METHODS ARTICLE

ECOPT[2]: An adaptable life cycle assessment model for the environmentally constrained optimization of prospective technology transitions

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Abstract

Life cycle assessment (LCA) is a method to evaluate the environmental impacts of technologies from cradle to grave. However, LCAs are commonly defined in terms of the consumption of a single unit of a product and thus ignore scaling issues in large-scale deployment of technologies. Such product-level LCAs often do not consider capital manufacturing capacity and supply chain bottlenecks that may hinder the rapid, widespread uptake of emerging technologies entering the market; emerging technologies often require the expansion of existing supply chains or the development of entirely new supply chains, such as the manufacturing of novel materials. As a result, such LCA studies are limited in their ability to realistically assess impacts at the macro-scale and thus to guide large-scale decisions. In this work, we present ECOPT[2], a generalized adaptable model that combines these constraints to the LCA approach using a mathematical programming approach and dynamic stock modeling. ECOPT[2] combines LCA factors with transition scenarios from energy systems models to determine the environmentally optimal deployment of new technologies while accounting for material circularity constraints and barriers to uptake. We also introduce the structure of the software tool and demonstrate its features using a stylized vehicle electrification scenario.

KEYWORDS
emerging technologies, fleet modeling, industrial ecology, life cycle assessment, mathematical programming, transformation pathways

1 | INTRODUCTION

There is increasing urgency to mitigate anthropogenic environmental impacts, particularly greenhouse gas emissions (IPCC, 2015; IPCC, 2018). There are many technological options for mitigation, and to guide policy toward the options with greatest effect, we must understand the full reach of these technologies' impacts and benefits. While energy system models (ESMs) and integrated assessment models (IAMs) can be used to assess

sector-wide or multisectoral transformation pathways to reach these mitigation goals, they generally do not include the full value chain, or indirect, impacts associated with technologies. However, as shares of low-carbon energy technologies increase, so does the significance of indirect impacts (Blanco et al., 2020) and material cycles, as the material intensity for these technologies is generally higher than for fossil-based energy (Hertwich et al., 2015). As a result, great focus has been placed on methods integrating ESM and industrial ecology methods such as lifecycle assessment (LCA) and material flow analysis (MFA) (Arvesen et al., 2018; Blanco et al., 2020; Kullmann et al., 2021; Pauliuk et al., 2017). Such integrations supplement the top-down coverage of the economy in ESM and IAMs with the higher level of environmental and value chain resolution found in LCA and MFA. As noted by Pauliuk et al. (2017), IAMs stand to benefit from linkages with industrial ecology methods, which introduce a representation of the biophysical basis of society to this family of models, including global supply chains, and the linking of services with stocks and flows and material cycles. Furthermore, LCA provides additional impact categories, which allows the evaluation of environmental trade-offs, in contrast to the climate focus of IAMs.

LCA is an analytical method developed to capture the environmental impacts over the lifetimes of products, processes, or services and those of their associated value chains. LCAs are commonly performed to assess the consumption of one unit of a product, thus giving a picture of the total environmental impacts induced by a single product's existence and use ("product-level" LCA). Commercial software, of which SimaPro (PRé Sustainability, n.d.) or GaBi (Sphera, n.d.) are examples, is frequently used to perform LCA. The capabilities of these software tools often reflect the popularity of singular-product type assessments in their feature set, in that they are generally restricted to these types of studies. These studies of singular products are useful for product design and cross-product comparisons (Haes et al., 2004), but limited in their usefulness to inform large-scale decisions, such as the transition to a new technology, which often encompasses transformational change within entire economic sectors.

In this section, we review in detail these shortcomings in common LCA applications and the limitations in results that consequentially arise from these shortcomings, and how previous literature has attempted to address them.

1.1 | Limitations of LCA for macro-scale decision-making

Below, we present three main limitations in current LCA approaches for these types of large-scale transition analyses, followed by a discussion of how previous work has attempted to address these limitations.

For one, product-level LCAs commonly model linear and unconstrained systems. The impact of introducing a thousand billion products is simply a thousand billion times the impact of a single product. The upscaling of single-product LCA results in this manner implies an idealized system where this upscaling occurs in isolation of the wider economy. Consequently, such idealized systems ignore the constraints imposed by limited material availability or capital manufacturing capacity. However, this limitation is becoming increasingly significant as the urgency for environmental action escalates; a necessarily rapid and large-scale response, that is, uptake or transition to new technologies, may be hampered by bottlenecks in raw material value chains, manufacturing capacity, or supporting infrastructure availability (Bergerson et al., 2020; Mäki et al., 2021). For example, as the more easily extractable resources are depleted, for example, those with higher ore grades, we turn to increasingly challenging resources, which in turn may cause higher impacts in their extraction and refining (Azadi et al., 2020; Gan & Griffin, 2018; Norgate et al., 2014). A second consequence becomes apparent when supply constraints restrict the rate of technology uptake; the environmentally optimal solution will prioritize technology deployment in regions where the greatest overall environmental benefit will be achieved. Given the current urgency for climate action, it may in fact be advantageous to favor a technology with higher climate impacts but with no deployment bottlenecks over a technology with lower impacts, but which cannot immediately achieve its full deployment potential due to supply limitations. Adding such constraints thus allows for more realistic macro-scale applications of LCA studies, as the technology is not assessed in isolation from the wider system.

The second limitation is that LCAs often evaluate only a restricted set of parameters, for example, varying electricity mixes used, or assumed product lifetime. Studies also often investigate the effect of these parameters one at a time, and thereby do not investigate the cumulative effects of changing several of these options concurrently. The most obvious weakness of such an approach is that the full spectrum of possible outcomes is not explored, particularly in complex systems. Consequently, scenarios that minimize the environmental impacts might not be identified because they may include parameter values or parameter combinations not investigated in the study (Yang & Heijungs, 2018). Part of the reason for these limited sensitivity analyses is the cumbersome set-up of common LCA software tools, which require the manual definition of every investigated scenario.

A third limitation of product-level LCA studies is that they represent static, or steady-state, systems. The results from these studies represent a static snapshot of a product; in a rapidly evolving world, these results quickly become outdated and are inadequate for assessing the potential of a technology in the immediate future due to gains in economies of scale and rapid technological improvements and developments in the supply chain. This issue is exemplified in the rapid decarbonization of the production of lithium-ion batteries in the past decade since their introduction to the market (Philippot et al., 2019). Furthermore, while any given technology is evolving, other systems in the background are concurrently undergoing their own transitions, which in turn affect the technology in question (Gibon et al., 2015; Mendoza Beltran et al., 2018). These dynamic background effects are often not captured or only superficially treated in product-level LCAs and are not currently implemented in the commercial software commonly used in performing LCAs (Cardellini et al., 2018).

