

Towards Energy and Material Transition Integration – A Systematic Multi-scale Modeling and Optimization Framework

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ABSTRACT

The energy transition is driven both by the motivation to decarbonize as well as the decrease in cost of low carbon technology. Net-carbon neutrality over the lifetime of technology use can neither be quantitatively assessed nor realized without accounting for the flows of carbon comprehensively from cradle to grave. Sources of emission are disparate with contributions from resource procurement, process establishment and function, and material refining. The synergies between the constituent value chains are especially apparent in the mobility transition which involves (i) power generation, storage and dispatch, (ii) synthesis of polymeric materials, (iii) manufacturing of vehicles and establishment of infrastructure. Decision-making frameworks that can coordinate these aspects and provide cooperative sustainable solutions are needed. To this end, we present a multiscale modeling and optimization framework for the simultaneous resolution of the material and energy value chains. A case study focusing on the transition of mobility technology towards electric vehicles in Texas is presented. The key contributions of the proposed framework are (i) integrated network design and operational scheduling, (ii) the tracking of disparate emissions, (iii) simultaneous modeling of the material and energy supply chains, (iv) implementation on `energy`, a python package for the multiscale modeling and optimization of energy systems.

Keywords: energy transition, material transition, mixed integer programming, multiscale modeling, carbon accounting

INTRODUCTION

The ongoing energy transition towards net-carbon neutrality has various challenges, not limited to (i) managing the storage for intermittent renewables, (ii) accounting for emissions from disparate sources, (iii) managing the cost to consumers, (iv) coordinating the transition of technologies for different applications such as the generation of power, transportation and production of dense energy carriers (DECs) (v) meeting the material requirements for establishing infrastructure sustainably [1]. Addressing these challenges requires a holistic view of multiple interdependent supply chains and the synergies between them.

Moreover, decarbonization requires both direct and

indirect emissions to be accounted for. Direct emissions occur from the release of pollutants at the operational level by processes, whereas indirect emissions occur due to the refining and procurement of materials and resources as well as the establishment of processes and infrastructure. Further, indirect emissions occur at the onset of establishing infrastructure, while direct emissions can occur over a protracted temporal horizon throughout the lifetime of technology. Decision-makers planning energy systems of the future need to coordinate both aspects to determine optimal transition pathways.

Materials such as minerals, metals, and polymers are required to establish infrastructure. The refining and processing of these is a contributor to emissions. However, polymers can also act as a carbon sink and, in the

context of the circular economy, provide an opportunity for the valorization of the carbon vector.

Given our contemporaneous dependence on carbon-based feedstock for both power generation and production of polymers, the oil & gas (O&G) industry plays a central role in enabling both the energy and material transition. The repurposing of the O&G industry towards the manufacturing of polymeric materials through captured carbon dioxide will also preserve established production infrastructure and capital. Furthermore, polymers offer a durable alternative to metallic materials which have a high energy demand for refining, produce toxic refuse during mining, and have challenges in terms of recycling and reuse in some cases. For example, passenger vehicle designs have evolved to include a larger amount of polymers in their interior while achieving improvements in efficiency and safety due to lower density and higher impact resistance respectively [2].

The use of hydrocarbon feedstock to produce polymers for electric vehicles (EVs) as opposed to transportation fuels for internal combustion engine (ICE) vehicles can also reduce direct carbon emissions as they can act as a sink for carbon that would be otherwise emitted as greenhouse gases (GHGs) [3]. Readily available polymers such as polypropylene (PP), polyamide (PA), polystyrene (PS), polycarbonate (PC), polyurethane (PUR), polyvinyl chloride (PVC), polyethylene (PE), and polyethylene terephthalate (PET) all find use in automobile production. Moreover, polymers are also needed for insulation in grid infrastructure, power conversion systems, and also for ancillary infrastructure in solar and wind farms.

