

# Optimization of Circular Supply Chains for Electric Vehicle Batteries

Kaapo Kopra<sup>a</sup> and Iiro Harjunoski<sup>a\*</sup>

<sup>a</sup> Aalto University, Department of Chemical and Metallurgical Engineering, Espoo, Finland

\* Corresponding Author: iiro.harjunoski@aalto.fi

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## ABSTRACT

The increasing popularity of electric vehicles (EVs) leads to an expected rise in the quantity of end-of-life lithium-ion batteries (LIBs) that require efficient management. This paper presents a State Task Network (STN) based optimization model to analyze and optimize the supply chain for LIBs, allowing for the selection of optimal processing routes, facility locations, capacities and re-integration of recovered materials, as well as analyzing the possible trade-offs between different end-of-life management strategies. Based on available data from the literature, the model is demonstrated with the LIB supply chain considering both primary production and different end-of-life strategies for spent LIBs (recycling and reuse). The case study reveals that mechanical pretreatment followed by hydrometallurgical recycling is the optimal pathway and it outperforms the linear supply chain in both costs and emissions. The cost optimal solution opts for more centralized collection and disassembly, whereas when minimizing the total greenhouse gas emissions, the optimal collection and disassembly center locations are decentralized. The model can aid in the design of circular supply chains to select and locate the optimal processes and to examine how the network should evolve over time.

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**Keywords:** Batteries, GAMS, Optimization, Supply Chain, Circular Economy

## INTRODUCTION

The recent energy transition to renewable energy sources has resulted in increased demand for metals such as lithium, cobalt, nickel and manganese that are needed to produce lithium-ion batteries (LIBs) used mainly in electric vehicles (EVs). At the same time, the natural mineral deposits are reaching critical concentrations of these valuable metals and thus increasing the environmental impacts associated with metals extraction via the conventional primary production routes [1]. As only a limited fraction of LIBs are currently recycled [2], a wider adoption of recycling processes and advancements in circular economy (CE) could help alleviate future supply-demand disparities for battery materials, reduce environmental burdens, and lower the production costs by decreasing the required amount of primary production of battery metals.

The concept of circular economy (CE) has been gaining popularity in businesses, government and the research community [3]. In contrast with linear production

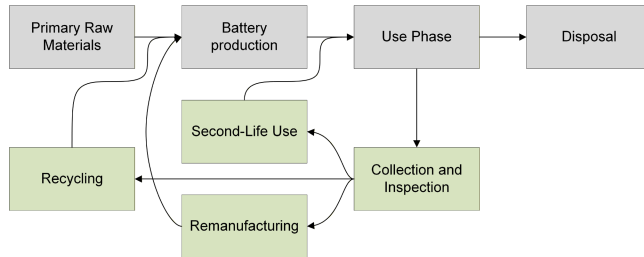
systems, the aim of circular economy is that materials never become waste. It is based on the following principles: to eliminate waste and pollution, to circulate products and materials and to regenerate nature [4]. Aligned with the principles of CE, end-of-life (EOL) EV LIBs can be managed through several alternatives to disposal: reuse in second-life applications, remanufacturing suitable battery cells, and recycling to recover valuable materials from EOL LIBs. The general structure of the circular LIB system is presented in Figure 1.

A vast amount of research has focused on designing recycling processes for LIBs to recover valuable materials and facilitate closed-loop recycling of battery materials. Currently, mechanical pretreatment processes, hydrometallurgical processes and pyrometallurgical processes are conducted on an industrial scale, whereas emerging direct recycling processes are currently on a pilot or laboratory scale level and thus lack industrial maturity [5].

- Mechanical pre-treatment: involves discharging, crushing and separation stages for the LIBs to

obtain black mass powder which contains valuable metals, mainly from the cathode active material.

- Hydrometallurgical recycling: the black mass is leached, and the battery metals are selectively separated and purified.
- Pyrometallurgical recycling: the spent LIBs are fed into a high-temperature process to produce a metal alloy as well as a slag phase as a byproduct.



**Figure 1.** Schematic representation of the circular LIB system.

## METHODOLOGY

The need for systematic methods to assess and optimize circular economy networks has been recognized in the process systems engineering literature [3]. Recent examples include the design and optimization of circular economy networks for polyethylene terephthalate (PET) [6] and the optimization of circular food supply chains [7].