These limitations have been partly addressed using several approaches. The early literature on change-oriented LCAs that strive to capture the consequences of a perturbation, or "consequential LCAs" (CLCA), recognized the issue raised by constrained supply. Guidelines for CLCAs recommended the manual exclusion of obviously constrained suppliers from value chains, as these could not increase production to meet an increase in demand (Ekvall & Weidema, 2004; Thomassen et al., 2008). Nevertheless, to this day, the vast majority of CLCAs follow modeling guidelines that consider only small, marginal changes in technology mix and consumption choices[1] (Dandres et al., 2011; Palazzo & Geyer, 2019); suppliers are exogenously identified by the analyst as either constrained, and therefore excluded from the analysis, or unconstrained and therefore part of the marginal mix (Weidema, 2003). A more explicit modeling of resource and production constraints was introduced to environmental modeling by the body of literature on the World Trade Model (Duchin, 2005) and the RCOT model (Duchin & Levine, 2011), where increasing demand is modeled as having to rely on progressively less environmentally attractive sources as supply constraints are reached. To our knowledge, this approach has been mostly limited to macro-economic modeling rather than high-resolution LCA models, with the exception of the exploratory work by Kätelhön et al. (2016). While this stochastic technology-of-choice model was subsequently adopted in other work (Larrea-Gallegos et al., 2019; Lee et al., 2019), it has not been extended to tackle the dynamic evolution of constraints and demand levels over time. This question of the dynamic evolution of constraints in LCA was partly addressed in Watari et al. (2019) using linear optimization. Watari et al. (2019) combine a dynamic stock-driven fleet model with LCA factors to investigate how constraints on lithium availability limit the rate at which electrification can occur. However, the Watari et al.'s (2019) study did not constitute a full LCA as well-to-wheel emissions were used and therefore excluded the vehicle production cycle, which also omits the emissions associated with primary material extraction.

Because linear optimization acts as a type of sensitivity analysis and determines the combination of parameters resulting in minimized environmental impacts among *all* possible combinations, the method also presents a solution to the second shortcoming of LCA, namely the frequently "manual" approach to parameterization and scenario analysis. The benefits of joint LCA and optimization approaches are two-fold: it allows the inclusion of supply constraints, and by default, the optimization approach finds the combination of decision variables that result in the lowest environmental impacts. Examples of joint LCA-optimization studies generally involve the selection of technologies by minimizing environmental impact, and using as decision variables, for example, the mix of substitutable products with limited supply as in Budzinski et al. (2019), Saner et al. (2014), and Steubing et al. (2016), among others. These studies, however, have been static in nature and do not identify a transition pathway. Another approach by Milovanoff et al. (2021), while not a true mathematical programing model, constrains emissions to a target and uses transport activity as the decision variable and uses a "search-and-try" approach. Similarly, Gao and You (2018) perform a dynamic multi-criteria approach optimizing resource use, environmental impact, and costs of the shale gas supply chain, while Vadenbo et al. (2014) optimize environmental and economic performance of waste and resource management in industrial networks. These implementations avoid the issues associated with an unconstrained approach to upscaling LCAs, while also determining the optimal scenario for minimizing environmental impacts. However, none of these studies combine a generalized approach (i.e., are case-studies of specific contexts that cannot be applied to other systems), dynamic systems, multi-region assessments, and open-source development.

To date, two main approaches to incorporating transition dynamics in LCA have been adopted, tackling the third shortcoming of LCA previously mentioned. In the first, researchers incorporate results from energy models, including IAMs, as a means to include the consequences of energy transitions (Cox et al., 2020; García-Gusano et al., 2017; Gibon et al., 2015; Mendoza Beltran et al., 2018; Pedneault et al., 2021; Vandepaer et al., 2019). These approaches attempt to model the evolution of the physical economy on which the product under study depends, also called the "background" in LCA terminology. With a dynamic approach, the evolution of this background system, for example, with progressively decarbonizing energy mixes, can be captured in the prospective LCA of a technology reliant on such energy mixes.

Another approach to incorporating dynamics is to adopt stock cohort-based analysis in the representation of a specific technology (Field et al., 2000). This approach has been applied most notably to building stocks (Göswein et al., 2019; Lausselet et al., 2021) and vehicles (Baptista et al., 2012; Choma & Ugaya, 2017; Garcia et al., 2015; Milovanoff et al., 2019; Stasinopoulos et al., 2012). The stock cohort-based approach accounts for the change in emissions intensity over time, for example, as vehicles are retired and replaced by more fuel-efficient models, and which are produced using more efficient processes than their predecessors. The dynamic cohort analysis often builds upon, or is linked to, dynamic stock models from material flow analyses (Liu et al., 2013). To our knowledge, few authors have combined both stock modeling and a dynamic LCA background; Pauliuk et al. (2021), Sigüenza et al. (2021), and Gibon et al. (2015) describe such an approach. Many existing IAMs and ESMs also incorporate a basic stock model; however, as previously discussed, these models generally lack the lifecycle perspective and often do not consider the flows of materials in the system.

