NORTHWESTERN UNIVERSITY
TRANSPORTATION CENTER

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LOwering CO2: Models to Optimize Train Infrastructure, Vehicles, and Energy Storage (LOCOMOTIVES)

Northwestern University Freight Rail Infrastructure & Energy Network Decarbonization (NUFRIEND) Framework

Final Technical Report

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Final Technical Report

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Section A - Executive Summary

The goal of this project was to develop a tool to aid railroads and other stakeholders assess and approach the decarbonization of freight rail operations by identifying new, viable low-carbon energy storage and conversion systems for future locomotive systems and how they should be deployed on the existing US freight rail network.

In the first quarter, the project focused on collecting data, establishing a simulation workflow, and engaging industry through the creation of the Industry Advisory Board (IAB). In the second quarter, the project focused on selecting fuel pathways and powertrain technologies, setting performance targets, conducting a techno-economic analyses, and developing the simulation framework that would serve as the backbone of the future toolhead. The third quarter involved developing an industry-oriented interactive dashboard powered by a five-step sequential framework, as well as holding industry advisory board meetings as per the initial technology-to-market plan. In the remaining project quarters, the NUFRIEND dashboard were fine-tuned with the help of IAB member feedback and in-depth scenario analyses were conducted to support the techno-economic analysis of energy sources. Additionally, dashboard documentation, project insights, and open-source code on GitHub were prepared and released. Throughout the project, the team completed testing and analysis of all model components, integrated all initial test scenarios, and conducted stakeholder engagement.

Lower-carbon drop-in fuels can be deployed as admixtures and are considered uniform across the network at a desired penetration rate, while hydrogen and battery-electric technology deployment poses a more complex problem as they require significant investments to be made in the siting of refueling/charging facilities and the replacement of locomotive fleets. Thus, strategies for locating and sizing refueling/charging facilities on a railroad's network to meet their energy demands were developed to inform deployment decisions. To address this challenge, the Northwestern University Freight Rail Infrastructure & Energy Network Decarbonization (NUFRIEND) framework presents a five-step sequential framework to select O-D paths, locate facilities, reroute flows, size facilities, and evaluate the deployment for alternative energy sources that require locomotive powertrains to be converted and new refueling infrastructure to be deployed.[1]

The NUFRIEND Framework is an industry-oriented tool for simulating the deployment of new energy technologies across the US freight rail network. The framework provides a comprehensive network-level optimization and scenario simulation tool for decarbonizing the freight rail sector, addressing the uncertainties surrounding technological developments by supporting sensitivity analyses for different operational and technological parameters through a transparent and flexible input module. It offers practical alternatives to diesel locomotives and can be applied for any railroad considering the specific network structure and freight demand, outputting evaluation metrics for the associated emissions and costs relative to diesel operations.

A number of relevant simulation scenarios were run and analyzed for key insights on the value of different alternative technologies for freight rail decarbonization. The project developments and findings have been presented at numerous conferences and events.

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[1] https://www.transportation.northwestern.edu/research/featured-reports/locomotives.html

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Section B - Accomplishments and Objectives

The actual performance against the stated milestones is summarized below:

Table 1 - Key milestones and deliverables compared against the actual performance

WBS	Milestone Title	Summary
M1.1	Data collected	**Milestone:** Acquire and transfer time series data for a range of scenarios required for software development and validation. Associated train and route data will also be collected. Define full data requirements. Document is submitted for PD approval. **Actual Performance:** (Q1) GIS data acquired from the FRA, approval for the use of Confidential Carload Waybill Sample (CCWS) granted from the STB, key railroad inputs obtained from Industry Advisory Board, energy and emissions inventory development and cost data collection for various technology pathways.
M1.2	Test scenarios defined	**Milestone:** The scenarios for validation are identified and they represent wide range of operating conditions including extreme scenarios. Define technology options and roll out strategies to be analyzed under each of the three categories. For each scenario category, determine key parameters that form the basis of the cost and impact analysis. Document is submitted for PD approval. **Actual Performance:** (Q2) Fuel pathways and powertrain technologies selected. Scenario specification approach outlined. List of inputs used to specify a scenario detailed.
M1.3	Performance metrics	**Milestone:** Identify performance metrics targeted. These may include computational performance (i.e., hardware specifications, computing cost targets, solution time, solution quality, as well as operational performance metrics). The Full rollout model (FRM) is expected to include many time-dependent parameters, including but not limited to projected ES performance and cost, freight rail fleet turnover, manufacturing scale/capacity, infrastructure buildout, diesel, and other fuel costs, etc. Document is submitted for PD approval. **Actual Performance:** (Q2) Performance target set for industry deployment, objectives linked to emission, cost, and operating requirements, and sensitivity analysis planned for computation and uncertainty in parameters.

WBS	Milestone Title	Summary
M2.1	Simulation Framework Defined	**Milestone:** A simulation framework template for the software modules, which includes formally defined variable naming conventions and other coding standards is submitted for PD approval. This includes platform workflow, customer interaction points and data flow. This should detail how the software model components interact and pass information as well as how a central management system keeps track of various algorithm progress and results. An appropriate open-source platform repository with enforced peer review is established for the team to facilitate efficient co-editing. Define base system including details on existing practices. Provide details of new approach including details on modification to existing practices and additional data requirements. Provide mathematical formulation(s) for new approach. Document is submitted for PD approval. **Actual Performance:** (Q1) Simulation workflow established, inputs and outputs defined, key interfacing points identified.
M3.1	Alpha Framework	**Milestone:** The initial simulation framework that coordinates simulation modules, establishes a data bus structure, and maintains simulation time. Alpha placeholders for each module are connected to this simulation framework. Data flow through the model is confirmed and incremental code testing method established. I/O table is documented. Performance metric defined in M1.3 assessment validated through test scenarios defined in M1.2. **Actual Performance:** (Q2) Simulation framework established with the definition of data flow and parameters, major components completed with testing and analysis done throughout. All initial test scenarios were run and all model components were integrated.
M3.2	Beta Framework	**Milestone:** Beta level submodules have been created for each component and integrated into the framework. This includes models for the physical train energy, the rail network, infrastructure, operations, ES technology, and output metric calculators, including target level of GHG, and LCOTKM. Life cycle analysis (LCA) of various fuels/powertrain technologies - based on GREET model, will expand tool and will calculate the carbon reduction potential (in gCO2e/MJ and gCO2e/Mt-km)) for each fuel/locomotive technology pathway compared to conventional diesel locomotive for freight and passenger rail applications on various duty cycles. Roll-out strategy is documented, as well as I/O user interface per FOA request. Performance metric defined in M1.3 assessment validated through test scenarios defined in M1.2. **Actual Performance:** (Q3) Beta framework implemented with an industry-oriented interactive NUFRIEND Dashboard powered by a five-step sequential framework including network models, LCA, and TEA to capture rail network, freight demand, energy source technological parameters and other inputs to simulate and optimize facility locations and sizing, and outputting emissions, costs, and operational performance metrics.