While the modeling and optimization of different aspects of the energy transition has been an active field of research [4,5,6,7], the parallel transition of materials has not received equal attention. In this publication, we introduce a framework for the simultaneous modeling of the material and energy transition, allowing the identification of solutions that reduce emissions across disparate emission scopes. The system is represented through the resource task network (RTN) methodology augmented for the consideration of different material options for process infrastructure. The emissions arising from disparate sources such as material synthesis, resource consumption and utilization post discharge, and production are considered. The mathematical programming framework is modeled as a mixed integer linear program (MILP) with binaries assigned for the establishment of processes and the choice of material modes for said processes. Moreover, the model does simultaneous network design and scheduling which is able to account for renewable intermittency and optimize energy storage.

The publication is organized as follows: first the details of the considered mobility transition supply chain are discussed, next the modeling and solution methodology are elucidated upon and certain aspects of the general

formulation are discussed, followed by the results and ongoing work.

A MOBILITY TRANSITION SUPPLY CHAIN

The mobility transition with respect to passenger vehicles entails the adoption of EVs to replace ICE vehicles. Using a simple linear forecast to predict EV sales for Texas, more than 900,000 units will be sold in 2050 considering an annual sales growth rate of 16% [8], and about 12 million EVs will be on the road. EVs differ from ICE vehicles in both the energy source for their function, as well as the supply chains involved in making energy available. Fossil fuels utilized in ICE vehicles cause emissions at the point of use. Conversely, EVs have no direct emission but can cause emissions as a result of power generation through fossil fuel-based power generation. Moreover, while power can be generated through renewable means, materials required to establish power generation and distribution infrastructure are still privy to emissions. The transition to EVs will need to be supported by an expansion of the grid and power generation infrastructure.

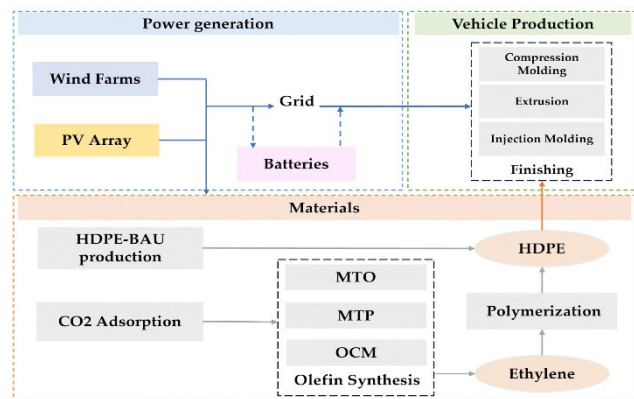


Figure 1. A schematic of the mobility transition supply chain.

The transition of mobility infrastructure requires the transition of technologies for 1) transportation 2) manufacturing, 3) power generation, and 4) polymer production. As a whole, three distinct blocks can be considered as shown in Figure 1, viz. 1) Power generation which include solar photovoltaics (PVs) and wind farms (WFs), 2) Polymer production wherein High Density Polyethylene (HDPE), 3) the production of vehicle parts through a combination of different molding methods. As a whole, we look at two different technology pathways:

1. The business as usual (*BAU*) pathway where in HDPE is produced from fossil feedstock such as natural gas and oil
2. The carbon capture utilization and sequestration (*CCUS*) pathway which necessitates the direct air

capture (DAC) of CO₂ followed by one of three processes for the production of olefins, with polymerization of produced ethylene as the final step

The three pathways for olefin production considered are:

- **Methanol to Olefins (MTO):** In this route, methanol is synthesized from CO₂ hydrogenation and converted into olefins (ethylene and propylene).
- **Methanol to Propylene (MTP):** In this process, the major product is propylene, which is synthesized from CO₂.
- **Oxidative Coupling of Methane (OCM):** This process produces mainly ethylene through oxidative coupling of methane derived from the hydrogenation of CO₂

The MTO and MTP processes represent successful initiatives aimed at reducing reliance on petroleum for olefin production. In the MTO process, methanol is transformed into olefins with a carbon selectivity ranging from 78% to 82% at approximately 500 °C and 250 kPa, utilizing a SAPO-34-type zeolite catalyst. The by-products include propylene, C4 fraction, and liquified petroleum gas (LPG).

Similarly, in the MTP process, methanol is converted into propylene with a carbon selectivity of around 71% at temperatures between 400 and 500 °C and a pressure of 150 kPa, employing a zeolite-based catalyst [9]. LPG, propylene, and C5 fraction are by-products.