While many of the above examples present good case studies in addressing some of the shortcomings of the LCA method, the community still lacks an approach that combines these approaches such that it can be adapted to various technologies and stocks. In this paper, we present the Environmentally Constrained Optimization of Prospective Technology Transitions (ECOPT[2]) adaptable model. With this work, we aim to describe the model workings and provide an open-source software tool[2] for evaluating technologies using LCA and to address the limitations of linearity, static analysis, and narrow scope commonly seen in product-level LCAs. We illustrate the use of this tool for informing transport electrification policy by modeling the optimal electrification pathway with respect to climate change impacts while accounting for stock dynamics and constraints to uptake. We adapt LCA to macroscale by capturing the dynamic interactions at the stock level while accounting for system-level constraints that may alter the supply mixes and environmental intensity of value chains or impede the mass-scale rapid rollout of technologies. To this end,
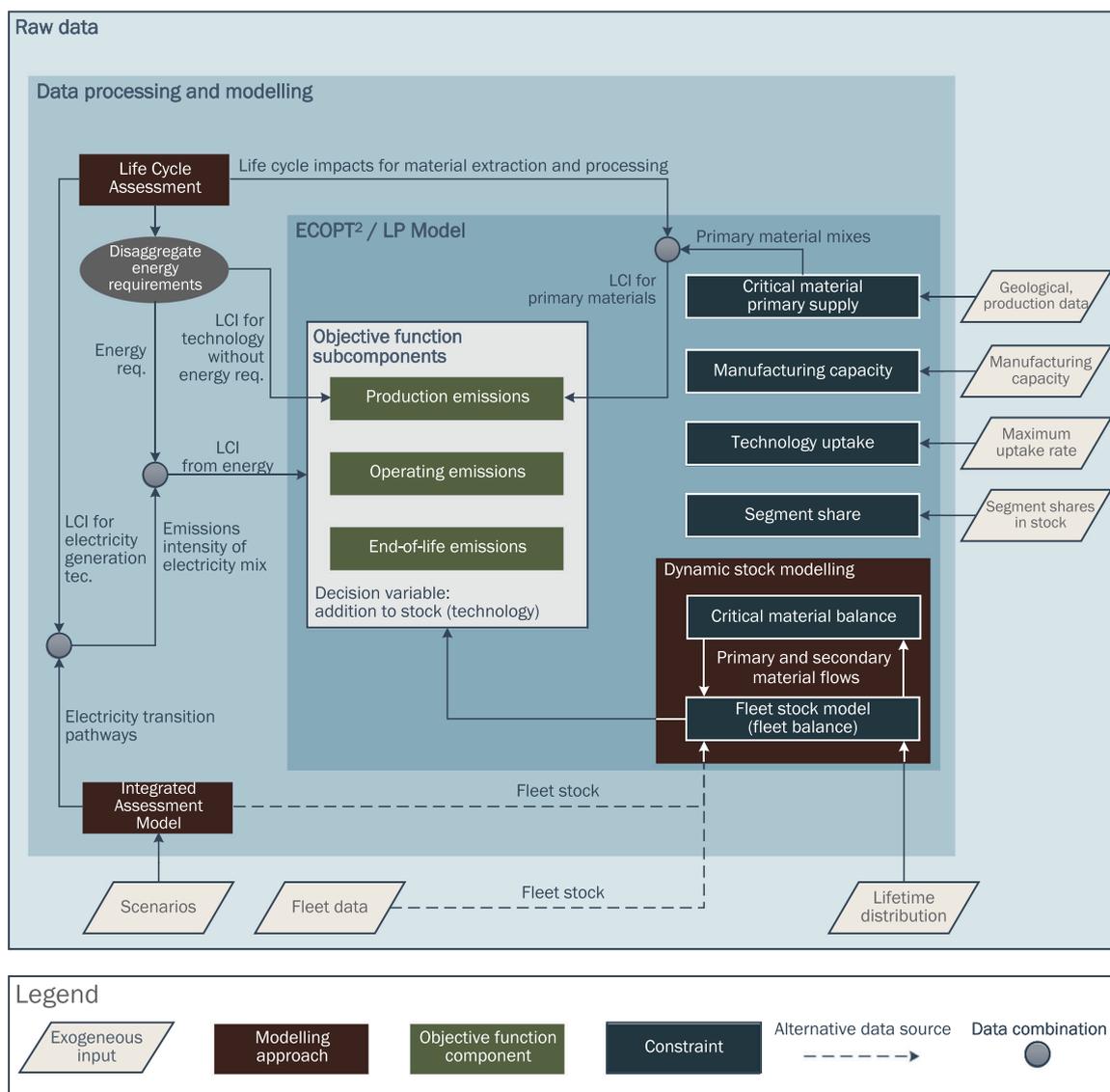
FIGURE 1 ECOPT² structure overview. LCI: Lifecycle impacts

we investigate electrification pathways compatible with climate targets that result in the lowest climate emissions given physical and temporal barriers to uptake, for example, restrictions to supply, market uptake, and the effects of temporal lag and technological lock-in. This model also includes technological, segment, and regional differentiation. Finally, this work also aims to add to the growing portfolio of partially or fully open source integrated LCA and industrial ecology frameworks (Cardellini et al., 2018; Ciroth, 2007; Mutel, 2017; Pauliuk & Heeren, 2020) with the addition of an optimization approach.

The remainder of this paper begins with a conceptual overview and mathematical formulation of the model in Section 2. We present a stylized example of an analysis using the model in Section 3 to illustrate the model capabilities. Finally, in Section 4, we conclude with a discussion of potential use and future work.

2 | CONCEPTUAL MODEL OVERVIEW

As mentioned, current LCA tools have weaknesses that make them ill-suited for informing large-scale decision-making processes. ECOPT², a generalized adaptable model, which applies LCA principles while introducing system constraints and a dynamic approach, allows for realistic scenario evaluations of technology diffusion. The model (Figure 1) consists of a core optimization problem (in our case, a linear program) wherein the objective is to minimize life cycle impacts of the technology stocks (e.g., light duty vehicle (LDV) fleet) by deploying novel technology capital (e.g., novel powertrain technologies) to different competing market segments (e.g., vehicle size segments or final use sectors) in user-defined regions. Parametrized inputs include energy transition pathways from energy models such as IAMs, life cycle impact factors for the technology capital and

associated sectors, such as electricity generation, fuel chains and raw materials, and available stocks of key critical materials. By combining these data, the model describes prospective technological transformation pathways resulting in the lowest total environmental impacts, and which are consistent with the desired climate and socioeconomic scenarios.

The structure of ECOPT^2 allows practitioners to optimize over several impact categories using endpoint or single-score indicators, if so desired. An alternative means to evaluate multiple impact categories is to implement additional constraints to restrict the values of non-optimized impact categories by using the ε-scaling method. For example, they may implement a constraint whose impacts in other categories may not exceed a given level over the base year value, or an absolute user-provided value.

The model can be used to represent sectors that may need a rapid technological shift to decarbonize. While we present this model applied to the question of electrification of the LDV fleet, other examples of potential applications of ECOPT^2 are mentioned in section 2.3. The linear program represents the LDV stock with resolution on powertrain technology, energy carrier (fuel), region, vehicle segment (size), and vehicle age (cohort). Life cycle impacts for the vehicle stock are computed, with manufacturing impacts occurring in the year of introduction, annual operating emissions, and end-of-life impacts occurring in the year of vehicle retirement. The objective function minimizes total emissions over the entire model time horizon, thereby assuming perfect foresight on the part of the decision-maker. The ECOPT^2 software tool (Hung et al., 2022) is implemented in Python and GAMS. A discussion of key aspects of the software implementation, including data handling, class structure, and operational features, can be found in the Supporting Information S1.

2.1 | Mathematical formulation

The list of indices, parameters, and variables used in the LP can be found in Table 1.

2.1.1 | Objective function

The objective function in ECOPT^2 minimizes total fleet impacts of the target impact category, c_{opt}, over the full model period and all life cycle phases (Equation (1)). Production impacts in their entirety are allocated to the year of introduction (at $a = 0$, see Equation (6)). Definitions for ε^{prod}, ε^{op}, and ε^{EOL} are found in Equations (6)–(8).

$$\text{minimize } \varepsilon = \sum_{t \in T} \sum_{s \in S} \sum_{r \in R^{LDV}} \sum_{y \in Y} \left(\varepsilon^{prod}_{c,t,s,r,y} + \varepsilon^{op}_{c,t,s,r,y} + \varepsilon^{EOL}_{c,t,s,r,y} \right) \text{ for c} = c_{opt} \tag{1}$$

2.1.2 | Stock–cohort balance model

The fleet model is stock-driven (Müller, 2006), where the inflow of vehicles in year y is the sum of the number of vehicles retired and the increase of total vehicles required in the fleet from year y-1(Equation (2)). The stock in any given year is thus the sum of the stock from the previous year and the additions to stock (θ, see Equation (9)), less the vehicles retired (ρ, Equation (3)).

$$\sigma_{t,s,r,a,y} = \sigma_{t,s,r,a-1,y-1} + \theta_{t,s,r,a,y} - \rho_{t,s,r,a,y} \tag{2}$$

where

$$\rho_{t,s,r,a,y} = \left(\theta_{t,s,r,a-1,y-a} \, g \, (a-1) \right) \tag{3}$$

The number of vehicles required in the fleet is exogenously defined by the user and implemented as a constraint (see Equation (9)). The retirement function $g(a)$, defined in Equation (4), is the survival function normalized by age such that $\sum_a g(a) = 1$, and thus represents the share of vehicles for each age cohort a that is removed from the stock in that year. For example, if $g(2) = 0.05$, then 5% of 2-year-old vehicles are retired.

$$g(a) = 1 - \frac{\tilde{S}(a+1)}{\tilde{S}(a)}, \tag{4}$$

where $\tilde{S}(a)$ is the normalized survival function (Equation (5)):

$$\tilde{S}(a) = \frac{S(a)}{\sum_a S(a)}, \tag{5}$$

where S(a) is the survival function for a normal distribution.

