should	≥ 283 Wh/kg
Cycle Life	Shall	≥ 12,000 cycles at 70% DOD before reaching 70% BOL capacity.
	Should	≥ 12,000 cycles at 90% DOD before reaching 70% BOL capacity.
	Shall	Be capable of being consistently cycled until reaching 70% BOL capacity without cell fallout.
Calendar Life	Shall	≥10 years at 25°C at 50% SOC before reaching 80% of BOL capacity
	Should	Support 15yr. Calendar life at 25°C

Here 'Shall' represents the minimum requirements and 'Should' represents the target requirements of the project.

The total energy delivered by a cell is determined by the Li^+ storing capacity and the operating voltage. The capacities of the commercially available cathode materials are in general, less than the capacity of anode materials. Additionally, the operating voltage vs Li/Li^+ is significantly higher for cathode than anode materials. Thus, the energy content of a cell is primarily determined by characteristics of the cathode material.

4. INPUT PARAMATERS OF THE MODEL

The Umicore internal material to pack model is based on a 60Ah high energy pouch cell. The methodology of the model is similar to published reports [1].

Figure 2 shows a representative schematic of the cell.

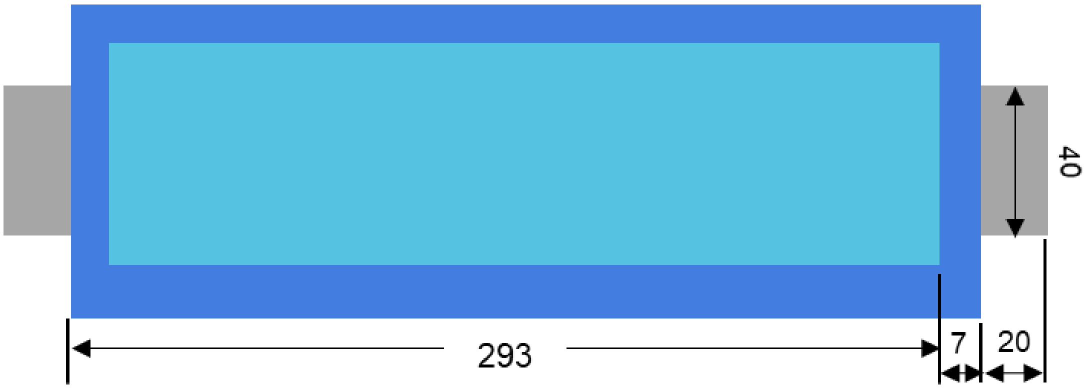

Figure 2. Schematic of the 60Ah high energy pouch cell used in Umicore model. All the dimensions are in mm.

Table 2 shows the characteristics of an assumed electrode design.

Table 2. Characteristics of The Electrode Design in the High Energy Pouch Cell.

Parameters	Cathode	Anode
Active material, wt%	96	95
Electrode Density, g/cc	3.3	1.6
Design	Double Sided	Double Sided
Coating Thickness (1 side), µm	85	*
Areal Loading, mg/cm^2	28	*
Thickness of current collector, µm	12	8

* Changed according to the reversible capacity of the cathode material.

5. SIMULATION RESULTS ON ENERGY REQUIREMENTS

As a cathode material, Nickel Manganese Cobalt oxide (NMC) has been proven the best material to achieve high energy cell. High capacity and voltage are the characteristics of NMC cathode materials. There are several categories of NMC materials according to the relative amount of Nickel, Manganese and Cobalt. By increasing the Ni content relatively higher capacity can be achieved.

Several simulations are executed with a cathode material of different capacities. In the simulation, physical properties such as density of the cathode is assumed to be like NMC. The anode material is graphite for all cases. The operating voltage windows is assumed as 3-4.2V.

