Towards a Stochastic Representation of Optimal Pathways for Automotive Batteries at End of Life

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Introduction

Batteries at the end of their automotive life have many options: (remanufacturing, repurposing, recycling [1]. Pathways may be inherently constrained by whether the battery was under warranty, how the battery was operated, and the battery's chemistry [2]. The overall environmental and economic impact of the EOL pathway further depends on the application for the repurposed battery [3,4], the chemistry of the battery, method of recycling, and the business model of all such activities [1,5]. Much research has focused on particular aspects within the complex network, providing a skeleton of how to prepare for the ever-increasing flow of lithium-ion batteries at the end of automotive life (EOL), which may reach 26 GWh globally by 2025 [6].

A model can be parameterized to suggest a “likely” annual stock and flow of batteries with an understanding of the range of economics tied to different EOL pathways. In understanding the stocks and flows of batteries, informed by an optimal planning model, relevant authorities (Regulators and OEMs, repurposers and recyclers, etc.) may better prepare and accommodate this future “waste” flow. Scant work has observed the optimal pathways automotive batteries will take, primarily due to the inherent complexity along with every decision point. Thus, this work is novel in formulating a holistic optimization of end-of-life pathways but indeed a progression towards an optimal solution rather than a finite solution. Given this, the bulk of the proceeding work will focus on framing the problem and suggesting a methodology for parameterizing and deriving an optimal solution

Lit Review: Identifying Relevant EOL Processes

The proceeding focus will be on describing the relevant parameters for this problem and describing their existing uncertainties and evolving uncertainties: battery health, repurposing costs, repurposing benefits, recycling costs, and recycling benefits.

Battery Health

Battery state of health (SOH) has many implications in optimizing EOL pathways; a cursory definition of SOH typically refers to the remaining capacity within a battery, once subject to degradation [7]. Battery degradation is the decrease in battery charge capacity over time. LiBs experience degradation for many reasons, some of which are understood and some not [8]. Of those that are understood, several are from routine usage of the battery, abuse of the battery, and some even occur simply over time with no relation to battery use. Every part of the battery is subject to degradation: anode, cathode, electrolyte, separator, current collector, etc. Essential parameters affecting the health of a battery are charge rate (C-rate), Depth of discharge (DoD), total cycles, and operating temperature [9]. In the context of this optimization, SOH is most important for defining the usefulness of a battery (how much it can store or discharge) but also crucial for implying how close it is to the aging “knee” or a rapid decline of the battery’s usefulness [7]. The aging knee is also little understood but is typically parameterized to be around 60% SOH when such decline occurs [10,11].

There are many existing and evolving uncertainties in parameterizing SOH. The battery's age at the onset of EOL is uncertain and can be subject to stochastic events, such as a car crash. If a battery is in a vehicle that crashes in the first year, the battery will have had little cycling and minor calendar aging but may be taken out of the car. Another uncertainty is the battery's operation during its automotive life, which relates to DoD and C-rate. For example, if a driver is prone to aggressive driving with excessive acceleration and braking, the instantaneous discharge rates may be higher on the whole. Thus, when at EOL, this excessive use of the battery may cause it to fail quicker. The climate or operating temperature a battery exists in may cause it to accelerate degradation or hamper its performance (e.g., [12]). Additionally, all these parameters related to SOH may rapidly evolve in the coming years. For example, a broad evolving uncertainty related to operating an electric vehicle is the dawn of autonomous vehicles. If a substantial proportion of cars on the road are autonomous, the large-scale expectations for these health-related parameters may change remarkably. An example of how these parameters may evolve assumes that autonomous vehicles will decrease automotive accidents and provide more controlled and optimal driving patterns. With decreased automotive accidents, the number of batteries that arrive at EOL with higher SOHs due to premature vehicle retirement will likely decrease. Vehicle autonomy will likely lead to a higher SOH for batteries at EOL with increased control and optimal driving patterns. One other radical change that is imminent is a large-scale adoption of new anode technologies that will dramatically increase the lifetime of a substantial number of LI-ion chemistries [13,14]. Large-scale adoption of this technology would modulate the stock of available batteries at EOL over a particular time horizon.