TABLE 1 List of indices, parameters, and variables in the linear programming model

Symbol	Description	
Indices/sets		**Example set elements**
$y \in Y$	Year	{2020, 2021…2080}
$t \in T$	Technology	{ICE, BEV}
$T^{new} \subset T$	Emerging technology or technologies	{BEV}
$e \in E$	Energy carrier	{FOS, ELC}
$s \in S$	Segment or size	{A, B, C, D, E, F}
$j \in J$	Critical material species	{Lithium, Cobalt}
$i \in I$	Primary critical material producers	{Li_1, Li_2, … Co_n}
$m \in \{(j, i)\}$	Primary critical material producers of material j	{(Li_1, Li), (Li_2, Li), … (Co_n, Co)}
$r \in R$	Country or region	{Region LOW, Region HIGH…$PROD_n$}
$R^{stock} \subset R$	Regions relevant for technology operation	{Region LOW, Region HIGH…}
$R^{prod} \subset R$	Regions relevant for technology manufacturing	{PROD…$PROD_n$}
$a \in A$	Age cohort	{0, 1, 2, 3…a_{max}}
$c \in C$	Environmental impact category	{greenhouse gases, acidification potential}
Parameters		**Example units**
d_y	Annual use of technology in year y (e.g., distance traveled per vehicle in year y)	km vehicle^{-1}
$\kappa_{t,s}$	Amount or size of key components in each technology t of segment s (e.g., assumed battery size for segment s)	kWh
α_s	share of segment s in stock	%
$\xi_{t,m,y}$	Material intensity for critical material m in technology t in year y	kg kWh^{-1}
$\gamma_{t,y}$	Recovery rate of components from technology t in year y	%
$\eta_{m,y}$	Yield of material m from component recycling process in year y	%
$\hat{\sigma}_{r,y}$	Total stock of vehicles in year y and region r	vehicle
$\chi^{prod}_{c,t,s,y}$	Impact intensity of production without electricity, for vehicle of technology t, segment s in year y	kg CO_2-eq vehicle^{-1}
$\chi^{energy}_{c,e,r,y}$	Life cycle impact intensity of energy carrier e in region r in year y	kg CO_2-eq kWh$_{fuel}^{-1}$
$\chi^{mat}_{c,m,i,y}$	Impact intensity of production for primary material m, by supplier i in year y	kg CO_2-eq kg$_{material}^{-1}$
$\chi^{EOL}_{c,t,s,y}$	Impact intensity of end-of-life, by technology t, segment s in year y	kg CO_2-eq vehicle^{-1}
$\omega^{prod}_{t,s,y}$	Electric energy intensity of production for technology t, segment s in year y	kWh$_{el}$ vehicle^{-1}
$\omega^{op}_{t,s,y}$	Energy intensity of operation for technology t, segment s in cohort y	kWh$_{el}$ vehicle·km^{-1}
Constraints		
υ_t	Maximum technology diffusion rate of technology t^{new} due to willingness to adopt, etc.	%
$\phi_{i,y}$	Available supply of primary material from supplier i, in year y	kg
$\mu_{t,y}$	Annual manufacturing capacity for technology t^{new} in year y	kWh
Variables		
ε	Total impacts. Objective function.	t CO_2-eq
$\varepsilon^{prod}_{c,t,s,r,y}$	Total production impacts from vehicles of powertrain t and size segment s in region r and year y	t CO_2-eq
$\varepsilon^{op}_{c,t,s,r,y}$	Total operation impacts from vehicles of powertrain t and size segment s in region r and year y	t CO_2-eq
$\varepsilon^{EOL}_{c,t,s,r,y}$	Total end-of-life impacts from vehicles of powertrain t and size segment s in region r and year y	t CO_2-eq
$\sigma_{t,s,r,a,y}$	Total stock in region r, of powertrain t, segment s and age a in year y.	vehicle

(Continues)

TABLE 1 (Continued)

Symbol	Description	
$\theta_{t,s,r,a,y}$	Vehicles added to stock in region r, of powertrain t and size segment s in region r and year y. Decision variable.	vehicle
$\rho_{t,s,r,a,y}$	Vehicles removed from stock of powertrain t, size segment s and age a in region r and year y	vehicle
$\lambda_{i,y}$	Mix of primary material producers i used in year y. Decision variable.	$kg_{material}$ producer^{-1}
Formulae and other		
g(a)	Normalized probability of vehicle retirement, as a function of age	
S(a)	Survival function	
$\tilde{S}(a)$	Normalized survival function	
K	Constant; seed for technology uptake constraint	

Note: Note that the model equations are explained in context of the stylized case study presented in section 3, which demonstrates the use of ECOPT^2 for the deployment of electric vehicles.

The survival function $\tilde{S}(a)$ (Equation (5)) is a normalization of the survival function $S(a)$. $S(a)$ is calculated using the mean and standard deviation of the vehicle lifetime, assuming a normal distribution of vehicle ages. However, other distribution functions, such as the Weibull distribution, may be used. The mean and standard deviation of vehicle lifetime are both assumed to remain constant across the entire system and modeling period and are the same for both vehicle powertrain technologies.

2.1.3 | Impacts

Life cycle impacts are calculated by life cycle phase (manufacturing, use and end-of-life) for greater generality. Manufacturing impacts (Equation (6), ε^{prod}) are the sum of impacts from the use of primary critical materials ($\lambda\chi$), impacts arising from electricity use in manufacturing, and the remaining production impacts ($\theta\chi^{prod}$). Impacts from primary critical materials are affected by the mix of primary suppliers (Equation (11), λ), as the suppliers may differ in impact intensity (χ^{mat}). Impacts from electricity use in manufacturing are the product of the number of vehicles added (θ), energy intensity of production process (ω), and impact intensity of the electricity used in the producing country (χ^{energy}). Similarly, the remaining impacts are the product of vehicles added (θ) and the impact intensity of remaining production processes (χ^{prod}), excluding the critical material and electricity inputs.