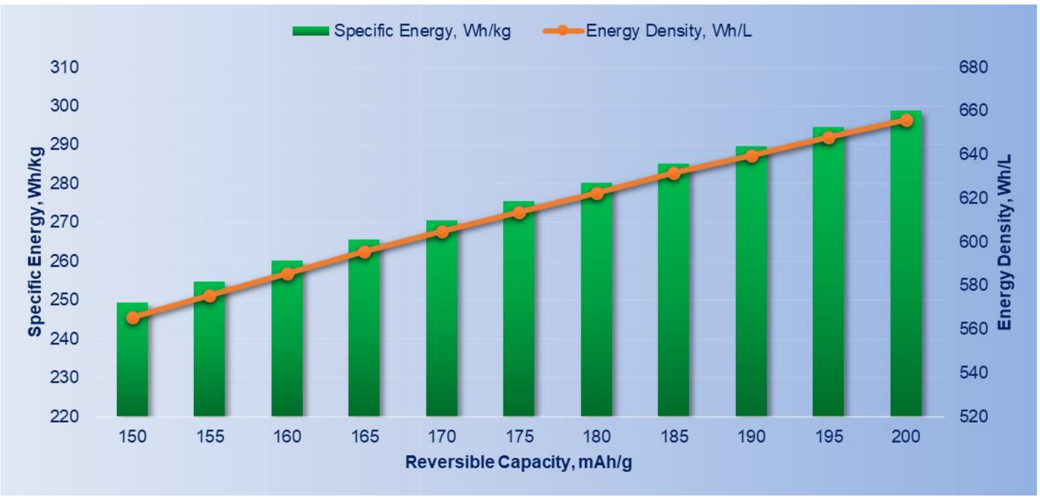

Figure 3. Specific energy and energy density evolution of cells with cathode materials of different capacities.

It is clear from the Figure 3 simulation to meet the minimum specific energy requirement (242 Wh/kg), at the full cell level, the cathode must deliver a reversible capacity of 150 mAh/g or higher. To reach the specific energy of 283 Wh/kg, the cathode reversible capacity must be 180 mAh/g or higher.

It is well known that in NMC cathode material, the deliverable capacity depends on the Ni content. Figure 4 shows the impact of different elements (Ni, Mn, and Co) on the performance of NMC material.

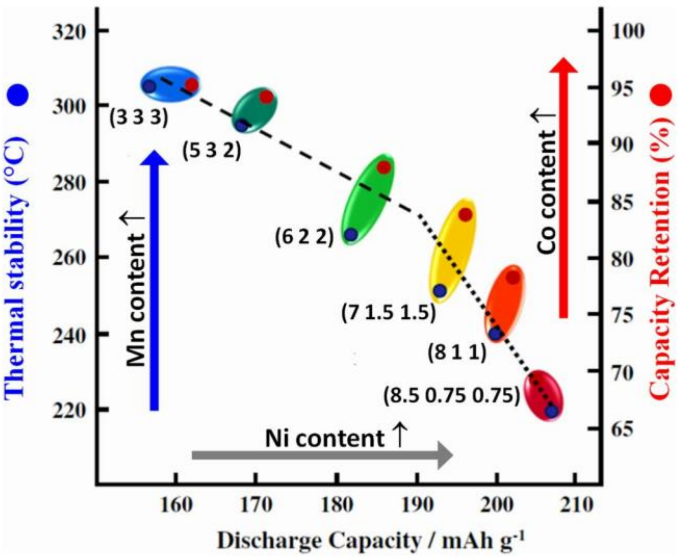

Figure 4. A map of relationship discharge capacity (black), thermal stability (blue) and capacity retention (red) of Li/Li[NixCoyMnz]O2 compounds with number in brackets corresponding to the composition (Ni Mn Co). [2]

Important to mention here, the figure represents the discharge capacity in a half-cell (Li metal anode) and typically charged to 4.3V. If converted to a full cell, the reversible capacity corresponds to 5-10% inferior to the one of half-cell. Thus, to meet the minimum specific energy requirement NMC 333 can be used. However, NMC 811 or higher Ni NMC must be used in order reach the specific energy target of >283Wh/kg. In case of NMC811, due to lower content of Mn and Co, the safety and cycle life of the material reduces significantly.

Considering capacity, safety, and cycle life, NMC622 delivers the most balanced performance. Detailed analysis on the cycle life requirements is presented in the next section.