Repurposing

Given the large capacity and high performance of modern vehicle batteries, retired batteries could still offer significant capacity in lower-power, secondary applications (e.g., battery storage for electricity grid applications). A growing body of research mainly examines the economic feasibility and environmental impacts of second-life [6,15,16]. While battery packs from EVs will be retired for several reasons [16–18], if warranty guarantees from early EV models are an indication, LIBs are likely to serve an 8-10 year useful life in a vehicle before being removed or replaced [19,20]. A typical retired EV battery may retain ~80% of its new storage potential. As LIBs are retired from use in EVs, some end-of-life (EOL) management is required. Previous research suggests second-life uses in less demanding applications like stationary energy storage may provide environmental benefits or cost benefits before recycling or other final disposal options [6,15]. While it may seem inevitable that second-life batteries would be cost-effective in stationary storage applications, there are potentially high costs for collecting, transport, and repurposing processes. Concurrently, the cost of new LIBs continues to fall dramatically, presenting a challenge to the cost-competitiveness of second-life LIBs [21,22].

Many uncertainties exist in repurposing costs. As a result of the novelty of repurposing an automotive battery, most studies have derived costs from process-based models in place of empirical evidence (e.g., [16,23–25]). Recurrent findings have suggested procurement costs of spent batteries, labor, and transportation costs as critical uncertainties. The procurement costs of spent batteries are entirely dependent on the business model of the repurposing operation. For example, under a leasing scenario in which the battery's original equipment manufacturers' (OEM's) own the battery within a given vehicle and plan on repurposing the battery, they could circumvent these procurement costs [20]. This process is also very laborious. A repurposer will have to unpack a battery, test its health through various charge/discharge procedures, potentially swap out cells that are damaged and repack the battery [9,26]. This procedure is modeled to take as long as 4 hours [16]. Transportation of spent or repurposed batteries (e.g., in/outflow) is subject to significant uncertainty because batteries are heavy and potentially hazardous [27]. Concerning the latter, there's an ongoing debate as to whether batteries should be classified as universal waste or hazardous waste, which could either severely limit options for transport or modulate the costs [28]. Given these critical uncertainties, the distribution of repurposing costs across the literature is vast. Not unlike parameterizing battery SOH, these uncertainties are liable to change substantially.

As alluded to before, there are substantial uncertainties in batteries' benefits once they've been repurposed. Since providing powertrain to an electric vehicle is so demanding, the cascading options for repurposing are plentiful. Thus, three sources of uncertainty for parameterizing benefits from repurposing exist: many different applications with varying benefits, uncertainty in benefit because costing energy storage technologies is nascent, and uncertainty as to the performance of repurposed batteries (as a function of SOH). Despite other potential applications, stationary storage is most commonly considered for repurposed batteries [15]. There are various services (and thus benefit streams) a battery can provide, but recent work suggests that the likely most cost-competitive options are small-scale behind-the-meter deployments. Mainly in contrast to large-scale deployments that can substantially benefit from economies of scale, repurposed batteries may appear cost-competitive (Steckel et al., in prep). Even when just considering BTM deployments, significant discrepancies exist as a function of how customers use their system. Annual data collection efforts are actively trying to quantify received benefits from BTM storage systems qualifying for the Self Generation Incentive Program in California, which perhaps bests illustrate this range of benefits as a function of the customer [29]. Not much work has been done on further calibrating the benefits of repurposed batteries performing these same tasks. However, it may seem obvious given the relationship between battery SOH and the performance of a battery and the presumption that repurposed batteries are initially more degraded (e.g., [30]).

Recycling

Recycling and recovering the materials in Lithium-ion batteries decreases the need for raw materials, lowering the battery's life-cycle impact and improving energy security by reducing imports. However, there is little data on recycling rates for LIBs in the United States, and estimates are persistently low and potentially inaccurate [20]. LIB recycling is still a small industry. Specific data on the cost of recycling batteries or industrial recovery rates are uncertain and insufficient. In contrast to other battery recycling, LIB cells must first be separated into their individual components before recycling can recover materials [31]. Given this intricacy, different methodologies exist for the final stage of recycling broadly described as pyrometallurgical, hydrometallurgical, and advanced hydrometallurgical (advanced hydrometallurgical is also referred to as direct cathode recovery; [1]). Generally speaking, many of the economic uncertainties in repurposing automotive batteries apply to recycling (e.g., logistics).