WBS	Milestone Title	Summary
M3.3	Full Rollout Model	**Milestone:** Full roll-out model validation. Data collected are used to conduct train model energy estimation validation over a varying set of conditions and characterize the model accuracy. Illustrative examples of full roll-out model scenarios are documented. Using the inputs from previous tasks, such as the adoption rates of transitional technologies, refueling cost, etc., we will further analyze the best locations and build-out roadmaps for deploying the fueling infrastructure such as charging stations, battery storage, hydrogen refueling to support the roll-out of new ES technology adoption spatially and temporally different decarbonization scenarios. The results are the fleet-wide aggregated energy consumption and GHG emissions of selected or all possible ES systems and fuel pathways to identify the decarbonization options with rail freight. Document is submitted for PD approval. **Actual Performance:** (Q4) Full roll-out model developed based on Beta Framework. Interactive dashboard is hosted on servers allowing public access. Model validation with collected data and example documentation completed.
M4.1	Initial technology to market plan submitted to ARPA-E	**Milestone:** Initial T2M plan. Submission of draft Impact Sheet that describes the desired impact the project team would like to have by the end of the project. Assess value of technology based on market impact to determine appropriateness of further work. Document submitted for PD approval. **Actual Performance:** (Q1) Collaboration with Industry Advisory Board commenced, with particular consideration on impact of infrastructure and asset replacement costs.
M4.2	Techno-economic analysis	**Milestone:** Based on existing techno-economic framework (HDRSAM) this task will evaluate the levelized cost of hydrogen for fuel cell locomotives (in $/kg_H2) and electricity for fast charging of battery electric locomotives (in $/kWhe). Document submitted for PD approval. **Actual Performance:** (Q2) Levelized fuel costs for diesel and drop-in fuels, levelized cost of charging battery electric locomotives for different battery charging schemes, and levelized cost of refueling hydrogen locomotives for different hydrogen dispensing types were conducted with application of TEA tools to rail flows and test scenarios.
M4.3	Stakeholder engagement	**Milestone:** Industry advisory board briefing and input on scenarios. The document on stakeholder engagement (value proposition, barriers and criteria for adoption), model structure, functionality, tech demonstration of planned capabilities, and IP strategy for open-source is submitted for PD approval. **Actual Performance:** (Q2) Industry views and latest energy source studies incorporated in the model design and requirements with topic-specific interviews in progress to keep track of development, interviews with rail operations and equipment professionals conducted.

WBS	Milestone Title	Summary
M4.4	First iteration of T2M plan	**Milestone:** Industry advisory board briefing and input on methodology and scenario data. Revised T2M plan submitted to PD for approval. **Actual Performance:** (Q3) Several industry advisory board meetings held for industrial perspectives and feedback regarding the development of the NUFRIEND Framework and Dashboard. The revised T2M plan submitted in quarterly reports.
M4.5	Levelized cost of ES technology	**Milestone:** This task will develop estimates of the cost components to establish a firmer basis for costs such as capital cost, maintenance and repair, depreciation, and operating costs for rail. Document submitted for PD approval. **Actual Performance:** (Q4) Techno-economic analysis of energy sources produce cost estimates regarding capital and operations of refueling/charging facilities, energy costs, and delay costs. Techno-economic analysis of energy sources produce cost estimates regarding capital and operations of refueling/charging facilities, energy costs, and delay costs.
M4.6	Release Open-Source Code	**Milestone:** The open-source software code is prepared and publicly released on an appropriate open-source platform. Documentation of the code is provided. A getting started tutorial will guide new users through setting up and running a simulation. A set of example assumptions, that reflect the most current public information, are provided with example results. **Actual Performance:** (Q4) Software code is prepared on GitHub with documentation. Compilation and checking of the codes have been completed. A demonstration video is produced.

Section C - Project Activities

The goal of this project was to develop a tool to aid railroads and other stakeholders assess and approach the decarbonization of freight rail operations. The NUFRIEND framework was developed to address the project goals as a network-level optimization and scenario simulation and evaluation tool. The NUFRIEND framework is a comprehensive industry-oriented tool for simulating the deployment of new energy technologies across the U.S. freight rail network. In it, scenario-specific simulation and optimization modules provide estimates for carbon reduction, capital investments, cost of carbon reduction, as well as operational impacts for any given deployment profile. The NUFRIEND dashboard, along with supporting documentation and reports have been made publicly available.[2]

A no-cost extension was granted for this project to be extended by one additional quarter.

Section D - Project Findings

Section D.1 - Introduction

The transportation sector is the largest contributor to greenhouse gas (GHG) emissions in the US, contributing 27% of the emissions in 2020 [1]. Many transportation modes, particularly in the freight sector, have been difficult to decarbonize due to their massive energy requirements and the associated investments that would be necessary for that purpose. However, recent advances in lower-carbon fuels, battery technology, and hydrogen fuels have provided potentially viable alternatives to diesel for these traditionally hard-to-decarbonize modes.

In 2019, the US freight rail sector accounted for approximately 40% of the national freight ton-miles and emitted nearly 40 megatons of CO_2 into the atmosphere in the process, an amount equivalent to the emissions of all the passenger vehicles in Texas alone [2], [3]. Though freight rail offers about four times greater energy efficiency than trucking [4], recent strides in the electrification of trucks [5] may significantly reduce rail's environmental advantage and cause freight demand to shift away to less energy efficient modes. As rail freight's importance in the overall supply chain continues to grow in the era of e-commerce [6], freight demand is forecast to grow rapidly in the coming decades [7], which may counteract railroads' investments in engine efficiency improvements. External pressures have also been mounting to decarbonize freight rail as local governments have considered regulations on locomotive idling in urban areas [8] and large shippers such as Amazon and IKEA have committed to net-zero carbon emissions by 2040 which include those produced by the shipment of their goods [9].

Diesel-electric locomotives have dominated US freight rail operations since the 1960's [10] and have seen significant improvements in powertrain efficiencies since that time [11]. With the exception of a few corridors in the Northeast, track electrification has been limited to passenger rail as it would place a significant economic burden on private freight railroads to deploy electrical infrastructure in mostly rural stretches of the country and upgrade the many track segments that cannot accommodate overhead rail due to height constraints [12]. Advancements in alternative

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[2] https://www.transportation.northwestern.edu/research/featured-reports/locomotives.html

energy storage technologies in recent decades—particularly in lower-carbon drop-in fuels, battery chemistries, and cleaner hydrogen pathways—offer a practical alternative to track electrification for decarbonization. Railroads and fuel chemists now have a larger portfolio of lower-carbon diesel replacements (e.g., biodiesel, electric-fuels, renewable-diesels) than they did a decade ago [11]. Innovations in battery chemistry have led to increased volumetric and gravimetric energy densities, while reducing their overall cost per energy storage capacity [13], making this technology sufficiently mature to power electric locomotives [14]. Hydrogen combustion and fuel cell experimentation has made the technology viable for locomotive applications [11], while experimentation in fuel production has yielded many different kinds of hydrogen fuel pathways (e.g., steam-methane reforming, electric, nuclear, renewable), each with differences in their environmental impacts and costs of production [15]. Each of these alternative technologies provide distinct benefits and challenges to their implementation and must be compared on the economic, environmental, and operational impacts of their deployment to appropriately assess their value.

Several high-profile pilot studies have been conducted in partnership between multiple railroads, locomotive manufacturers, and local and state governments to test the viability of alternative technologies on revenue service [11], [16], [17]. The 2019 BNSF-Wabtec battery-electric pilot ran a battery-electric locomotive in a diesel-hybrid consist on revenue service between the 300-mile Stockton-Barstow route in California, showing emissions reductions of approximately 15% [16]. In partnership between the Pacific Harbor Line and Progress Rail, a battery-electric switcher locomotive was run in the Port of Los Angeles and Long Beach to investigate its performance while reducing carbon emissions and eliminating all localized pollutant emissions [17]. The Union Pacific Railroad has purchased 20 battery-electric locomotives for use as yard switchers, making it the largest commercial investment in the technology to date [18]. After running a hydrogen fuel cell locomotive pilot, Canadian Pacific has committed to expanding its fleet of hydrogen locomotives and constructing two hydrogen production facilities to supply their operations [19].