In the OCM process [10], methane (CH₄) and oxygen (O₂) undergo an exothermic reaction on a catalyst bed, resulting in the formation of ethylene (C₂H₄), ethane (C₂H₆), water (H₂O), and heat. Traditional reactors, such as packed bed reactors (PBR) and fluidized bed reactors, have been commonly employed for this purpose. However, there is a current exploration of Fluidized Bed Membrane Reactor (FBMR) options to assess the potential improvement in selectivity. The operating conditions for this technology involve temperatures of approximately 800 °C and pressures of 200 kPa. Further, all three processes require the provision of steam, cooling water, oxygen, and hydrogen besides power.

Produced ethylene is converted into HDPE via polymerization through different technologies such as CSTRs, loop slurry, fluidized-bed gas phase, and stirred-bed gas phase reactors. Various processes have been marketed by companies such as LyondellBasell, Mitsui Chemicals, Chevron Phillips Chemicals, Univation, Lummus Novolen, etc. Nevertheless, as data for such processes is not publicly available, the average data from Europe for such processes is considered [11]. Both HDPE production routes, BAU or CCUS, are subject to the finishing processes; a combination of compression molding

(CM) 24.25%, extrusion (EX) 9.25% and injection molding (IM) 66.5% [8].

Currently, the energy demand for EVs and production of resources is met through a mix of fossil fuel (coal and natural gas), and renewable (wind and solar) power generation. In the transition scenario, renewable power will replace fossil fuel-based power generation. Moreover, requisite power generation and management systems can be established through different material alternatives as well. PVs, for example, can be made from monocrystalline or polycrystalline silicon, lithium for lithium-ion batteries can be sourced either through rock or brine lithium, and wind farms can be offshore or land-based each with different material requirements. The other materials required for construction include glass, steel, concrete, aluminum, silicon, copper, and cast iron.

Polymers in EVs account for about 13% of the mass of the vehicle. In the illustrative example, we only consider the need for HDPE which accounts for about 2.7 kg (1.4%) mass of the total amount of polymers used in cars [12], the total car mass considered is 1481 kg. The objective of the considered study is to analyze the network designs of the current HDPE demand for the ~1.3 million passenger vehicles produced annually in Texas through renewable means. Of key interest are 1) the identification of optimal cost and emission technology pathways, 2) the quantitative determination of the trade-offs between cost and emission, 3) identification of optimal material modes for the establishment of infrastructure.

The region of Houston is used as a proxy for the entire state of Texas for the collection of wind and solar data. The GREET model is used to source parameters for natural gas, oil, electricity use, and related process emissions [12], while the Ecoinvent version 3.9.1 database is used to assign a global warming potential (GWP) for every material considered in the study [13].

METHODOLOGY AND FORMULATION

The framework is multiscale in that it models spatiotemporally disparate phenomena such as renewable intermittency and augmentations in technology costs and efficiency. Moreover, the operational and network planning decisions are modeled simultaneously as well. Emissions are considered from: 1) resource consumption, 2) resource discharge, 3) material procurement for establishing infrastructure. The framework can also consider emissions from construction or manufacturing processes, but this is not modeled in the presented case study given the lack of reliable data. Note, that the framework can also account for different environmental indicators, namely, global warming, ozone depletion, acidification, and eutrophication (marine, terrestrial, freshwater). However, the presented case study only accounts for the global warming aspect of emissions.

For energy technologies, power generation processes are modeled alongside energy storage, and different material modes are considered. The lithium-ion battery (LiI), for example, can use lithium sourced from brine or rock. Each option has different associated emissions due to the process of mining these materials differ significantly. Similarly, different combinations of materials such as steel, cast iron, silicon, concrete, etc. are considered for establishing PVs and WFs.