Given the nascent industry, the costs of recycling are highly uncertain. Thus, uncertainty in recycling costs will depend heavily on subsidies, method of recycling, and scaling of facilities. Perhaps the most critical and non-linear uncertainty is whether recycling operations will be subsidized and the extent [27]. In fact, there is still uncertainty as to whether or not recycling is economical without subsidies [31]. As for methodology, Ciez and Whitacre find this to be a massive driver of both economic uncertainty and the overall environmental cost. In their process-based model of recycling facilities, advanced hydrometallurgical is found to be the optimal recycling method. Like repurposing, recycling will benefit from economies of scale and lower per-unit costs [32].

The benefits from recycling batteries are constrained to uncertainty surrounding the value of constituent materials. Recyclers mainly recover higher value materials (such as copper, cobalt, and nickel) or easily recycled materials (steel or aluminum parts); the remaining electrode materials, primarily lithium and aluminum, are reduced to slag [33]. Thus, the value of these recycled materials fluctuates as the value of the virgin materials fluctuates. Two potential uncertainty drivers in parameterizing the benefit of recycling automotive batteries include changes in commodity prices of critical minerals like cobalt or lithium and then the changing bill of materials in automotive batteries. Cobalt is the most notable of cathode materials that experience marked volatility, given geopolitical instability from the region it originates [1]. This volatility and a generally high price have prompted an industry-wide shift away from cobalt-heavy chemistries [20,34]. This industry-wide shift also highlights the uncertainty inherent in recycling benefits when the mix of constituent materials embedded in automotive batteries is constantly changing.

Lit Review: Parameterization

The review of relevant literature provides a good overview of the necessary parameters to input the optimization model. Thus, to populate these parameters, current literature is scanned to populate a probability distribution for every relevant parameter. In this initial simplification of EOL management, these parameters are sought: available battery capacity (MWh) for every year, battery SOH, average automotive lifetime, costs of repurposing, discounted benefits of repurposing, time for the repurposed battery in an application, annual degradation in an application, costs of recycling, and benefits of recycling. The benefits of repurposing are the only costs that are discounted; other costs are represented as occurring in one time step. The parameters are shown here in Table 1. In the proceeding results, the distributions are all represented as normal distributions, but this distributions' modulation can easily be done. After an initial search of available battery capacity (MWh) for every year, battery state of health at EOL, automotive lifetime, time for the repurposed battery in an application, and annual degradation in an application were decided to be represented as discrete exogenous variables in the optimization formulation, hence only one value.

parameter	**mean or discrete value**	**standard deviation**	**source**
Repurposing cost	36.6	14.8	(Steckel et al., in review)
Recycling cost	29.3	20.8	[1,32,35–37]
Repurposing annual benefit	25	35.4	[4]
Recycling benefit	30	11.3	[1,32]
2021 EOL capacity	2567		(Dunn et al., in review)
2022 EOL capacity	2956		(Dunn et al., in review)
2023 EOL capacity	3668		(Dunn et al., in review)
2024 EOL capacity	5855		(Dunn et al., in review)
2025 EOL capacity	7730		(Dunn et al., in review)
2026 EOL capacity	19085		(Dunn et al., in review)

2027 EOL capacity	16625		(Dunn et al., in review)
EOL battery SOH	0.8	0.1	[20]
Automotive lifetime	8		[20]
Time in repurposed application	7		(Steckel et al., in review)
Annual degradation	0.02		(Steckel et al., in review)

Table 1) parameters with mean and discrete values, standard deviations (where applicable) and source.

Methodology

The bulk of this research effort was to parameterize the resulting optimization model to decide optimal pathways; that said, the resulting model is purposely underspecified and is meant to be a skeleton for comparing different pointed scenarios. In its current state, this function model is a linear program with probabilistic objective function coefficients. Thus, expected values populate the coefficient vector c_{ti}. Admittedly, without additional constraints the optimal solution is very simple in that if $c_{t1} > c_{t2}$ the optimal solution will be that X_{t1} will increase throughout iterations of the optimization until it reaches a binding constraint and vice versa if $c_{t1} < c_{t2}$. Another point is that because all values are presented as present values, both the recycling and repurposing costs are the sum of their individual costs and benefits. Thus, the expected value coefficient vector c_{t1} can be formulated according to this equation (eq. 1).

$$\sum_{i=1}^{T} EV(c_{t1})X_{t1} \;\; (eq. 1)$$

The second vector, relating to net repurposing cost, is slightly more complicated as alluded to prior. The cost function is calculated identically, but the repurposing benefit is a function of both battery SOH (eq. 2) and a net present value function (eq. 3). The values modulating the benefit function are exogeneous and can be used readily to inform discrete scenarios. For example, the number of years a repurposed battery, t_{rep}, can serve in an application is used to generate scenarios later in the paper.