Use phase impacts (Equation (7), ε^{oper}) are the product of annual mileage (d_y), vehicle fuel efficiency (ω^{op}), and fuel or electricity well-to-wheel impact intensity (χ^{energy}). Well-to-wheel impacts represent the life cycle impacts of the fuel or electricity chain, from extraction, refining, and combustion, and include the impacts from related infrastructure, and therefore allow for a consistent comparison of BEV and ICEV use phase.

End-of-life impacts (Equation (8), ε^{EOL}) are the product of retired vehicles and the impact intensity of end-of-life treatment, χ^{EOL}.

$$\varepsilon^{prod}_{c,t,s,r,y} = \lambda_{i,y}\chi^{mat}_{c,i,y} + \theta_{t,s,r,a,y}\left(\omega^{prod}_{t,s,y}\chi^{energy}_{c,\dot{e},\dot{r},y} + \chi^{prod}_{c,t,s,y}\right), \text{ where } \dot{r} \in R^{prod}, \dot{e} = \text{electricity}, a = 0 \qquad (6)$$

$$\varepsilon^{op}_{c,t,s,r,y} = \sum_{a=0}^{a_{max}}\left(\sigma_{t,s,r,a,y}\right)d_y\,\omega^{op}_{t,s,y-a}\,\chi^{energy}_{c,t,s,y} \qquad (7)$$

$$\varepsilon^{EOL}_{c,t,s,r,y} = \sum_{a=0}^{a_{max}}\left(\chi^{EOL}_{c,t,s,y}\,\rho_{t,s,r,a,y}\right) \qquad (8)$$

2.1.4 | Constraints

Stock-balance constraint

The transport demand in passenger-kilometers (p·km) or number of vehicles (σ) is met. This constraint is implemented by exogenously defining the total fleet size by region ($\hat{\sigma}$) over the studied time period and using this to determine the number of units added in a given year (Equation (9)). In the

case of p·km, the total transport demand is divided by an assumed annual mileage and occupancy factor to obtain the size of the total fleet.

$$\sum_{t \in T} \sum_{s \in S} \sum_{a \in A} \sigma_{t,s,r,a,y} = \left(\hat{\sigma}_{r,y} - \hat{\sigma}_{r,y-1} \right) + \sum_{t \in T} \sum_{s \in S} \sum_{a \in A} \rho_{t,s,r,a,y} \tag{9}$$

Manufacturing constraint

The demand of new batteries in a given year is measured in terms of energy storage capacity and is a function of the battery size (κ) for each battery electric vehicle (BEV) segment and the number of BEVs added to the fleet in that year (Equation (10)). This demand must be less than or equal to the manufacturing capacity, μ, for batteries. If this constraint is binding, the ECOPT^2 introduces fewer BEVs, that is, θ_{BEV} is reduced so as to respect the availability of new batteries.

$$\mu_{t,y} \geq \sum_{s \in S} \sum_{r \in R^{stock}} \left(\kappa_{t,s} \theta_{t,s,r,a,y} \right), \text{ where } a = 0, \ t \in t^{new} \tag{10}$$

Critical material balance constraint: Total supply

The sum of supply from all primary producers (i) of each critical material (m) used in capital manufacturing (λ) must be equal to the total amount of material needed for the addition to stock (θ), less the amount of recycled material made available for production from retired stock (ρ) at collection rate γ and recycling yield η (Equation (11)). The production mix of primary suppliers, λ is a decision variable, where suppliers with lower impact intensity are preferentially selected.

$$\sum_{i \in I} \lambda_{i,y} = \sum_{t \in T} \sum_{s \in S} \sum_{r \in R^{stock}} \sum_{a \in A} \left(\kappa_s \xi_{t,j,y} \right) \left(\theta_{t,s,r,\dot{a},y} - \gamma_{t,y} \eta_{j,y} \rho_{t,s,r,a,y} \right), \text{ where } \dot{a} = 0, \ t \in t^{new}, \ \{i,j\} \in m \tag{11}$$

Critical material primary supply constraint

Each critical material m consists of a primary production mix, λ, of producers of primary materials, i (Equation (12)). The materials from each supplier have a maximum annual supply, ϕ. This constraint ensures that the available supply from each primary producer i is not exceeded. If this constraint is binding, ECOPT^2 has exhausted all supplies of primary material(s) i, and additions of BEVs, θ_{BEV} to the stock is curbed.

$$\phi_{i,y} \geq \lambda_{i,y} \tag{12}$$

Technology uptake constraint

In practice, the market share of a new technology or innovation grows (the technology is said to "diffuse" (Meade & Islam, 2006)) at a rate affected by many factors, including willingness of consumers to adopt (Rao & Kishore, 2010). In the case of BEVs, this willingness is in turn affected by the lack of charging infrastructure, consumer range anxiety, governmental incentives and subsidies, or a lack of vehicle model features satisfying consumers' needs (e.g., all wheel drive, trailer hitch), and so on (Fluchs, 2020; Mukherjee & Ryan, 2020; Singh et al., 2020; Zambrano-Gutiérrez et al., 2018). ECOPT^2 represents limits on the diffusion rate as a technology uptake constraint (Equation (13)), expressed relative to the addition to stock from the previous year. A constant, k, is added as a "seed" to allow for the first year of introduction (i.e., when the year before has no additions of the new technology)

$$\theta_{t,s,r,a,y} \leq \left(\theta_{t,s,r,a,y-1} \right) \left(1 + \upsilon_{max} \right) + k, \text{ where } R \in R^{stock}, T \in T_{new}, \ a = 0 \tag{13}$$

Segment share constraint

As a simplification in this study, the market share of vehicle segments, α_s, remains constant throughout the model time horizon (Equation (14)) and is the same as the segment shares of the initial stock. It is also assumed that segment shares are the same in all regions and for all powertrains, that is, consumers have the same vehicle segment preference for BEVs as ICEVs.

$$\sum_{t \in T} \theta_{t,s,r,a,y} = (\alpha_s) \left(\sum_{t \in T} \sum_{s \in S} \theta_{t,s,r,a,y} \right), \text{ where } s \in S, R \in R^{stock}, \ a = 0 \tag{14}$$

2.2 | Data sources, handling and flow

As illustrated in Figure 1, a model run is populated by exogeneous data from several sources. Scenarios such as the shared socioeconomic pathways (SSPs) can be used as input to the ESM or IAMs to provide a consistent basis for the electricity transition pathways and the technological fleet ($\hat{\sigma}_{r,y}$). For the latter, some IAMs may not have the technological resolution necessary to provide these data. Historical growth trends can be used instead in these cases. Data for the constraints in the LP may be user-defined, use other expert judgment, or be based on historical statistics or trends. The appropriate data sources for these parameters are dependent on the research question at hand. Lifetime distribution may be calculated using statistical distributions, such as lognormal or Weibull distributions.