The system is represented and modeled through an augmentation of the resource task network (RTN) methodology, which considers the materials required to set up processes [14]. This representation is christened the resource task material network (RTMN). Resources, by definition, can be consumed, discharged, stored, transported, or produced. On the other hand, materials are utilized solely for the establishment of infrastructure such as transport linkages and processes. The need for this strict distinction between materials and resources stems from: (i) unlike resources, materials are not converted, (ii) disparate temporal nature of use, wherein resources are used continuously over the scheduling scale and materials are used only in time periods over the network scale when technologies are established, (iii) convenience of reporting emissions in terms of scopes. As a whole, this streamlines the system representation as well as the mathematical modeling. As an example, in the mobility transition supply chain, HDPE is a *resource* produced through the culmination of a set of processes, whereas the concrete required to establish a wind farm is a *material*.

The planning horizon is considered at two distinct discretizations: 1) a scale for network level decisions, 2) a scheduling scale with 8760 discretizations to capture the intermittency of renewables and the flow of resources. Given that a single period is considered for network level decisions, the capital cost or emissions related to material utilization are not annualized. However, the model can be easily expanded to consider multiple network periods along with associated changes in technology costs. Further, while the example presented models a single location, multiple locations along with associated transportation modes between these locations can also be considered.

The framework simultaneously optimizes network design and process scheduling. Mixed integer programming is used with binaries for decisions such as locating processes and determining optimal material modes. Continuous variables capture the mass balance, and monetary aspects. Some important constraints such as the material balance, emission constraints, and network design are discussed here. Network design is achieved through constraints (1 and 2). Material constraints (3-5) allow the model to choose between different available material modes. Each material mode in turn has an

associated consumption of materials (ϕ) per unit capacity. Notably, emissions can also occur through 1) the consumption or use of produced resources, and 2) direct process emissions as shown in emission constraints (6-9). Inventory balance in every time period in the scheduling horizon is done through constraint 10, wherein each variable is bounded by either a parameter (S^{max} for S, C^{max} for C), or by a variable in the network scale (Cap^S for Inv , Cap^I for P).

sets	definition
$l \in L$	location
$i \in I$	process
$r \in R$	resource
$m \in M$	material
$w \in W$	material modes
$e \in E$	emissions
$t \in T^N$ or $t \in T^S$	network or scheduling scale

variables	definition
$Cap_{l,i/r,t}^{I/S}$	process/inventory capacity
$Em_{l,e,r/i/m,t}^{r/i/m}$	resource/process/material emission
$Em_{l,e,t}^{(L)}$	Emission (total at location)
$C_{l,r,t}^{(L)}$	Resource consumption (total at location)
$S_{l,r,t}^{(L)}$	Resource discharge (total at location)
$Mat_{l,i,mt}^I$	Material utilized for process
$Mat_{l,m,t}^L$	Material utilized at location
$Cap_{l,i,m,t}^{I-W}$	Capacity of material mode
$X_{l,i,m,t}^I$	Binary for locating process
$X_{l,i,w,t}^{I-W}$	Binary for choosing process mode
$X_{l,r,t}^S$	Binary for storage facility
$Inv_{l,r,t}$	Inventory level for resource
$P_{l,i,t}$	Production level for process

parameters	definition
$Cap_{l,r/i,t}^{S/I-min/max}$	max/min inventory/process

	capacity
$EP_e^{r/m}$	resource/material emission
$\phi(m, w)$	material consumption
$\eta(r, i)$	conversion

$$Cap_{l,r,t}^{s-min} \cdot X_{l,r,t}^s \leq Cap_{l,r,t}^s \leq Cap_{l,r,t}^{s-max} \cdot X_{l,r,t}^s \quad (1)$$

$$Cap_{l,i,t}^{l-min} \cdot X_{l,i,t}^l \leq Cap_{l,i,t}^l \leq Cap_{l,i,t}^{l-max} \cdot X_{l,i,t}^l \quad (2)$$

$$Mat_{l,i,m,t}^l = \sum_{\forall w \in W} (\phi(m, w) \cdot Cap_{l,i,w,t}^{l-w}) \quad (3)$$

$$Cap_{l,i,t}^{l-min} \cdot X_{l,i,w,t}^{l-w} \leq Cap_{l,i,w,t}^{l-w} \leq Cap_{l,i,t}^{l-max} \cdot X_{l,i,w,t}^{l-w} \quad (4)$$