Ahmed et al. [6] proposed a State Task Network (STN) modeling approach for the optimal design of circular economy networks and applied it to a case study on polyethylene terephthalate (PET) networks with a one-year assessment period. Baratsas et al. [7] presented a systems engineering framework for the optimization of circular food supply chains using a Resource Task Network (RTN) representation. Finally, Iakovou et al. [8] presented an RTN-based approach for the optimal design of reverse logistics networks for photovoltaic recycling.

The multi-period modeling of the supply chain for batteries is crucial, especially given the growing availability of EOL materials. By modeling the entire supply chain, we can examine how different end-of-life management strategies can be efficiently integrated with the primary production processes.

### Model formulation

The optimization model is based on the State Task Network representation first introduced by [9] for short-term scheduling of batch processes. The State Task Network representation allows for flexible representation of production processes where materials are represented as states that are transformed in processes referred to as tasks. Thus, the framework allows for the preparation

of a superstructure, which includes all the possible production processes that can be used to produce the required products in the supply chain. As the STN formulation inherently allows for material circulation in the network, a complete supply chain network can be represented which includes both primary production processes and all possible processes to treat end-of-life batteries, as well as the possible reintegration routes in the supply chain.

The goal is to be able to present the holistic supply chain model for lithium-ion batteries that allows the investigation of optimal EOL LIB treatment options and how the recovered materials can be integrated back into the different stages of the battery production supply chain.

### Sets, Parameters and Variables

The nomenclature used in the optimization model is summarized in Tables 1-3.

**Table 1:** Sets used in the optimization model.

|                 |                                  |
|-----------------|----------------------------------|
| $c \in C$       | Capacity selection               |
| $d \in D$       | Delay time periods               |
| $i \in I$       | Processing tasks                 |
| $l \in L$       | Locations                        |
| $s \in S$       | Materials                        |
| $t \in T$       | Time periods                     |
| $S^F \subset S$ | Subset for final products        |
| $S^V \subset S$ | Subset for primary raw materials |

**Table 2:** Parameters used in the optimization model.

|                      |   |
|----------------------|---|
| $Cap_{i,c}^{Max}$    | Maximum capacity for processing task                          |
| $Cap_{i,c}^{Min}$    | Minimum capacity for processing task                          |
| $CostP_{s,t}$        | Cost of purchased materials                                   |
| $CostS_{s,t}$        | Cost of sold/sink materials                                   |
| $CTrans$             | Transportation cost   |
| $Dem_{l,s,t}$        | Material demand   |
| $Dist_{l,l'}$        | Distance between locations                                    |
| $E_i$                | Emissions of processing tasks                                 |
| $EPur_s$             | Material procurement emissions                                |
| $ETrans$             | Transportation emissions                                      |
| $FC_{i,c,t}$         | Fixed costs of processing tasks                               |
| $Sink_{s,t}^{Max}$   | Maximum sink for materials                                    |
| $Supply_{s,t}^{Max}$ | Maximum supply of materials                                   |
| $VC_{i,t}$           | Variable costs of processing tasks                            |
| $\rho_{s,i}$         | Conversion of materials in processing tasks                   |
| $\rho_{s,i}^+$       | Generation of material $s$ in $i$ , ( $\rho_{s,i} > 0$ )      |
| $\rho_{s,i}^-$       | Consumption of material $s$ in $i$ , ( $\rho_{s,i} < 0$ )     |
| $\alpha_{i,d}$       | Fraction of outputs from process $i$ released after delay $d$ |

**Table 3:** Variables used in the optimization model.

|                 |  |
|-----------------|--|
| $B_{i,l,t}$     | Flow through processing task $i$ at location $l$ during time period $t$ .  |
| $P_{l,s,t}$     | Purchasing of material $s$ in location $l$ during time period $t$ .  |
| $S_{l,s,t}$     | Selling/sink of material $s$ in location $l$ during time period $t$ .  |
| $Tr_{l,l',s,t}$ | Transportation of material $s$ from location $l$ to location $l'$ during time period $t$ .                         |
| $Y_{i,l,t,c}$   | 1 if processing task $i$ with capacity level $c$ is selected at location $l$ during time period $t$ , 0 otherwise. |

### Objective Functions

To evaluate the potential trade-offs between economic performance, environmental impacts, and supply chain circularity, three objective functions are considered: supply chain costs, greenhouse gas emissions generated and the consumption of primary raw materials.