The LCA impact factors for at least three sectors are needed in ECOPT^2: the electricity generation sector, primary critical material extraction and processing, and for the technologies being studied. These LCA factors may be obtained by the practitioner performing the LCAs, or by using literature. However, in using literature LCA data, the practitioner must take care to ensure that the impact characterization method and system boundaries are consistent. In addition to this caveat, the lifecycle inventories or LCA data must have high enough resolution to disaggregate the amount of electricity input and the resulting impacts. This is a requirement for the life cycle impacts of the studied technologies (e.g., BEVs and ICEVs from the case study); however, the factors for materials processing and electricity-generation technologies should also have electricity disaggregated if such resolution is available. Systems in which electrification is being compared to other energy carriers such as fossil fuels, also require LCA factors for these, which should be "well-to-wheel" (including extraction, refining, distribution, and combustion emissions) in scope.

The life cycle impacts of material extraction and processing are distinguished against suppliers, which may be individual actors, supply regions, ore types, and so on, as appropriate. The life cycle impacts for electricity generation should be technology-specific (i.e., not average grid mixes, but rather consider fuel types, etc.) and regionalized, if possible, to account for geographical differences in efficiency, fuel sources, transport losses, and so on.

2.3 | Adaptation to other systems

While ECOPT^2 is presented in the context of electromobility, the model itself is technology agnostic and can therefore be used to assess the dynamics of any sector where technologies in an early commercialization phase are being introduced. For example, a rapid transition in the energy system with the large-scale adoption of solar photovoltaic and wind power technologies would require an entirely different set of materials and capital manufacturing facilities than the historical status quo of fossil fuel-based power stations. These materials might include cement, copper, steel, and rare earth minerals (Goodenough et al., 2018; Hertwich et al., 2015), and may additionally require the installation of large-scale stationary batteries for improved grid operation at higher shares of intermittent energy sources (Choi et al., 2017; Gür, 2018). They may also be implemented at centralized utility-scale facilities, or as smaller components in a decentralized system, for example, rooftop photovoltaic systems, analogous to the vehicle-sized segments in the example application. Lastly, the efficiency of wind and solar power plants is highly dependent on the region in which they are installed, making regionalization aspects an important aspect to model. Other potential applications of ECOPT^2 could be the adoption of advanced materials in different applications (segments), or alternative energy carriers such as biofuels, hydrogen, or ammonia across multiple sectors (Table 2).

3 | DEMONSTRATION/APPLICATION

To illustrate the model function and utility, we present here a stylized scenario with two fictitious regions (Table 3). In this scenario, one region starts with an electricity mix with high carbon intensity ("HIGH"), and the other with relatively low ("LOW"). Region HIGH has a strong decarbonization policy in place and drastically decarbonizes the electricity sector toward 2050. There are two suppliers each of lithium and cobalt as the constraining critical materials. The input files for this scenario are included with the software package and can be run using the demo "switch" in *main.py*. In this scenario and in the following figures, the optimization period is from 2021 to 2050, with the 2000−2020 period representing user-provided data.

Figure 2 demonstrates the evolution of the LDV market shares (new vehicles) over the modeled period. Each color represents a different vehicle size segment, with the darker shade representing BEVs. In it, we see that BEV introduction is prioritized for mini and medium segments in LOW, with a sharp increase in market share at the beginning of the optimization period (2021). We can also see that the introduction of BEVs is quickly constrained, as illustrated by the slowdown of introduction in the larger segments after 2027. Additionally, most of the size segments are electrified in LOW while HIGH only electrifies the mini segment.

Figure 2 also shows that in LOW, the BEV market share growth is constrained and slows down or reverses in the medium, large, executive, and SUV size classes. Thus, in this example scenario, given the assumed constraints on supply chains for BEVs as an emerging powertrain technology, there is a prioritization for electrification both in terms of vehicle segments and in terms of region. In the stylized scenario, results indicate that under the defined constraints, the HIGH region should delay electrification of its LDV fleet and rather concentrate on rapidly decarbonizing the

TABLE 2 Examples of how other research areas can be implemented in ECOPT[2]. Empty cells in the table can be implemented as single-element sets

Research area ↓	Set			
	tec	seg	enr	mat_cats
Intermittent electricity generation technologies	• Wind • Solar pv • Stationary batteries	• Utility-size facilities • Decentralized /private installations	• Electricity • Fossil fuels	• Rare earth minerals • Cement • Copper • Silicon
Hydrogen economy	• Vehicle fuels • Electricity generation • Industry		• H_2 feedstocks • Natural gas (natural gas reforming) • Electricity (electrolysis)	• Platinum • Natural gas • Potable water
Waste management and energy recovery (deployment of circular economy strategies)	• Energy recovery • Hydrometallurgy • Pyrometallurgy • Chemical recycling	• Residential districts • Commercial districts	• Waste-to-energy • Electricity • Fossil fuels	• Household waste sources • Industrial waste sources
Muti-modal passenger transport	• Battery electric • Fuel cell electric • Internal combustion	• Passenger vehicles • Passenger rail • Busses • Plane	• Electricity • E-fuels • Hydrogen • Fossil fuels • Biofuels	• Rare earth minerals • Lithium • Cobalt • Platinum • Natural gas • Fossil fuels • Cropland

TABLE 3 Key input parameters for stylized scenario

		Region LOW	Region HIGH
Fleet size, 2020		300 000	200 000
Growth in total fleet, annual	%	0.5%	1.5%
Carbon intensity of electricity mix, 2020/2050	g CO_2e/kWh	500/350	1000/450

electricity mix. While the LOW region electrifies the LDV fleet as much as the imposed constraints allow, there is a prioritization for the mini and small segments, as the difference in impacts between BEVs and ICEVs in these segments is largest in the scenario; more emissions are therefore avoided by electrifying these segments first. Given these types of insights, policymakers can tailor measures to encourage fleet development toward this optimized scenario, for example, specifically incentivizing uptake of smaller electric vehicles.

Figure 3 plots the co-evolution of vehicle fleet and life cycle impacts. The upper panel shows the technological evolution of the combined fleet of both regions and the corresponding evolution of emissions by life cycle phase. We can see the fleet impacts shift from being operation-phase dominated when ICEVs are the main technology, but as BEVs are introduced, the share of operation emissions decreases as the production impacts increase. Compared to a business-as-usual case where there is no uptake of new technology, the stylized electrification scenario results in a modest reduction in overall fleet emissions over the entire model period, despite a slight increase of impacts due to the higher production impact intensity of the new technology at the beginning of the optimization period.