Picking the right mix and schedules to invest and deploy the next-generation of energy technologies is a challenging process. Technological uncertainties, network effects, regional economics, and economies of scale all render mathematical optimization formulations of the problem essentially intractable. Decarbonization decisions will no-doubt have far-reaching environmental, operational, and financial impacts on railroads, shippers, regulators, and other stakeholders in the greater supply chain. While previous research focused on conventional fuel types and highly simplified railroad networks, there is a significant research gap in developing optimization models to support the deployment of infrastructure to support rail decarbonization.

Section D.2 - NUFRIEND Framework

The Northwestern University Freight Rail Infrastructure & Energy Network Decarbonization (NUFRIEND) Framework was developed to assist the rail industry in planning and evaluating the adoption of alternative fuels for decarbonization efforts. Scenario-specific simulation and optimization modules provide estimates for emissions reduction, capital investments, cost of carbon reduction, and operational impacts for any deployment profile.

The framework relies on two different approaches to capture the characteristics and requirements of the two main groups of energy technologies:

1. **Drop-in fuels (Figure 1)**: Lower-carbon drop-in fuels can directly replace diesel fuel in locomotives and refueling stations. We assume no significant changes to existing assets or infrastructure are required for their deployment. Figure 1 shows the flowchart of the framework developed to analyze drop-in fuel deployment scenarios.
2. **Energy storage fuel technology (Figure 2)**: Hydrogen and battery-electric technology deployment poses a more complex problem as they require significant investments to be made in the siting of refueling/charging facilities and the replacement of locomotive fleets. Thus, strategies for locating and sizing refueling/charging facilities on a railroad's network to meet their energy demands must be developed to aid deployment decisions. However, jointly locating and sizing facilities quickly becomes a combinatorial problem due to the interconnectivity of the many potential facility locations seen on networks as well as the fact that regional economics and economies of scale both affect the cost of a facility deployment strategy. To reduce the problem complexity, we decompose the facility location and facility sizing problems from each other and insert a flow routing module in between to assign freight flow that must be served by the selected facilities. Figure 2 depicts a flowchart highlighting the five-step framework developed to address the deployment of the refueling/charging infrastructure to support hydrogen or battery-electric locomotives.

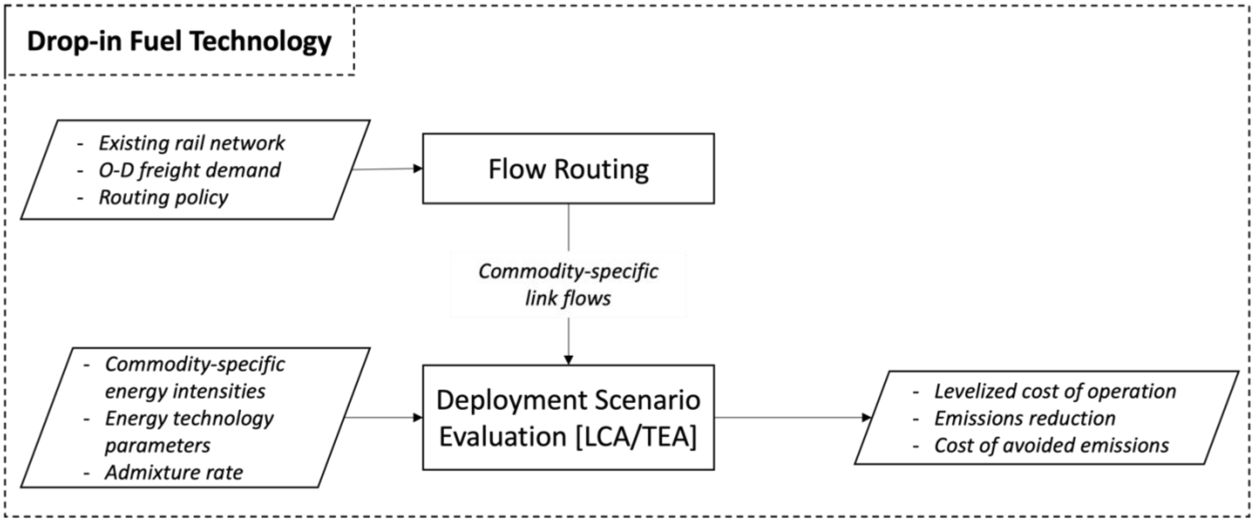


Figure 1 - Flowchart of framework to support the deployment of lower-carbon drop-in fuels on the rail network.