First, the total supply chain costs are minimized that consists of fixed and variable processing costs, transportation costs, and material purchasing costs and revenues generated from selling materials.

$$\min \sum_i \sum_l \sum_t B_{i,l,t} \cdot VC_{i,t} + \sum_i \sum_l \sum_t \sum_c Y_{i,l,t,c} \cdot FC_{i,c,t} + \sum_l \sum_{l'} \sum_s \sum_t CTrans \cdot Tr_{l,l',s,t} \cdot Dist_{l,l'} + \sum_l \sum_s \sum_t (P_{l,s,t} \cdot CostP_{s,t} - S_{l,s,t} \cdot CostS_{s,t}) \quad (1)$$

Second, the environmental sustainability of the supply chain is addressed by minimizing the total emissions that consists of process emissions, transportation emissions and emissions related to material procurement.

$$\min \sum_i \sum_l \sum_t B_{i,l,t} \cdot E_i + \sum_l \sum_{l'} \sum_s \sum_t ETrans \cdot Tr_{l,l',s,t} \cdot Dist_{l,l'} + \sum_l \sum_s \sum_t P_{l,s,t} \cdot EPur_s \quad (2)$$

Finally, as proposed in [6], the total purchasing of primary raw materials is minimized and is considered as a proxy for material circularity in the supply chain.

$$\min \sum_l \sum_{sv} \sum_t P_{l,s,t} \quad (3)$$

### Constraints

Net flow through each processing task cannot exceed the maximum production capacity at the selected capacity level.

$$B_{i,l,t} \leq \sum_c Y_{i,l,t,c} \cdot Cap_{i,c}^{Max} \quad \forall i, l, t \quad (4)$$

Net flow through each processing tasks must exceed the minimum production capacity level.

$$B_{i,l,t} \geq \sum_c Y_{i,l,t,c} \cdot Cap_{i,c}^{Min} \quad \forall i, l, t \quad (5)$$

Material purchases in the supply chain cannot exceed the maximum supply of materials.

$$\sum_l P_{l,s,t} \leq Supply_{s,t}^{Max} \quad \forall s, t \quad (6)$$

Material sales in the supply chain cannot exceed the maximum allowed sink of materials.

$$\sum_l S_{l,s,t} \leq Sink_{s,t}^{Max} \quad \forall s, t \quad (7)$$

The demand for the final products must be satisfied in the supply chain. In a circular system, the final products are consumed by the demand zones.

$$\sum_i -B_{i,l,t} \cdot \rho_{s,i}^- = Dem_{l,s,t} \quad \forall l, s^F, t \quad (8)$$

The mass balance at all locations and all time periods is formulated based on material generation or consumption, transportation and the purchasing or selling of materials. As in the case of electric vehicle batteries, the use phase introduces a time delay before the material becomes available for end-of-life processes. Accordingly, the material generation term is modified to model this delay as a fractional release, where each task with a delay generates materials in predetermined fractions.

$$\sum_i \sum_d B_{i,l,t-d} \cdot \rho_{s,i}^+ \cdot \alpha_{i,d} + P_{l,s,t} + \sum_{l'} Tr_{l',l,s,t} = \sum_i -B_{i,l,t} \cdot \rho_{s,i}^- + S_{l,s,t} + \sum_{l'} Tr_{l,l',s,t} \quad \forall s, l, t \quad (9)$$

For each processing task and each time period, at most one capacity level can be selected.

$$\sum_c Y_{i,l,t,c} \leq 1 \quad \forall i, l, t \quad (10)$$

The selected production capacity of the processing tasks at time  $t$  cannot be lower than at previous time period  $t-1$ .

$$\sum_c Y_{i,l,t,c} \cdot Cap_{i,c}^{Max} \geq \sum_c Y_{i,l,t-1,c} \cdot Cap_{i,c}^{Max} \quad \forall i, l, t \quad (11)$$

Thus, the objective functions defined in Eqs. (1-3) are used to study trade-offs in circular supply chain design, and the resulting MILP formulation can be expressed as:

$$\begin{aligned} & \min Z \\ & \text{s.t. Eq. (4) - (11)} \end{aligned} \quad (12)$$

$$B_{i,l,t}, P_{l,s,t}, S_{l,s,t}, Tr_{l,l',s,t} \geq 0, Y_{i,l,t,c} \in \{0, 1\}$$

By constraining the material flows through selected echelons and by fixing the location of existing facility locations in the supply chain, the model facilitates "what if" analyses and enables the investigation of different scenarios.