$$X_{l,i,t}^l = \sum_{\forall w \in W} X_{l,i,w,t}^{l-w} \quad (5)$$

$$Em_{l,e,r,t}^r = EP_e^{r-cons} \cdot C_{l,r,t}^l + EP_e^{r-use} \cdot S_{l,r,t}^l \quad (6)$$

$$Em_{l,e,m,t}^m = EP_e^m \cdot Mat_{l,m,t}^l \quad (7)$$

$$Em_{l,e,i,t}^i = \sum_{\forall i \in I} EP_e^r \cdot \eta(r, i) P_{l,i,t}^l \quad (8)$$

$$Em_{l,e,t}^L = \sum_{\forall r \in R} Em_{l,e,r,t}^r + \sum_{\forall m \in M} Em_{l,e,m,t}^m + \sum_{\forall i \in I} Em_{l,e,i,t}^i \quad (9)$$

$$\sum_{\forall i \in I} \eta(r, i) P_{l,i,t}^l + C_{l,r,t} + Inv_{l,r,t-1} = Inv_{l,r,t} + S_{l,r,t} \quad (10)$$

The implementation in *energiapy* [15] utilizes a component based architecture with temporal horizon, resources, materials, processes, locations, and scenarios serving as modeling components. Various material modes can be declared for each process, wherein the material consumption for the establishment of said infrastructure on a per unit basis is provided as attributes. The associated GWP is declared as an attribute of each material and resource in the object-oriented programming framework. A small example is available in the package documentation to guide users on the application.

RESULTS AND DISCUSSION

The framework can be optimized to various objectives, the two objectives discussed here are to 1) minimize system costs, and 2) minimize system emissions. First a base case is established wherein the system is optimized only to minimize the system cost while not restricting emissions. The network design for the base case as shown in Figure 2 consists of WF, Lil, HDPE production from the BAU pathway and the molding processes (extrusion, compression, injection). Moreover, the land-based material mode is chosen for establishing WF, and brine lithium is chosen for the Lil. The emissions resulting from the 2.7 kg requirement of HDPE per car is found to be 11.08 kg CO₂-eq. This includes 3.15 and 0.8 kg CO₂-eq from the purchase of natural gas and oil respectively, 5.12 from the venting of CO₂, and 2.00 from the material requirements for establishing the land-based WF and brine lithium based Lil.

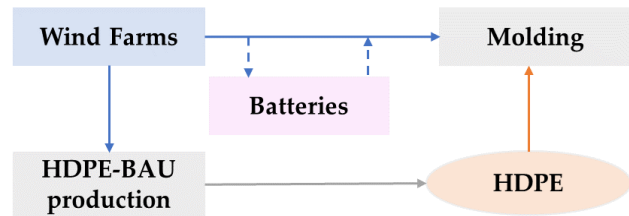


Figure 2. Low cost pathway for HDPE production.

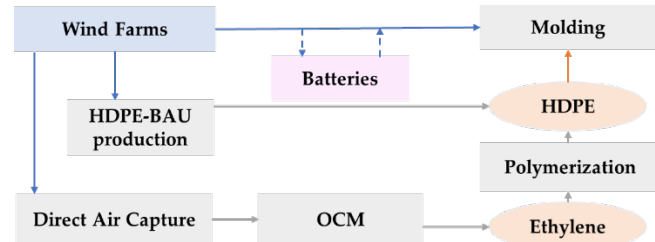


Figure 3. Low carbon pathway for HDPE production.

With the base case established, the network is then optimized towards the reduction of GWP. The maximum possible reduction in emissions is found to be ~9.07%. The cost optimal design for a ~9.07% reduction in emission tilts in favor of the CCUS pathway. The reduction entails a 2.2 factor increase in cost compared to the base case. Even in the minimum emission case, the BAU pathway for the production of HDPE is still utilized. This is due to the energy intense nature of the CCUS pathway which requires larger power generation and energy storage capacities, which are subject to both material emissions and cost. Further, the OCM process is considered. Note that the MTP and MTO processes both have LPG as a by-product which results in emissions at the point of utilization. The WF and Lil capacities are 1.86 and 3.74 times larger than the base case scenario.