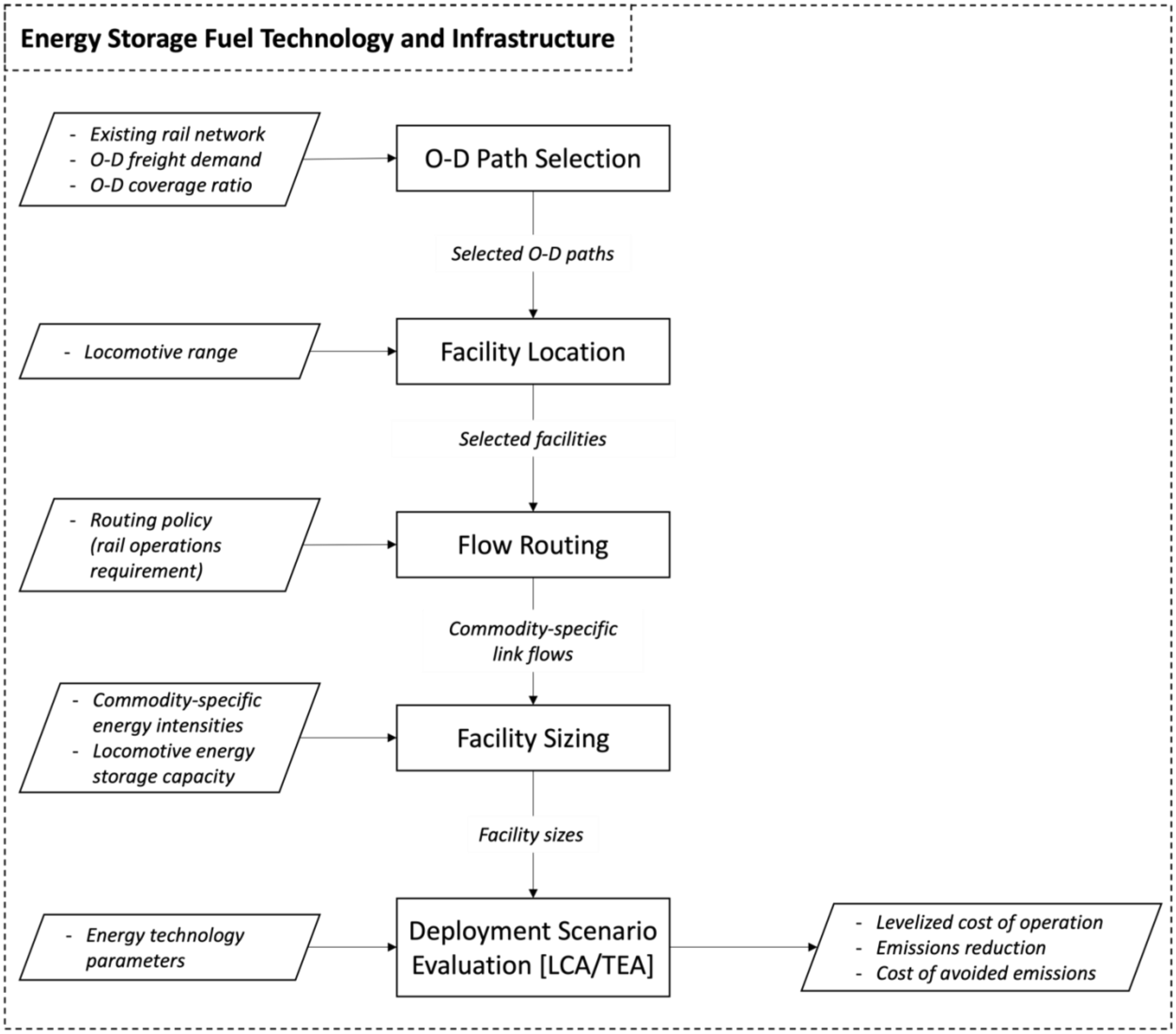


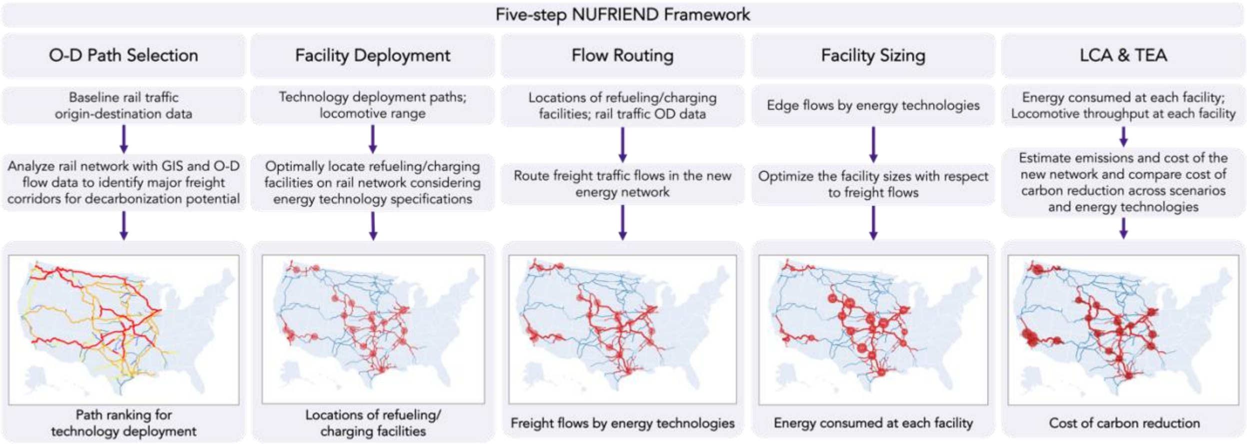
Figure 2 - Flowchart of five-step framework to support the deployment of refueling/charging infrastructure for hydrogen and battery-electric technologies.

The NUFRIEND framework aids stakeholders in analyzing alternative fuel technology deployments for freight rail operations. We assess and classify potential energy technologies based on deployment requirements and provide practical alternatives to diesel locomotives. The otherwise intractable facility location and sizing problem are solved with a five-step framework consisting of nominal problems from graph theory. A key advantage is the flexibility to apply the framework for any railroad considering the specific network structure and freight demand, outputting evaluation metrics for the associated emissions and costs relative to diesel operations. Equipped with the capability to efficiently simulate technology adoption scenarios with life-cycle analysis (LCA) and techno-economic analysis (TEA), this framework supports sensitivity analyses for different operational and technological parameters through a transparent and flexible input module, thereby addressing the uncertainties surrounding technological developments.

This framework simulates and evaluates the deployment of alternative fuel technologies on the rail network, and as such is dependent on the technological requirements of each energy technology. The energy technologies considered in this paper can be divided into two categories: (1) lower-carbon drop-in fuels such as biodiesels and e-fuels and (2) new energy storage technologies such as battery-electric or hydrogen.

Lower-carbon drop-in fuels are generally deployed as admixtures (e.g., 20% biodiesel and 80% diesel). Their deployment is considered uniform across the network at a desired penetration rate taken as the rate of the admixture. Thus, origin-destination (O-D) flows are simply routed by commodity group on the existing (baseline) network's links. These flows are used to calculate the costs and emissions associated with their deployment by weighing the relevant fuel parameters with their corresponding admixture rates. Figure 1 demonstrates the essential steps and flow of information.

However, for alternative energy sources that require locomotive powertrains to be converted and new refueling infrastructure to be deployed, we present a five-step sequential framework to (1) select O-D paths that leverage economies of density, (2) locate facilities along these paths, (3) reroute flows on the existing and alternative technology rail networks, (4) size the facilities in order to serve the rerouted flows, and (5) evaluate the deployment in terms of their emissions, costs, and operational impacts. The flow of information between each of the steps can be seen in Figure 2 with a visualization of each of the steps shown in Figure 3. The features of the NUFRIEND framework are highlighted in Figure 4.



Baseline rail traffic origin-destination data

Analyze rail network with GIS and O-D flow data to identify major freight corridors for decarbonization potential

Path ranking for technology deployment

Technology deployment paths; locomotive range

Optimally locate refueling/charging facilities on rail network considering energy technology specifications

Locations of refueling/charging facilities

Locations of refueling/charging facilities; rail traffic OD data

Route freight traffic flows in the new energy network

Freight flows by energy technologies

Edge flows by energy technologies

Optimize the facility sizes with respect to freight flows

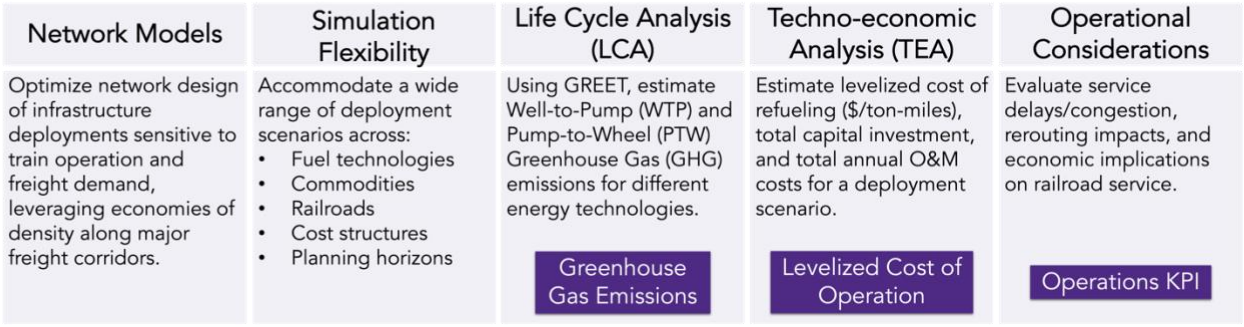
Energy consumed at each facility

Energy consumed at each facility; Locomotive throughput at each facility

Estimate emissions and cost of the new network and compare cost of carbon reduction across scenarios and energy technologies

Cost of carbon reduction

Figure 3 - Visualization for each of the steps of the five-step NUFRIEND Framework



Network Models	Simulation Flexibility	Life Cycle Analysis (LCA)	Techno-economic Analysis (TEA)	Operational Considerations
Optimize network design of infrastructure deployments sensitive to train operation and freight demand, leveraging economies of density along major freight corridors.	Accommodate a wide range of deployment scenarios across: • Fuel technologies • Commodities • Railroads • Cost structures • Planning horizons	Using GREET, estimate Well-to-Pump (WTP) and Pump-to-Wheel (PTW) Greenhouse Gas (GHG) emissions for different energy technologies.	Estimate levelized cost of refueling ($/ton-miles), total capital investment, and total annual O&M costs for a deployment scenario.	Evaluate service delays/congestion, rerouting impacts, and economic implications on railroad service.
		Greenhouse Gas Emissions	Levelized Cost of Operation	Operations KPI

Figure 4 - Features of NUFRIEND Framework

Section D.2.1 - Sequential Framework for Facility Location & Sizing

The joint facility location and sizing problem is a combinatorial problem to solve [20], especially over networks, where potential facility locations have many degrees of interconnectivity. To simplify the problem, therefore, we decouple and formulate variations of the facility location and sizing problems that capture important managerial concerns.