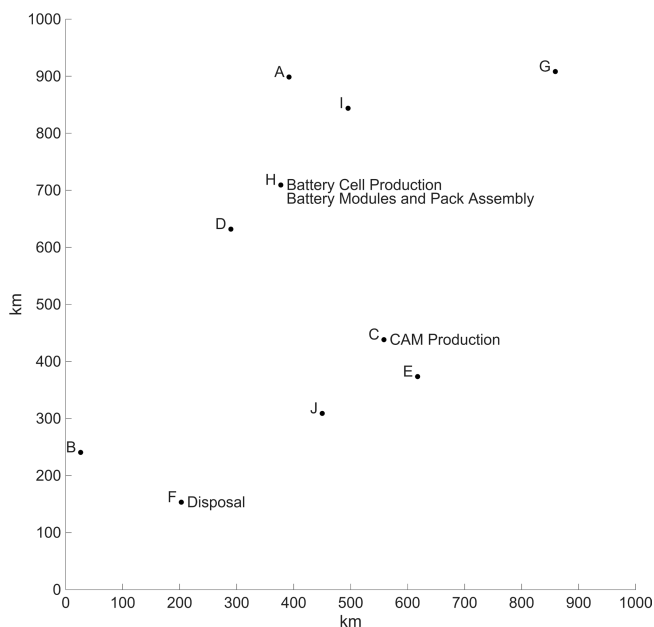
### CASE STUDY

To illustrate the proposed optimization model for circular supply chain design, a representative case study of NMC622 LIBs used in EVs is considered. The case study investigates the high-value metals present in the cathode active material of the LIBs: refined lithium, cobalt, nickel and manganese, while other materials in the lithium-ion battery cells and packs are considered to be inert. Model parameters are chosen to reflect typical

economic, environmental and process conditions that are reported in the literature ([10-12]). The case study considers 10 uniformly randomly generated locations within a 1000 x 1000 km grid, each associated with identical demand for LIBs with an annual demand growth rate of 1.5%. The supply chain is optimized for the time period of 30 years, assuming that no end-of-life LIBs are available at the initial time period. The main assumptions of the case study are summarized in Table 4, and Figure 2 presents the candidate locations and locations fixed in the linear reference scenario.

**Table 4:** The main assumptions used in the case study.

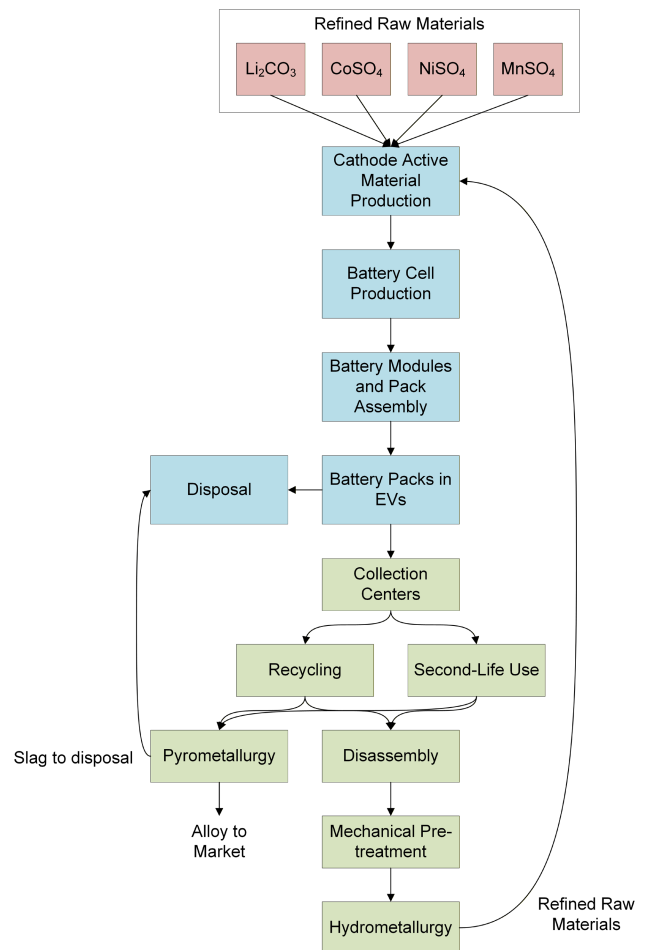
| Parameter                    | Value        |
|------------------------------|--------------|
| Cell chemistry               | NMC622       |
| Cell specific energy         | 0.218 kWh/kg |
| CAM to Cell ratio            | 0.324        |
| Cell to pack ratio           | 0.6          |
| Lifespan of EV batteries     | 10 years     |
| Lifespan of reused batteries | 4 years      |