6. LIFETIME REQUIREMENTS

The cathode material is primarily responsible for specific energy and energy density, while other components such as the anode, separator, electrolyte, binder, and fabrication process have an influence on its cycle and calendar life. Therefore, it is difficult to translate the precise lifetime requirements of a cell into the cathode characteristics only.

As explained in the previous section, Co content in NMC cathode material influences the cycle life. Calendar life has the similar impact. Figure 5 shows cycle life evolution. It is clear from the figure, NMC622 exhibit better cycle life than NMC811 but slightly inferior to NMC333.

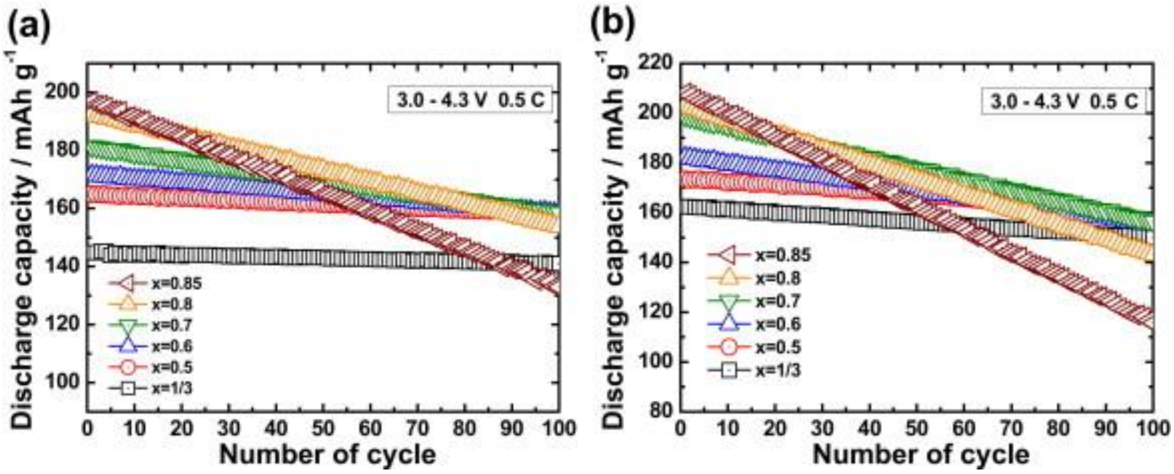

Figure 5. Discharge capacity vs. cycle number for the Li/Li[NixCoyMnz]O2 (x = 1/3, 0.5, 0.6, 0.7, 0.8 and 0.85) cells at (a) 25 °C and (b) 55 °C. The Co and Mn contents are – y=1/3,1/3,0.2,0.15,0.1,0.075 and z= 1/3,0.2,0.2,0.15,0.1,0.075. [3]

To demonstrate the required cycle and calendar life (Table 1), more than 10 years of characterization is required. As this is impractical to precisely test this within the timeline of this project an estimation is needed. Figure 6 shows the simulated cycle life and calendar life of 20 Ah cell with NMC333 cathode [3].