The panels in Figure 4 demonstrate results related to critical material supply. The left panel shows the demand of primary and secondary materials, the latter of which is assumed to be free of impacts, while the right panel shows the mix of primary suppliers, or supply mix, for each critical material. Each primary supplier has its own impact intensity for producing the material, which may be reflective of different mining, refining, and processing methods, as well as different ore grades. In this example scenario, the supply of primary cobalt is a constraining factor to BEV uptake as the primary cobalt being used in new batteries is equal to the total available supply of primary cobalt in the system. When these results are considered in parallel with Figure 2, we see that the availability of critical materials is constraining the uptake of the larger vehicle segments and thus causing the decreases in market share observed. The right panel provides more detail for the primary material supply mix, such as the relative shares of primary producers, the dynamics of when or whether each supplier reaches maximum supply capacity, and the excess supply capacity. The results of the material mixes can address whether and when supply chain constraints may occur in the scenario and consequently, the effect of these constraints on the total impacts. These dynamics exemplify the importance of understanding which constraints may delay the diffusion of these technologies onto the wider market; it is both useful to be aware of which factors in particular might limit the supply of the emerging technology in the future and how to best utilize this limited supply to maximize environmental benefits.
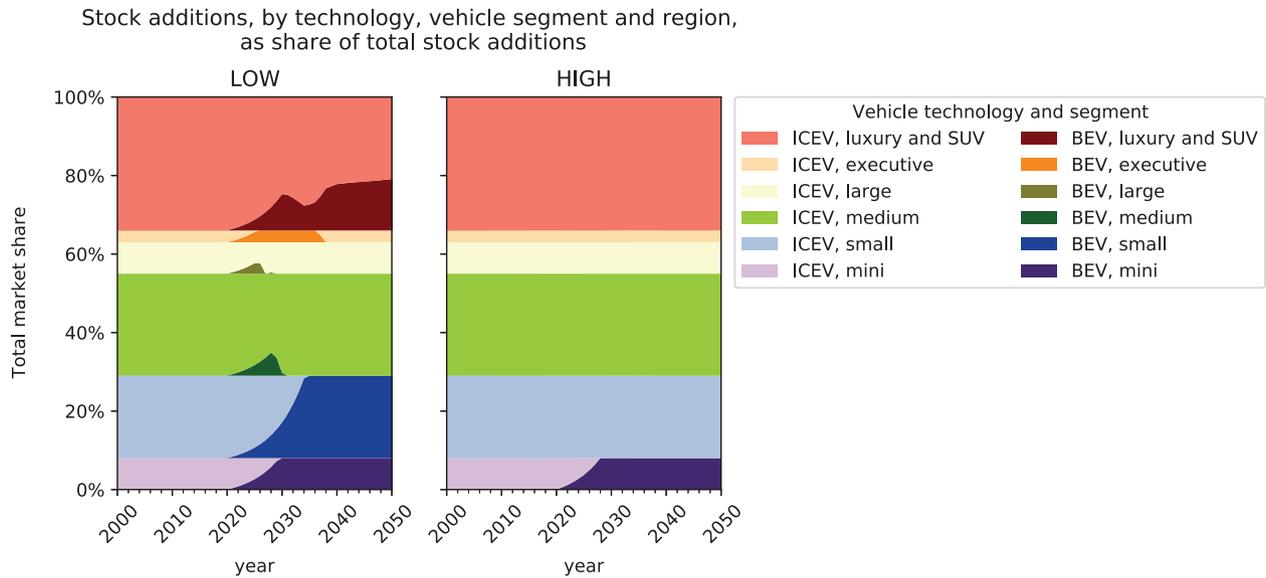
Stock additions, by technology, vehicle segment and region,
as share of total stock additions

FIGURE 2 Example visualization output of stock additions for a stylized scenario with two regions. Stock additions are distinguished by technology, vehicle segment, and region and are represented as share of total region stock
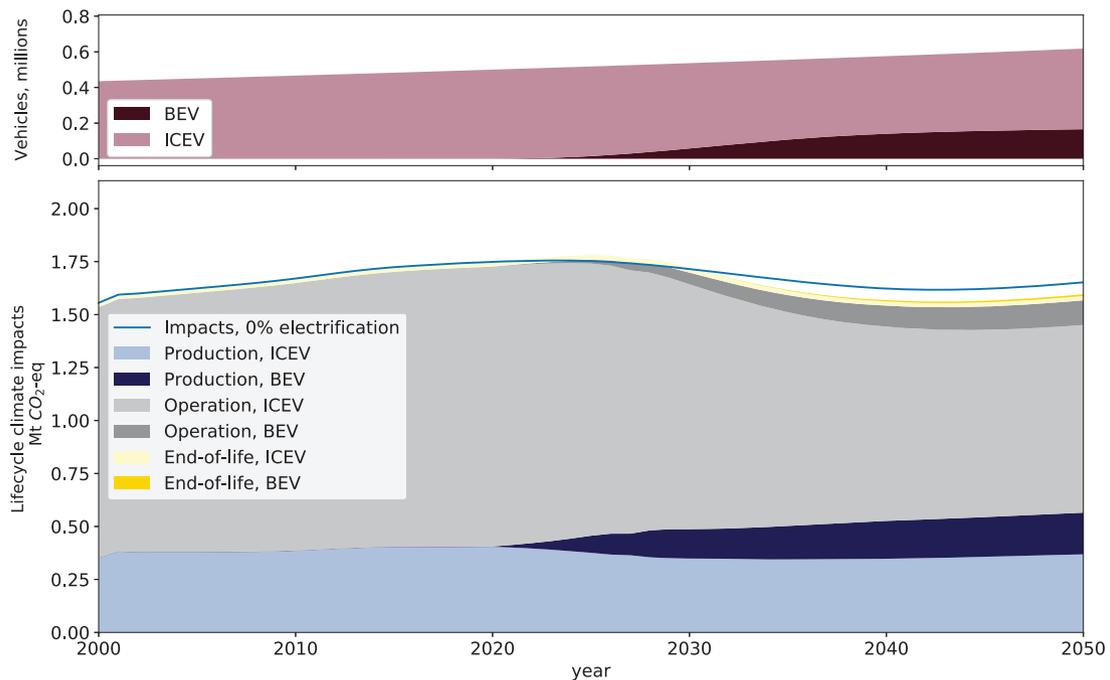

FIGURE 3 Example visualization output of co-evolution of total stock (upper panel) and life cycle impacts (bottom panel) from an LDV fleet. Production impacts are allocated to the year of vehicle production