**Figure 2.** Representation of the case study showing fixed battery production sites (C, F, H) and candidate locations.

In the case study, the production of LIB packs begins with the production of cathode active material (CAM) which consumes refined lithium, cobalt, nickel and manganese to produce the CAM. The CAM is then supplied to the cell production phase, which manufactures battery cells that are then assembled into battery modules and finally into battery packs in the assembly process. From the assembly, the produced battery packs are transported to demand zones where the battery packs

are used in electric vehicles. For the case study, a fixed lifetime of 10 years is assumed before the batteries become available for end-of-life treatment processes. Figure 3 illustrates the superstructure of the studied network.



**Figure 3.** Superstructure representation of the circular LIB network, focusing on the high-value refined battery metals present in cathode active material (CAM).

In the linear reference scenario, all EOL LIB packs are transported to the disposal facility located at F. In the recycling scenario, EOL LIB packs can be collected at collection and sorting centers, and either processed directly in pyrometallurgical recycling facilities or first disassembled into battery cells, followed by mechanical pretreatment to obtain black mass. The black mass can be subsequently treated in hydrometallurgical recycling facilities to recover refined battery materials that can be used in the CAM production. Finally, in the circular scenario, the EOL battery packs can be processed using the same recycling pathways, or a maximum of 20% can be sent to location F to be reused as stationary energy storage. Here we assume a fixed lifetime of 4 years as energy storage after which the LIBs are treated in downstream recycling processes. The analyzed scenarios in the case

study are summarized in Table 5.

**Table 5:** Studied scenarios in the case study.

| Scenario  | Description   |
|-----------|---|
| Linear    | Linear benchmark supply chain, where EOL LIBs are transported to disposal.  |
| Recycling | EOL LIBs can be processed in recycling processes.   |
| Circular  | EOL LIBs can be processed in recycling processes and a fraction reused in stationary energy storage applications. |

## RESULTS AND DISCUSSION

The optimization model is implemented in GAMS and solved using CPLEX solver version 22.1.1. The evaluated scenarios (Table 5) were run with all three objective functions (Equations 1-3) to assess the trade-offs in the optimal supply chain design. Further multi-objective optimization and pareto analysis was not conducted at this stage.

### Cost optimal solution

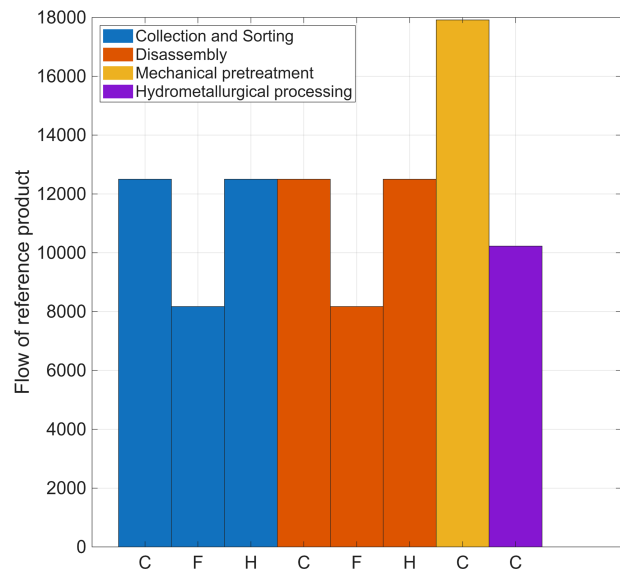
Compared with the linear supply chain, the recycling scenario reduced the total cost by 4.4% in the time periods studied. The optimal strategy was to use hydrometallurgical recycling for spent LIBs as it allows for cost savings due to smaller quantity of required raw material purchases. The cost-optimal supply chain uses centralized collection and disassembly and, at the final time period, requires three collection centers, three disassembly centers and a mechanical pretreatment center and a hydrometallurgical facility, as shown in Figure 4. Mechanical pretreatment and hydrometallurgical recycling are located at the same location as the CAM production to avoid transportation of the refined battery metals.