$$\sum_{i=1}^{T} EV(SOH) \;\; (eq. 2)$$

$$\sum_{i=1}^{t\_rep} \frac{(c_{t2})}{1 + r^{t\_rep}} \;\; (eq. 3)$$

So given that, the resulting value coefficient vector c_{t2} can be formulated according to this equation (eq. 4).

$$\sum_{i=1}^{T} EV(c_{t2})X_{t2} \;\; EV(SOH) \frac{(c_{t2})}{1 + r^{t\_rep}} (eq. 4)$$

The constraint set in this model's current form is fundamental. The first constraint set involves continuity, in that all batteries take a recycling or repurposing path at the onset of EOL (eq. 5).

$$X_{t1} + X_{t2} = b_t \ \ (eq. 5)$$

The last constraint set simply applies non-negativity to the decision variables (e.g., it would be impossible to have a negative number of batteries sent to repurposing in our formulation (eq. 6).

$$X_{ti} = 0 \ \ (eq. 6)$$

The ability to specify further constraints will allow more informed and realistic decisions. This paper was meant to formulate rather than solve this problem, so any further imposition of constraints would be arbitrary given the available data. A couple of constraints that could be implemented could be an infrastructure build component and marginal disposal cost. Implementing a relationship between additional decision variables (e.g., how many recycling/repurposing/hybrid facilities to build) and a constraint on how many batteries can take that pathway seems the most obvious next step. As discussed previously, the lack of recycling infrastructure in the USA makes this hard to parameterize. Also, given the desire of the model output, direct disposal (e.g., no recycling/repurposing) was not an option, but this constraint could be relaxed and replaced with a marginal cost in the objective function.

Results/Discussion

These results are preliminary but certainly interesting. Given our initial set of exogenous variables, the linear model suggests full routing to repurposing at EOL to be the optimal pathway (Table 2). This suggestion is not unexpected given the under specification of constraints. The model is essentially picking the smaller net costs between recycling and repurposing. One interesting thing that this model can show is a coarse sensitivity to exogeneous parameters, such as t_{rep}, the number of years a repurposed battery is used. Thus, the model suggests that recycling is the optimal output if a battery can only serve one year (Table 2). This procedure can likewise be repeated with any exogeneous variable, like SOH, at the onset of EOL.

t_rep yrs.	SOH mean	SOH sd	C1 ($/kWh)	C2 ($/kWh)	X11 (kWh)	X12 (kWh)	X21 (kWh)	X22 (kWh)	…
7	.8	.1	.00758	-45.2	0	2567000	0	2956000	…
1	.8	.1	.00758	15.5	2567000	0	2956000	0	…
2	.8	.1	.00758	-1.72		2567000	0	2956000	…

Table 2) Given the endogenous parameter set, the expected value cost parameters and decision variables are reported. The results are truncated in this table as the decision variable chooses all of one pathway for the given scenarios.

For many reasons, recycling should not be perceived as a sub-optimal pathway. Batteries with excessively low SOH, unforeseen damages, or repurposed batteries at the end of their second life will require infrastructure likewise to reclaim some value. Thus, the formulation of this optimization model, without constraints, may be somewhat misleading. As a result, two methods are suggested to derive a split-decision solution that the underspecified linear model cannot: an expected value optimal solution of Table 2 given a discrete and equal probability of all t_{rep} occurring and a Monte Carlo simulation given the same normal distributions for the model parameters. For the first contingent analysis, the resulting decision would reflect the optimal pathway to repurposing as 6/7 of the given year's capacity and 1/7 of recycling for the given year. The results from the Monte Carlo simulation are shown in Table 3.

t_rep	SOH mean	SOH sd	X_{11}	X_{12}	X_{21}	X_{22}	X_{31}	X_{32}	X_{41}	X_{42}	X_{51}	X_{52}	X_{61}	X_{62}	X_{71}	X_{72}
7	.8	.1	968	1600	1090	1870	1360	2300	2210	3640	2900	4830	7220	11900	6320	10300

Table 3) As in Table 2, however expected cost values and all decision variables are explicitly represented. Also, decision variables are no represented as MWh per computing limitations.