4 | CONCLUSION & FUTURE WORK

The ECOPT[2] adaptable model aims to fill gaps in commonly used product-level LCA approaches to increase the method's relevance to inform and guide macro-scale, regionalized technology transition strategies while retaining a high level of technological detail and granularity. Three of these gaps are the modeling of linear, unconstrained systems, the evaluation of piecewise, practitioner-selected effects, and the static nature of many traditional LCA approaches. This work fills these gaps by combining the life cycle perspective with a linear programming model, pathways detailed by energy models, introducing technological constraints and dynamic fleet stocks to the analysis, and using a dynamic background system in an open-source software tool.
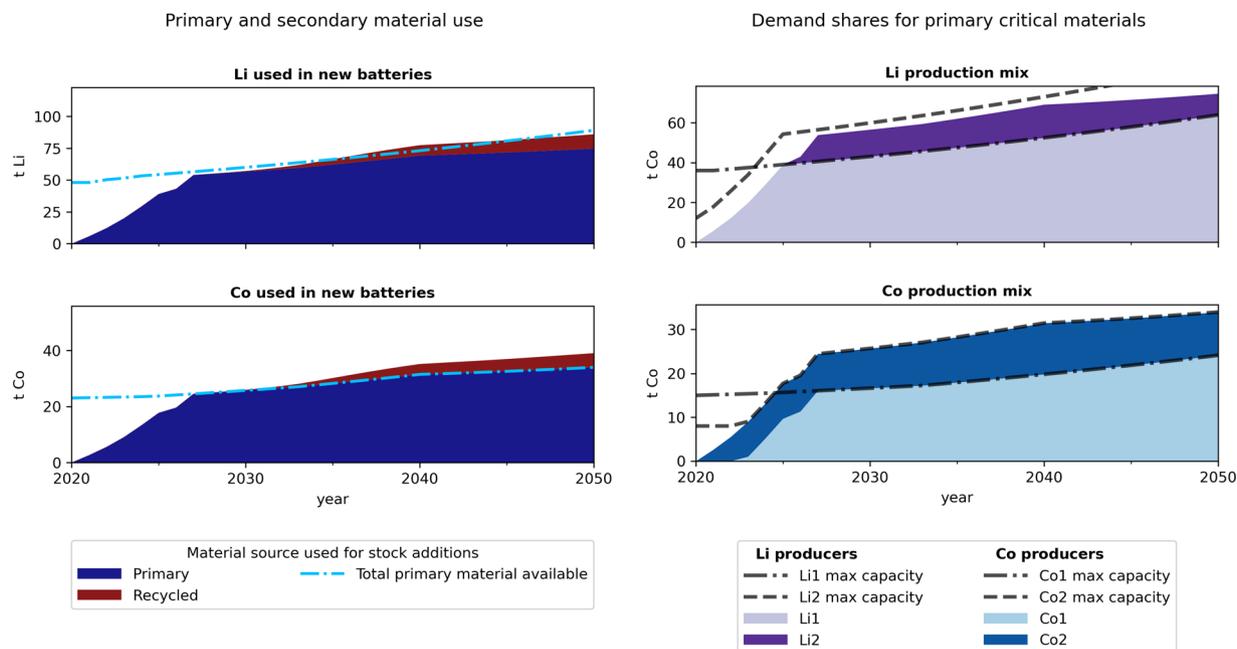
FIGURE 4 Example visualization of material dynamics for a stylized scenario. Left: Lithium and cobalt demand arising from BEV adoption in both regions, showing use of primary vs. recycled (secondary) material. Right: Production shares from different primary material suppliers of lithium and cobalt, given different carbon intensities for each producer

The ECOPT² model strives to model key causal links between a decision variable and its associated environmental impacts. Such causal links include competition between providers, substitution between products (especially substitution by secondary materials and byproducts), and so on. In that respect, it is well aligned with the objectives of a CLCA (Weidema, 2003). In contrast to typical CLCA practice, however, ECOPT² modeling does not start from the statement of a precise decision (e.g., replacing 20% of LDV by BEVs) before calculating the consequences of this decision within a given technological system. Rather, ECOPT² works in the opposite direction: given a technological system and its evolution, it identifies an optimal decision. Also, most CLCAs strive to capture the (marginal) effects of single decisions while keeping all other variables constant to isolate its effect (*ceteris paribus*). In contrast, ECOPT² assesses impact trajectories using scenarios, with changes in the backgrounds and the entire energy mix that occur independently from (and therefore are not a "consequence" of) the decision variable. Thus, by design, and contrary to typical CLCA practice, our analysis does not automatically exclude flows and processes that are not affected by the decision. Thus, ECOPT² aims to model the direct and indirect environmental impacts associated with an internally consistent technology transition scenario. While previous studies have combined some of these elements, such as combining LP and LCA, the focus of their work was to determine the environmentally optimal substitution mix for static systems (Budzinski et al., 2019; Saner et al., 2014; Steubing et al., 2016). In contrast, LP is used in ECOPT² toward understanding the dynamics of technology deployment while taking into consideration stock and material cycle dynamics.

The advantages of the approach used in ECOPT² is three-fold: first, the optimization endogenously influences the life cycle impact scores of the materials used in manufacture by selecting suppliers according to environmental performance. Second, rather than exogenously identifying constrained and marginal providers (as is typically necessary in consequential LCAs), the optimization simulates competition between providers with different production functions and limitations, thereby endogenizing a critical LCA modeling choice. Third, the constraints of the linear program serve not only to support the LCA but also to model a complete dynamic stock cohort model, and to naturally account for the increased availability over time of secondary materials and the environmental benefits that come from their substitution of primary production.

The incorporation of system dynamics such as bottlenecks in manufacturing or resource supply chains is essential to the wider understanding of the implications of policies that incentivize the uptake of new technologies. Given the restrictions to the ideal rollout of technologies, effective mitigation policies require these types of conclusions that are captured by models implemented in ECOPT². Thus, this work is an important step in adopting life cycle thinking, while explicitly acknowledging and working around potential obstacles to its adoption. With this work, we aim to provide a tool that facilitates integrated studies of complex systems by combining material dynamics, competition, LCA and IAMs.

Future iterations of ECOPT² could include a more comprehensive modeling of a dynamic economy beyond the energy and studied sectors (e.g., changes in material refining processes) for the LCA factors; this would further improve the prospective realism of the scenarios. ECOPT² in its current form acts as an ex-post analysis, using output from these models as exogenously defined data, without incorporating feedback dynamics. The implementation of such a feature could consist of a more direct linkage to existing ESMs such as those presented by Gibon et al. (2015) or Mendoza Beltran et al. (2018). The structure of ECOPT² also lends itself to integration with models based on the *ix*mod platform for IAMs (Huppmann et al., 2019; IIASA Energy, Climate, and Environment (ECE) program, n.d.); such integration would capture additional dynamics such as the cross-sectoral

feedbacks, while adding the industrial ecology perspective of full life cycles and material constraints to ESMs and IAMs. Other potential additions in future work include the explicit modeling of the associated infrastructure or auxiliary services, the expansion of additional environmental impacts, or by expanding the dimensionality of some parameters, pending data availability. The explicit modeling of inter-sectoral competition and feedback loops for, example, materials could also provide additional insights. Examples of such competition include the utility-scale adoption of batteries for stationary storage in competition with traction batteries and competing demand for permanent magnets for both electric motors and wind power turbines. The current implementation simplifies this competition as a single factor that allocates a share of total global resources to the LDV and transport sector for the modeled regions.

The ECOPT[2] approach allows for the realistic upscaling of LCA models from product level to a wider economy perspective. By including the potential barriers to new technology uptake, the model provides insight that can be used to better guide policy development and large-scale decision-making to ensure long-term planning toward the sustainable deployment of these technologies.

CONFLICT OF INTEREST
The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT
Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

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NOTES
[1] A notable exception being Dandres et al. (2011), who considered the economy-wide consequences of large-scale transition to renewable energy carriers in Europe.
[2] Note that while ECOPT[2] itself is open source, its current implementation uses GAMS commercial software to solve the mathematical program

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.