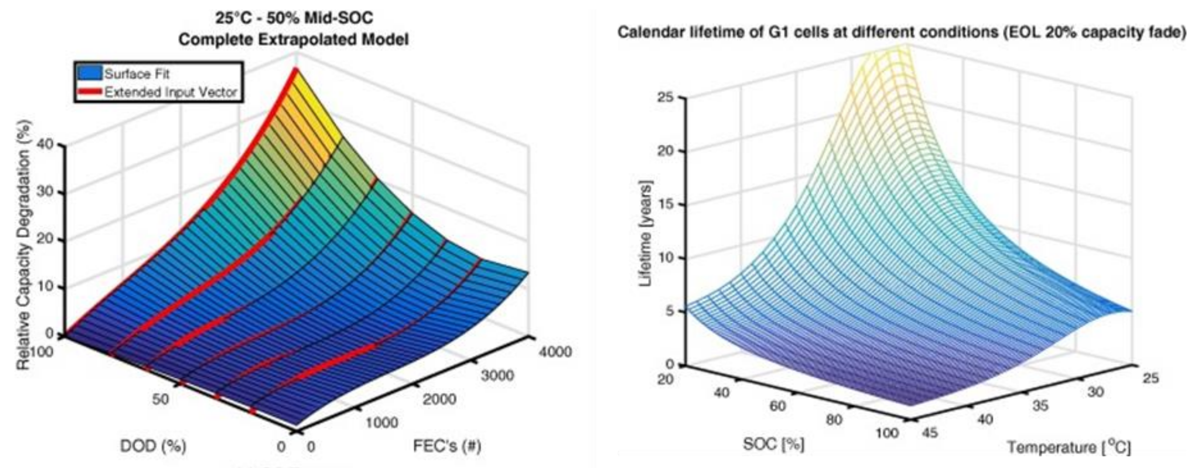

Figure 6. Simulated Cycle life (Left) and Calendar life(Right) of a high energy cell with NMC333 cathode[3].

According to this model, at 70% DoD, approximately after 4000 full equivalent cycle (FEC) or 5714 complete cycle, 20% capacity degradation is reached. With respect to the calendar life, at 50% SoC, approximately 20% capacity degradation is reached after approximately 10 years.

The capacity of the reported cell lost more than 5% after 1000 cycle at a discharge-charge rate of 1C-0.3C respectively (Figure 7). In comparison, a test cell (<1Ah) with Umicore NMC622 material showed approximately 8% degradation after 1000 cycle at a discharge-charge rate of 1C-1C.

Compared to the reported cell, Umicore's test cell was not commercially optimized. Moreover, the cycling was performed at a rate higher than accepted for Current Direct's application. It is well known that, higher charge/discharge current rate accelerates degradation [3].

Therefore, it is expected that, a commercially optimized cell with Umicore NMC622 should outperform the cycle and calendar life of the above reported cell under the expected application charge/discharge currents.

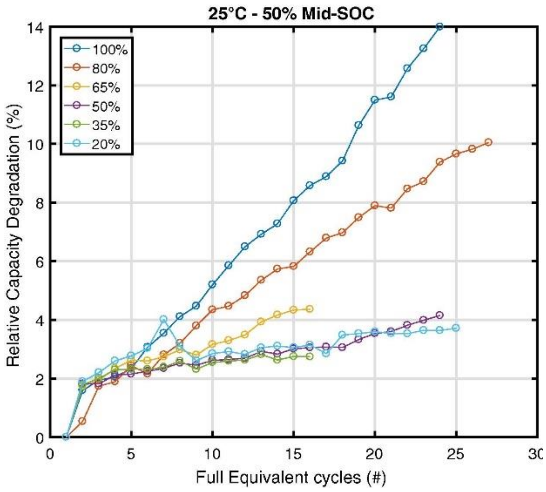

Figure 7. Cycle life evolution of a 20Ah cell with NMC333 cathode [3]**.**

Considering this estimation, the minimum cycle and calendar life requirement of the cell is expected to be met by Umicore's NMC622 material. To fulfill both energy and lifetime requirements, NMC 622 is the best choice due to its balance between energy and cycle life.

7. REFERENCES

[1] F. Duffner, M. Wentker, M. Greenwood, and J. Leker, “Battery cost modeling: A review and directions for future research,” *Renewable and Sustainable Energy Reviews*, vol. 127. Elsevier Ltd, p. 109872, Jul. 01, 2020, doi: 10.1016/j.rser.2020.109872.

[2] P. Rozier and J. M. Tarascon, “Review—Li-Rich Layered Oxide Cathodes for Next-Generation Li-Ion Batteries: Chances and Challenges,” *J. Electrochem. Soc.*, vol. 162, no. 14, pp. A2490–A2499, 2015, doi: 10.1149/2.0111514jes.

[3] H. J. Noh, S. Youn, C. S. Yoon, and Y. K. Sun, “Comparison of the structural and electrochemical properties of layered Li[NixCoyMnz]O2 (x = 1/3, 0.5, 0.6, 0.7, 0.8 and 0.85) cathode material for lithium-ion batteries,” *J. Power Sources*, vol. 233, pp. 121–130, Jul. 2013, doi: 10.1016/j.jpowsour.2013.01.063.