In the circular scenario, when the possibility of second-life use of LIBs was allowed, the optimal solution included using a fraction of the LIBs as energy storage in the allowed location F to generate more revenue, resulting in total supply chain cost decrease of 10.8% compared to the linear supply chain.

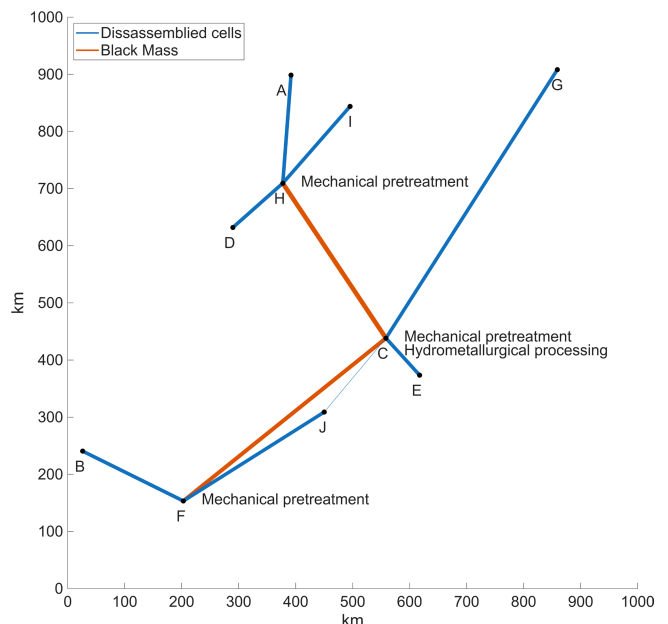
### Emission optimal solution

When the total supply chain emissions were minimized, the hydrometallurgical processing route was also selected, to reduce the supply chain emissions from raw material procurement. However, in contrast with the cost optimal strategy, the supply chain shifts towards a decentralized collection and disassembly to avoid emissions generated via transportation. The optimal supply chain for the recycling scenario consisted of collection and disassembly facilities at all locations, three mechanical pretreatment facilities at locations C, F, and H and a hydrometallurgical recycling facility at location C, as

presented in Figure 5. In the circular scenario, the model did not allocate any collected batteries to secondary use, as no environmental benefit was assigned to reuse.



**Figure 4.** Cost optimal capacities at the final period for the recycling scenario.



**Figure 5.** GHG-optimal decentralized supply chain for LIB recycling.

### Raw material optimal solution

For the studied generic pyrometallurgical and hydrometallurgical processes, the optimal solution for minimizing primary raw material procurement was to utilize the hydrometallurgical recycling route in all scenarios where recycling was permitted by the model constraints. By recycling EOL LIBs, the supply chain reduced its total refined battery materials consumption by 55% over the

studied time periods.

## CONCLUSIONS AND FUTURE WORK

The significant rise in the popularity of electric vehicles results in the increasing demand for lithium-ion batteries, consequently increasing the amount of EOL LIBs, which require efficient management. Thus, an optimization model is proposed as a tool to design and optimize the circular supply chain network for LIBs. The State Task Network based optimization framework allows for the optimal design of facility locations, technologies, capacities and the reintegration of recovered materials back into the different stages of the supply chain.

The results from the illustrative case study tested with literature data showed that both in terms of costs and emissions, the hydrometallurgical process is preferred. With the circular scenario, the optimal strategy was to utilize a fraction of the collected LIBs as stationary energy storage to generate more revenue. The case study revealed that the cost optimal solution prefers centralized collection, while the GHG optimal network prefers decentralized collection and mechanical pretreatment for LIBs. The preliminary results align well with the identified spoke-and-hub network recognized to reduce costs in LIB recycling [13].

Future work could involve developing a more realistic case study as well as studying different cathode active materials used in EVs. Also, considering the full bill of materials enables the optimization and assessment of the circularity of electrolytes and other materials present in LIBs.

## AUTHOR IDENTIFIERS

Author ORCIDs:

Kopra: 0009-0005-5428-1818

Harjunkoski: 0000-0003-0428-0751

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