The system can then be analyzed for the successive reduction of emissions up to 9.07%. Figure 4 shows

a Pareto front which compares the reduction of emissions to the cost as compared to the base case. Notably, the first 6% reduction in emissions comes at a marginal increase (16.44%) in cost. The network design also evolves with the reduction in emissions, this includes the choice of technologies, the choice of materials to establish said processes, and the process capacities.

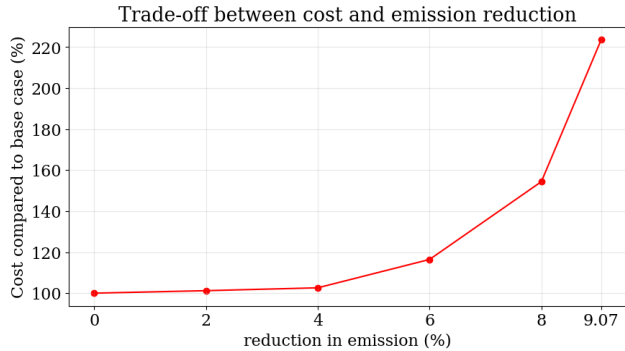


Figure 4. Trade-off between emission cost and emissions reduction.

The initial 4% reduction in emissions is achieved largely by setting up the energy intensive OCM process (refer to Table 1), and managing the capacity of the WF with a larger Lil. Beyond 4%, larger power systems are needed to accommodate the higher power demand. Given the higher cost of power infrastructure, system costs increase considerably.

Further, the consistent choice of land-based wind farms in both the minimum cost and minimum emissions represents a *win-win* scenario that offers the best solution across multiple objectives. Similarly, some options are never chosen such as the olefin production through the MTP and MTO route which are recognized as being both cost and emission intensive. As a reminder, processes can have different efficiencies based on the choice of materials, as well as different emission potentials based on the sourcing of materials (such as rock or brine lithium). Also, the cost of technologies are expected to reduce along with augmentations in efficiency resulting from adoption and research as the transition progresses.

It is also observed that a production capacity of HDPE from the BAU pathway is established even in the low carbon scenarios. This pathway is utilized on days with low wind availability given the low power requirement. If this pathway is not made available, the required power generation and energy storage capacity is significantly larger. In fact, to achieve a 6% reduction in emissions without the BAU pathway, the WF is sized at 28.98 MW and Lil is sized at 17.7 MW, representing an increase of 315% and 514.5% respectively. Meanwhile the cost of the system increases 388%. This highlights the trade-offs between direct and indirect emissions. The CCUS pathway utilizes significantly higher power which results in larger power generation capacities which in turn cause an increase in the emissions resulting from material utilization.

Figure 5 shows the disparate contribution to emissions. The largest source of emissions is direct CO₂ discharge. The lower emission scenarios have a larger contribution from WF and Lil as they are sized at a larger capacity. Natural gas (NG) and oil consumption decreases with the lower reliance on the BAU pathway and hence the emissions resulting from their sourcing and purchase. It can also be noted that, in the given model, none of the sources of emissions can be entirely eliminated.

The framework also provides optimal schedules. For example in Figure 6, the schedule for power generation through WF is plotted alongside the power discharged from Lil, and the production through OCM is plotted alongside the production through the BAU pathway for the scenario with a GWP reduction of 6%. It can be seen that the constant demand for HDPE is met either through the OCM or BAU pathway. However, when the wind potential is high the OCM pathway is preferred. During periods of low wind availability, the BAU pathway is preferred with the power demand being met from the discharge of energy stored in the Lil. This is also reflected in the sizing of processes, wherein the BAU process has the same capacity as the OCM process (refer to Table 1).

Table 1. Process capacities for different scenarios.

