SmartCycling: Optimizing the circular economy of batteries with artificial intelligence aided designs



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Background and Motivation

• Adequate technical solutions for the circular economy must be based on analysis that are:

> Systemic, Quantifiable, Multidimensional

• A "circular" economy model is suitable to describe a value chain, but a "circular" engineering is not enough!

> A new type of engineering is required!

- **SmartCycling** will explore parameters that reflect the value of materials:
 - "Value" as the ability of materials to provide a functional service
 - Coupled with parameters for materials flow analysis such as statistical entropy
- SmartCycling will apply AI to process data:
 > re-design the recycling loop on a systemic level
 > perform multi-objective optimization wrt values





SmartCycling will use battery materials as case study due to their current industrial, economical and societal relevance

Impact

Al optimization for the systemic analysis of multidimensional engineering parameters for circularity is an entirely new area of research. Such an approach has not been tried before since there are no objective parameters for circular economy available to use as target functions of AI. It will allow us to **quantitatively** address the CE of critical materials.

- Scientific questions
 - In the systemic, multi-level view of material flow in the CE, can we identify the most relevant process variables at each level?
 - Can we encode these concepts into a sophisticated materials flow model that can be validated against existing practices and outcomes?
 - How can AI methods be employed to optimize the N-dimensional problem of battery material flows in the CE? Is there a single solution that satisfies multiple optimization objectives?
 - Do experimental outcomes agree with the model predictions?

Potential Outcomes

- A formal framework for modelling of battery materials recycling using a multidimensional and system-level analysis
- An original set of quantitative parameters that reflect the impact of transformative stages in the CE value chain
- An iterative framework for optimization of battery recycling processes, featuring Al algorithms for multi-objective optimization, experimental validation, and model feedback

SmartCycling project

- WP1. Process modeling and parametrization (M1-M36; Aalto; PhD1, PI Serna)
 - Task 1.1 Evaluation of parameters for value and functionality
 - Task 1.2 Data collection through simulation of LIB recycling processes
 - Task 1.3 Simulation of optimized recycling processes
 - Task 1.4 System optimization on process simulators
- WP2: AI optimization of recycling processes (M1-M48; Turku, PhD2, PD, PI Todorović)
 - Task 2.1 Comparative study of AI method performance for optimization over recycling processes
 - Task 2.2 Multi-objective AI optimization
 - Task 2.3 Model feedback and re-optimization
- WP3: Model validation (M25-M48; Aalto; PhD1, PD, PI Serna)
 - Task 3.1 Laboratory-scale experimental validation of models
 - Task 3.2 Validation of optimized solutions
 - Task 3.3 Characterization of recycled battery materials



SmartCycling activities and their position in the material life cycle (1. Processing, 2.Manufacturing, 3.Assembly, 4.Use and end-of-life). Waste (W) is generated throughout the life cycle. The various recycling processes can recover materials as chemical elements (E) or compounds (C), thus are reintroduced at different points of the life cycle.