The Monte Carlo simulation provides a more balanced EOL distribution and may be more appropriate than the underspecified linear model. The Monte Carlo simulation's nature seems more well equipped to capture the tails (e.g., batteries with low SOH) than the linear model that treats the cost coefficients as a discrete value for the entire analysis period. Contrastingly, the Monte Carlo procedure resolved decision-making at the MWh level (e.g., ~10000 decisions vs. ~10000000 decisions) and was repeated 100 times, giving much more diverse representation of the distribution of the model parameters. The suggested optimal pathways (X_{71} , X_{72}) are shown for an example year, providing a representative distribution (histogram) of optimal pathways to be interpreted if desired (Fig. 1). The suggested optimal pathways (X_{71} , X_{72}) are shown as a Sankey diagram also further to visualize the material flow (Fig. 2)

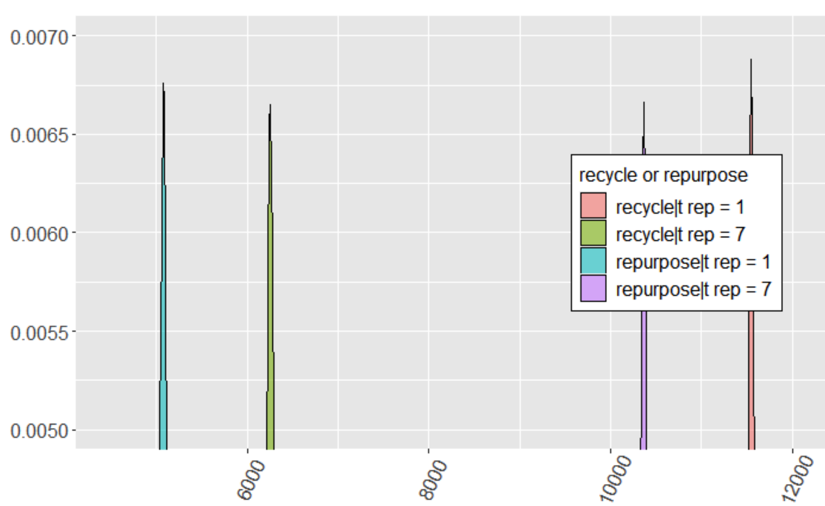

Fig. 1) Histograms of Monte Carlo simulation for optimal decision variables for recycling and repurposing for where $t_{rep} = 7$ (green, purple) and $t_{rep} = 1$ (red, teal).

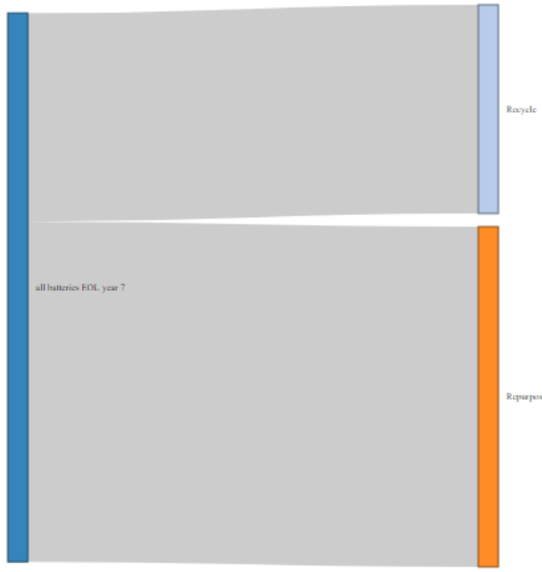

Fig. 2) Sankey diagram showing with weighted flows (MWh) in year 7 to recycling (blue) and repurposing (orange).

This project is preliminary and allows for many directions for future work: modulating the optimization approach, adding constraints, and modulating existing constraints. One alternative optimization approach would be representing this problem as a non-linear problem with penalty functions instead of constraints. With this formulation there would be more freedom to implement interactions between the decision variables and incorporating more complex economic constraints. The trade-off would then be having to solve with a gradient search procedure or other methodologies that would only identify local minima. As far as building upon the linear methodology, the constraints could be represented as chance constraints. This is a very likely direction as the discreteness of the annual battery capacity constraints is very unrealistic. These values were based off of vehicle warranties and are inherently very uncertain. As for further specification of the constraints, there are many directions to take this model. Additional constraints have already been mentioned earlier. Another major improvement to this model would be to have a more sophisticated time component. As in both constraints and cost parameters could be more time-dependent if coupled with evolving projections.

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