Scenario	DAC (tons)	HDPE-BAU (tons)	HDPE-CCUS (tons)	OCM (tons)	Lil (MW)	WF (MW)
Base	0	0.44	0	0	2.51	8.29
-2%	0.75	0.44	0.1	0.1	2.76	8.03
-4%	2.10	0.44	0.28	0.29	2.75	8.03
-6%	3.23	0.44	0.44	0.45	3.45	9.21
-8%	3.23	0.44	0.44	0.45	6.14	11.98
-9.07%	3.23	0.35	0.44	0.44	9.41	15.45

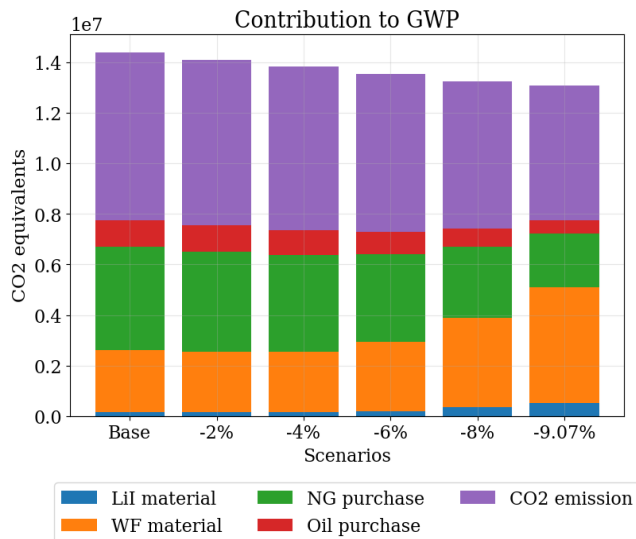


Figure 5. Contribution to GWP from source for each scenario.

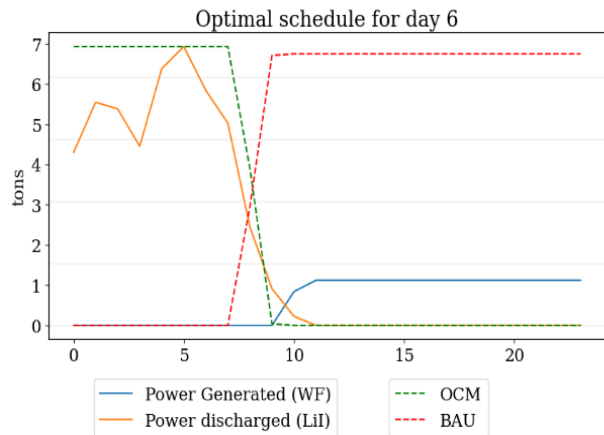


Figure 6. Schedule for power generation and discharge from energy storage.

Caution should be exercised when interpreting the results due to two limitations: 1) the unavailability of material use data for some processes causing a possible bias in results where values are assumed, and 2) the GWP associated with materials can vary by literature source. Nevertheless, the framework can be interrogated to quantify the sensitivity of the solution to parameter values.

The framework preserves the simultaneous scheduling and network design capability of earlier frameworks in literature [4,5,6,7] while allowing: 1) the estimation of emissions from disparate sources, and 2) identifying optimal material choices for the establishment of processes. Moreover, the framework is applied to a novel case study wherein the material and energy supply chains are modeled simultaneously. This provides a more holistic view of the system, thus enabling decarbonization across the different scopes of emissions. In principle, this framework can be applied towards the optimal

design of systems bearing awareness to life cycle considerations.

FUTURE WORK

While only GWP is considered in the presented work, other environmental effects such as ozone depletion and acidification potential can also be modeled. The optimization of multiple criteria using multi-objective optimization (MOO) can be reported. In its current form, the emission accounting methodology cannot be considered a comprehensive life cycle assessment (LCA) [7] given the lack of focus on process lifetimes and circularity of materials [16]. A challenge that needs to be addressed in the RTMN methodology is the fact that resources and materials are often not distinct. For example, while HDPE is treated as a resource in the considered mobility example, it may also serve as a material for the establishment of grid infrastructure.

Furthermore, the sensitivity of the model solution to considered parameters can also be assessed. The framework can also be run for longer temporal horizons which will allow the consideration of reductions in technology cost over the temporal horizon. Moreover, only HDPE is analyzed in the presented work, future iterations of the framework will also assess the role of other polymers utilized in the manufacturing of vehicles. Power is also required for charging EVs which can be modeled in tandem. Besides renewable intermittency, the framework can also accommodate variability in the cost of resources such as NG and oil and resource demand. Case studies considering the aforementioned aspects will be presented in future publications.

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