We formulate the facility location integer program as an extension of the Set Covering Problem [21]. The solution yields the minimum number of facilities on the network required to fulfill continuous trips along the paths between a pre-specified set of O-D pairs. These O-D pairs are selected from the network based on the flows between them. Each O-D pair is ranked in descending order by the value of the ton-miles of goods moved between them, from which a subset is selected based on the input O-D coverage ratio (see Figure 2). Paths are generated between each O-D pair in this subset and are used, along with the input locomotive range, to specify the coverage constraints for the integer program. To locate facilities, the existing rail network is represented as a directed graph in which the nodes represent candidate locations—rail yards with the capacity to service trains—for refueling/charging facilities and the arcs represent the railroad tracks between the candidate facility locations. The selected facilities are used to create a subnetwork enabled by the alternative technology. To represent where flows can be served by the alternative technology, the enabled arcs on this subnetwork are either (1) along paths between facilities with a distance below the maximum given range or (2) on paths with a distance of no more than half the given range (i.e., the in-and-back-out distance from a facility does not exceed the range).

As flows are assumed to originate and terminate at any candidate facility location on the rail network, they may be assigned to the alternative technology enabled subnetwork. The actual assignment of flows depends on the specified routing policy, which may or may not allow for flows to be rerouted from their original routing on the baseline network, may have a maximum distance increase if flows are rerouted, or may only allow flows originating *and* terminating at enabled nodes to be served by the alternative technology. These, and other routing strategies can be accommodated, as specified by the input to the Flow Routing step. Importantly, as the alternative technology may not be able to serve all flows on the network, the baseline network, operated by diesel, is assigned any flows that cannot be served by the alternative technology. We assume that for a given O-D pair, the flows are served entirely by the alternative technology (if service is enabled), or entirely by diesel (as in the baseline case). The routing of flows on the two networks is used to compute the penetration rate (in percentage of ton-miles) of the alternative technology on the network.

As the energy intensities of moving different commodities are known to vary considerably [22], for each O-D pair, we route the flows between them for each of the nine main commodity groups as reported by the AAR [23]. The selected facility locations and commodity-specific link-flows for the alternative technology subnetwork are critical inputs for the sizing of facilities (i.e., the specification of facility energy capacities). We build on the minimum cost network flow problem structure [24] to formulate a facility sizing problem which provides the energy flows at each of the refueling/charging facilities that minimizes the total cost of energy consumption for the network. The constraints for this formulation ensure the energy required to move all goods (calculated by commodity) is dispensed by the selected facilities. Peak link-wise energy requirements are calculated as the product of the commodity-specific peak flows assigned to each link and the commodity-specific energy intensities. The model outputs the peak facility size (in kWh/day for battery and kgH_2/day for hydrogen) of each selected facility that is required to provide service to the goods routed on the alternative technology's network as well as the average energy consumption (kWh/day or kgH_2/day) and locomotive throughput (locomotive/day). These outputs are critical to calculating each facility's utilization rate as well as the emissions, cost, and operational impacts of a particular deployment.

Section D.2.2 - Life-cycle Analysis (LCA) of Energy Technologies

In this study, we examine the GHG emissions of different energy technologies with a system boundary covering both the well-to-pump (WTP) and pump-to-wheel (PTW) stages. The functional unit for the emissions was set as gCO_2/ton-mile. Together, WTP and PTW stages comprise well-to-wheel (WTW) analysis. While the WTP examines the environmental impact of production, transportation, and distribution of feedstock and fuels, PTW focuses on the vehicle operation. Note that the impacts from the vehicle manufacturing cycle, including stages such as material extraction, component manufacturing, assembly, and recycling of vehicle components, are out of scope for this analysis.

We use ANL's GREET model [15]—updated annually with the most up-to-date and detailed energy use and emissions data for petroleum refineries and electric power plants—to conduct the WTW analysis. For the diesel, biodiesel, e-fuel, and hydrogen (for various fuel pathways, e.g., steam-methane reformed or renewable hydrogen) technologies, we estimate the WTW GHG emissions factors (in gCO_2/Btu) using GREET 2021 [15]. The R-1 report published by Surface Transportation Board (STB) provides the annual diesel usage and associated revenue ton-miles for each of the Class I railroads [25]. Combining these values with the emissions factors from GREET, we estimate the railroad-specific WTW GHG emissions in gCO_2/ton-mile using Equation (1).

$$\begin{aligned} GHG\ emissions \left[\frac{gram\ CO_2}{ton-mile}\right] &= \frac{Total\ Diesel\ Use\ [gallons]}{Total\ Revenue\ Ton-Miles\ [ton-mile]} \\ &\quad \times\ Emission\ Factor\ from\ GREET \left[\frac{gram\ CO_2}{Btu}\right] \\ &\quad \times Lower\ Heating\ Value\ of\ Diesel \left[\frac{Btu}{gallons}\right] \end{aligned} \tag{1}$$

For battery-electric locomotives, we consider the GHG emissions associated with the upstream processes of electricity generation and the losses in the transmission and distribution system. For current and projected (Mid-case Standard Scenario) generation mixes, we capture the state-wise variation of electricity generation mixes in terms of gCO_2/kWh supplied to the charger station based on the results from [26].

We consider four different liquid hydrogen pathways in the WTW analysis of hydrogen powered locomotives. We used GREET's newly updated 2022 version to extract the WTW results for the following pathways:

1. Natural Gas
2. Natural Gas with CO_2 Sequestration

3. PEM Electrolysis - Solar
4. PEM Electrolysis – Nuclear

Figure 5 shows a comparison between these four pathways in terms of feedstock, fuel, and total GHG emissions. We further compare the WTW GHG emissions between current (2021) and future (2034) scenarios. Figure 6 compares the results for these two scenarios. For all four pathways, the future scenarios exhibit lower GHG emission compared to present cases, mainly due to the cleaner electricity used for hydrogen liquefaction.

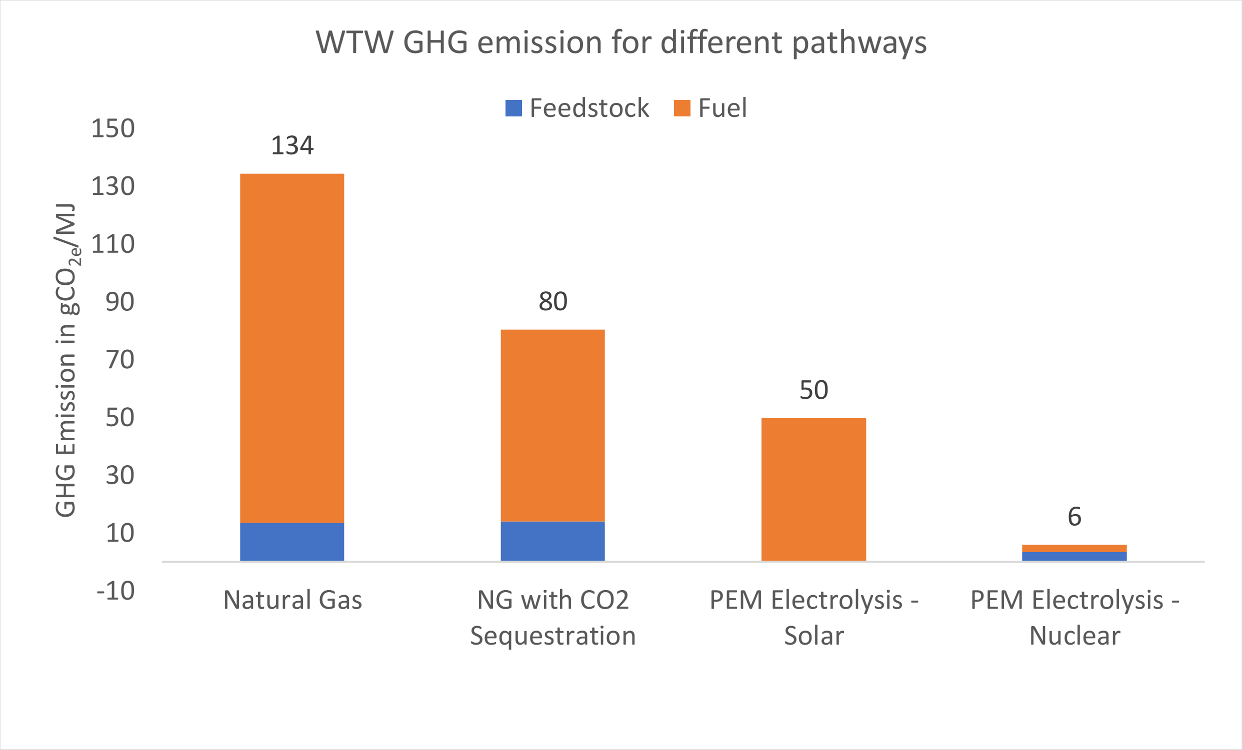


Figure 5 - WTW GHG emissions for different liquid hydrogen delivery pathways

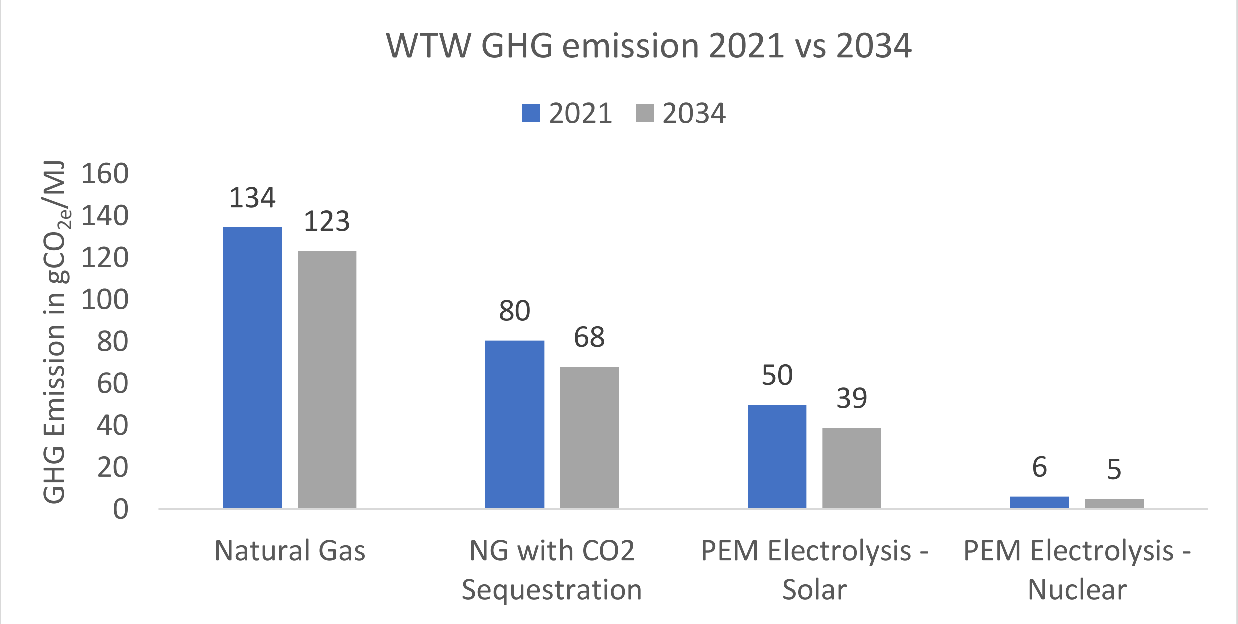


Figure 6 - Comparison of present and future scenarios for GHG emissions using different liquid hydrogen delivery pathways

Section D.2.3 - Techno-economic Analysis (TEA)

For conventional diesel, biodiesel, and e-fuels, this study focuses on the levelized cost of refueling only, as these energy technologies do not require additional infrastructure investments. We estimate the levelized cost of refueling by multiplying the commodity specific link flow, energy intensity, and fuel cost. For battery-electric and hydrogen technology, we consider the charging/refueling infrastructure cost in addition to the battery/hydrogen tender car capital investment and refueling costs. The sequential framework described in Section D.2.1 estimates the facility size based on the peak demand (in kWh/day for battery and kgH_2/day for hydrogen) at each location. Based on a given locomotive battery/hydrogen tender car capacity, the peak and average demand is used to estimate the peak and average locomotive throughput at each facility. From the peak locomotive throughput, we estimate the number of chargers/pumps needed at each location to support the peak demand, such that a provided maximum station utilization is not exceeded. ANL's bottom-up TEA tools, Heavy-duty Electric Vehicle Infrastructure Scenario Analysis Model (HEVISAM) for battery-electric, and Hydrogen Delivery Scenario Analysis Model (HDSAM) for hydrogen [27], provide the levelized cost of charging/refueling for a given fleet size and facility specification. We use HEVISAM to develop a functional relationship between the levelized cost of charging and number of locomotives for a given number of chargers. The levelized cost of operation for the battery-electric technology is calculated using Equation (2), while the levelized cost of operation for the hydrogen technology scenarios is represented in Equation (3).

$$\begin{aligned} &Levelized\ cost\ of\ operation\ \left[\frac{\$}{kWh}\right] \\ &= levelized\ cost\ of\ battery\ (ammortized\ capital\ cost\ of\ battery) \\ &+ levelized\ cost\ of\ charging\ (charging\ station\ contribution\ from\ HEVISAM) \\ &+ electricity\ price\ by\ state \end{aligned} \tag{2}$$

$$
\begin{aligned}
&\mathit{Levelized\ cost\ of\ operation}\left[\frac{\$}{kgH_2}\right]\\
&= \mathit{levelized\ cost\ of\ hydrogen\ tender\ car}\ (\mathit{ammortized\ capital\ cost\ of\ tender\ car})\\
&+ \mathit{levelized\ cost\ of\ refueling}\left(\begin{matrix}\mathit{delivery\ and\ refueling\ station\ capital\ cost}\\ \mathit{contribution\ from\ HDSAM}\end{matrix}\right)\\
&+ \mathit{hydrogen\ fuel\ price}\ (\mathit{production})
\end{aligned} \tag{3}
$$

The levelized costs of operation are estimated in terms of cost per quantity of energy (e.g., \$/kWh) or fuel (e.g., \$/kgH_2, \$/gallon) and are converted to cost per revenue ton-mile using energy intensity parameters from Table 3 and the results from the flow routing and facility sizing steps to determine the ton-miles served by a particular energy technology. The levelized cost per ton-mile provides a standardized way to represent alternative technology costs as an operational metric.

The WTW GHG emissions and the levelized cost of operation could be synthesized into one metric to compare across energy technologies. The cost of avoided emissions (CAE) of a particular technology is the ratio of the levelized cost of operations (in \$/ton-mile) and the WTW GHG emissions intensity (in kgCO_2/ton-mile), relative to the baseline diesel operations, as represented in Equation (**4**). The CAE serves as a key policy metric, as it provides the cost per unit of carbon reduced from emissions for a specific technology, a metric that can be compared to the social cost of carbon or carbon credit/tax schemes.

$$
\begin{aligned}
&\mathit{Cost\ of\ avoided\ emissions}\left[\frac{\$}{kgCO_2}\right]\\
&\qquad = \frac{\mathit{LCO\ alternative\ technology} - \mathit{LCO\ diesel}}{\mathit{WTW\ GHG\ alternative\ technology} - \mathit{WTW\ GHG\ diesel}}
\end{aligned} \tag{4}
$$

Section D.2.4 - Operational Implications

The NUFRIEND framework features operational impact metrics for associated deployment scenarios across several dimensions. The average delay associated with charging/refueling and potential congestion at charging/refueling facilities is an important factor for time-sensitive railroad operations which compete with trucking, such as intermodal. Commodity-specific flows are used to estimate the emissions reductions potential and levelized costs of shipping specific commodity groups by the alternative technology under consideration. Furthermore, different routing options are captured through three primary parameters: whether to allow rerouting from diesel to the alternative technology, the maximum allowable distance increase of such a rerouting, and whether goods can be switched to alternative technology locomotives as they become available at different sections of their trip, all allowing users to match their real operational practices and goals more closely. Related to this, we compute the average route distance increase over all shipments, which provides information on the scenario's impact on operations from re-routing goods through paths other than their shortest paths so that flows may be consolidated on alternative fuel service corridors.

Delay impacts are reported as average metrics, in both time and monetary units, for any scenario. These metrics provide the incremental delay relative to diesel refueling operations, which have negligible effects on current operations (in both time to refuel and congestion at stations). We break the delay time estimation into two steps. The first step involves a 0th order estimation of charging/refueling time, based on the technological specifications for the charging/refueling facility and energy storage capacity per locomotive as well as the flow of goods and locomotives through facilities and their energy/fuel states. This step provides the deterministic charging/refueling time for the deployment scenario. On top of this, we formulate a queuing model to capture the 1st order delays associated with the probabilistic nature of arrivals and service rates as well as the facility size. The queuing model applies the analytical results for the well-studied M/M/s queuing model. This provides estimates for the average time spent queuing per locomotive or car as well as the average length of the queue. These two values for delay time are then summed to determine the total average delay per locomotive or car. This delay value is converted to monetary units using estimates for the time-value of goods from [28] shown in Table 2.

Table 2 - Hourly Delay Cost per Train Car (in 2019 USD)

Trip distance (mi)	**0-1000**	**1000-1500**	**>1500**
Unit train	8.42	8.42	8.42
Manifest train	17.57	17.57	17.57
Intermodal train	26.06	26.95	28.36

Different freight commodities are known to have different shipment energy intensities due to both physical (e.g., density, and aerodynamics) and operational (e.g., shipment speed, time sensitivity, and geographic distribution) characteristics. For example, coal shipments are generally far less energy intensive than intermodal shipments, as these have considerably lower density and are frequently shipped at much higher speeds (due to their high value and time sensitivity). For this reason, the NUFRIEND framework allows for a more detailed analysis of deployment scenario results, using commodity groups as an additional dimension. For a particular commodity group, metrics are output on the share of flow served by the alternative technology on the network, the associated emissions, and the rescaled levelized costs of operation. These metrics allow users to glean a sense of the difficulty of decarbonizing specific commodity groups due to their physical and operational characteristics, which may be a useful piece of information for strategic rollout decisions.

Section D.3 - Compiled Data and Parameters

The framework presented above is next illustrated through application to evaluate alternative decarbonization scenarios for the US Class I railroads network. In this application, the parameters involved in modeling rail operations and energy sources collected from multiple sources are summarized in Table 3.

Table 3 - Parameters

A. Train Operations			
Parameter	**Western Railroads**	**Eastern Railroads**	**Source**
Freight demand	*(various, by O-D by commodity)*		[29]
Average number of locomotives per train	3.15	2.18	[25]

Average number of cars per train	74.6	68.5	[25]
Average tonnage per locomotive	1319	1403	[25]
Marginal battery cost per locomotive (¢/ton-mile)	0.12	0.19	[14], [25]
Marginal hydrogen tender car cost per locomotive (¢/ton-mile)	0.05	0.08	[25]
Average hydrogen locomotive range (mile)	1039	977	[15], [25, p. 1]
Diesel Energy Requirement for Various Commodities (BTU/ton-mile)			[15], [23], [25], [30], [31]
Agricultural & Foods	152	155	
Chemical & Petroleum	150	153	
Coal	107	109	
Forest Products	219	224	
Intermodal	875	893	
Metals and Ores	152	155	
Motor Vehicles	710	725	
Nonmetallic Products	128	131	
Others	553	565	

B. Battery-Electric

Parameter	**Value**	**Source**
Unit weight of battery tender car (ton)	150	[14]
Battery capacity (MWh)	14	[14]
Charging speed (MW)	3	[14]
Charging depth	80%	[14]
Battery energy efficiency	95%	[14]
Capital cost of battery + inverter + boxcar ($)	1,271,816	[14]
Future cost of battery ($)	452,908	[14]
Battery maintenance cost ($/day)	100	[14]
Battery lifetime (year)	13	[14]
Relative energy efficiency of battery-electric to diesel	2.44	[14]
Discount rate	3%	[14]
Time horizon (year)	26	[14]
Charging cost ($/kWh)	0.15	[15]
Electric grid carbon emissions (kg CO_2 eqv/kWh)	(various, by state by year)	[26]
Electric grid cost ($/kWh)	(various, by state by year)	[32]

C. Hydrogen

Tender car capacity (kgH$_2$)	4000	*Assumed*
Tender car capital cost (\$/kgH$_2$)	80	*Assumed*
Tender car lifetime (year)	20	*Assumed*
Relative energy efficiency of hydrogen to diesel	1.5	[33]
Hydrogen emissions (kg CO$_2$ eqv/kgH$_2$)	14.77	[15]
Hydrogen fuel cost (\$/kgH$_2$)	2.00	[27]
D. Drop-in Fuels		
Parameter	**Value**	**Source**
Diesel lower heating value (BTU/gallon)	129,488	[15]
Relative energy efficiency of drop-in fuels to diesel	1	[15]
Diesel emissions (kg CO$_2$ eqv/gallon)	12.36	[15]
Biodiesel emissions (kg CO$_2$ eqv/gallon)	3.50	[15]
E-fuel emissions (kg CO$_2$ eqv/gallon)	0.07	[15]
Diesel cost (\$/gallon)	2.47	[34]
Biodiesel cost (\$/gallon)	3.60	[34]
E-fuel cost (\$/gallon)	5.19	[34]

Section D.3.1 - Rail Network

The existing rail network was extracted from the North American Rail Network data set compiled by the Federal Railroad Administration (FRA) and the Bureau of Transportation Statistics (BTS) using work on rail facility classification done by Oak Ridge National Lab in WebTRAGIS [36]. These facility classifications allow for the number of nodes on the network to be reduced from the tens of thousands to hundreds as those nodes representing terminal, primary, and minor rail yards are kept and all others—representing grade crossings—were removed. Additionally, nearby nodes are clustered into super-nodes to simplify the network topology, while maintaining its overall structure. Operational data from the Annual Report of Finances and Operations (R-1 report) [25] on values for average train loadings, annual movements of goods and fuel consumption, locomotive fleet sizes, and physical train parameters were extracted for each of the Class I railroads. The relevant values that were calculated from these data are summarized in Table 3A.

Freight rail demand for 2019 was estimated from the STB's annually compiled Carload Waybill Sample (CWS) [29], which samples a subset of all rail movements in the U.S. and provides movement-specific data on railroad, routing, and costs. Though this framework can be applied to any individual railroad, the CWS data was aggregated to the three-railroad level in accordance with STB policy to preserve confidentiality in the illustration of results that follow. All operational parameters were also aggregated in a similar manner. As the aggregated CWS provides O-D flow data, these must be routed on the network following an assumed routing policy.

Section D.3.2 - Energy requirement

As the flow routing from the CWS provides estimates of the ton-miles of goods by commodity on the network, these must be converted into terms of energy from which fuel or electricity consumption can be calculated. The energy required to move a ton of goods one mile varies by commodity due to differences in physical characteristics (e.g., density) and operational practices (e.g., shipment speed), by railroad due to topographical and fleet variations, and by energy technology due to differences in powertrain designs [22]. As such, various factors must be applied to each ton-mile of goods based on its commodity type, the railroad that is moving it, and the locomotive's energy technology. A tool for calculating commodity-specific energy intensity factors was developed in [31], with the values updated for 2019 freight rail operations in [15]. Operational data from the R-1 report was used to regroup these commodity-specific energy intensity factors into the nine main commodity groupings recorded by the AAR [23]. Additionally, data on railroad-specific fuel consumption and ton-mile service from [25] was used to calculate railroad-specific energy intensities in [30], which were then reaggregated to the corresponding groupings used in the scenarios to follow. Finally, technology-specific energy efficiency ratios were taken from various sources. For biodiesel and e-fuels we assume the same energy intensity as for diesel. For battery-electric locomotives, the efficiency gain from battery was estimated as 2.44 the quotient of the battery round trip efficiency (assumed to be 95%) and diesel engine efficiency (assumed to be 39%) [14]. For Hydrogen locomotives, the energy efficiency gain compared to baseline diesel was taken as 1.5 [33]. These factors are shown in Table 3A.

Section D.3.3 - New Energy Sources

New energy sources are evaluated relative to diesel operations based primarily on their differences in cost and emissions. Baseline diesel cost and emissions data are extracted from the R-1 report [25]. Forecasts for drop-in fuel costs and emissions are based on [34] and are summarized in Table 3D. For battery-electric locomotives, the electric grid has geographically varying costs and emissions, which directly affect the evaluation of battery-electric deployment. State-specific commercial electricity rates from [32] and emissions values from [26] were used. In addition to electrical costs, the economic evaluation of the battery-electric scenario must consider the levelized capital cost of charging facility deployment. Thus, the TEA tool, HEVISAM, is applied using data found in Table 3B attained from prior work and personal communication with industry experts to estimate the levelized cost of operation for a given charging facility depending on its capacity and utilization rate. For hydrogen fuel locomotives, emissions values from [15] are used to estimate the WTW emissions associated with the use of steam-methane reformed hydrogen fuel, while refueling station capital costs and hydrogen fuel costs are provided by the HDRSAM tool using the parameters in Table 3C.

Section D.3.4 - Levelized Cost of Battery Tender Car

For the case of battery-electric locomotive deployment, the sizeable capital cost of the batteries must be captured. Building on assumptions and data from [14] on the cost of a 14 MWh battery tender car attachment for a locomotive, we calculate the levelized cost of battery tender car operation in dollars per ton-mile based on operational data from [25]. These values vary by railroad as seen in Table 3A and are a component of the complete levelized cost in Equation (2). The framework takes locomotive range as an input that is used to calculate the energy storage capacity assigned to each locomotive (in the form of additional battery tender cars) based on the average tonnage assigned to each locomotive. As the locomotive range increases, so does the required energy storage per locomotive, which in turn increases the energy capacity of battery tender cars per locomotive and levelized cost of battery operations.

Section D.3.5 - Levelized Cost of Hydrogen Tender Car

Due to considerably lower energy density relative to diesel, hydrogen fuel locomotives will require the use of a tender car for fuel storage. The storage of hydrogen fuel requires advanced temperature and pressure control systems, making hydrogen tender cars capital-intensive investments [37]. Using the techno-economic data summarized in Table 3C, we amortize the capital cost of the hydrogen tender car over its lifetime. Operational data from the R-1 report in [25] is then used to estimate the cost per ton-mile of hydrogen tender car operation, which vary by railroad as seen in Table 3A. These values are factored into the complete levelized cost of operation in Equation (3). From the assumption on fixed liquid hydrogen tender car capacities at 4000 kgH_2, we are able to estimate hydrogen locomotive range based on each railroad's average locomotive payload, as seen in Table 3A.

Section D.3.6 - Techno-economic Analysis (TEA) of Hydrogen

Similar to battery-electric locomotives, an economy of scale was observed for hydrogen locomotive refueling. Figure 7 illustrates the decrease in the total cost of locomotive refueling with increasing facility throughput. Moreover, cost decreases with increased station utilization, as fewer dispensers are assigned to a larger number of locomotives. In this study, we considered three different dispensing options for liquid hydrogen refueling. Results showed that low-pressure (10 bar) LH2 cryo-pump dispensing was usually the most economical option with the lowest levelized cost of refueling.

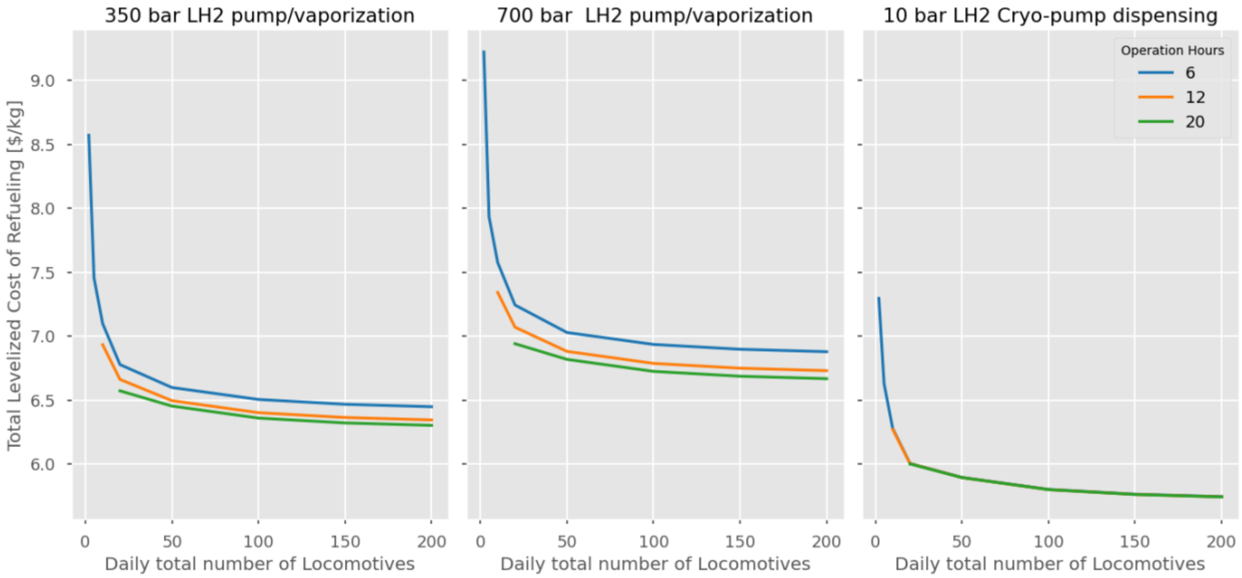


Figure 7 - Levelized cost of refueling hydrogen locomotives for different fleet sizes and dispensing options

The breakdown of the levelized cost is presented in Figure 8. For pump/vaporization options, the capital cost contribution of storage and compressor/pump plays a key role in the increased levelized cost in the liquid refueling station.

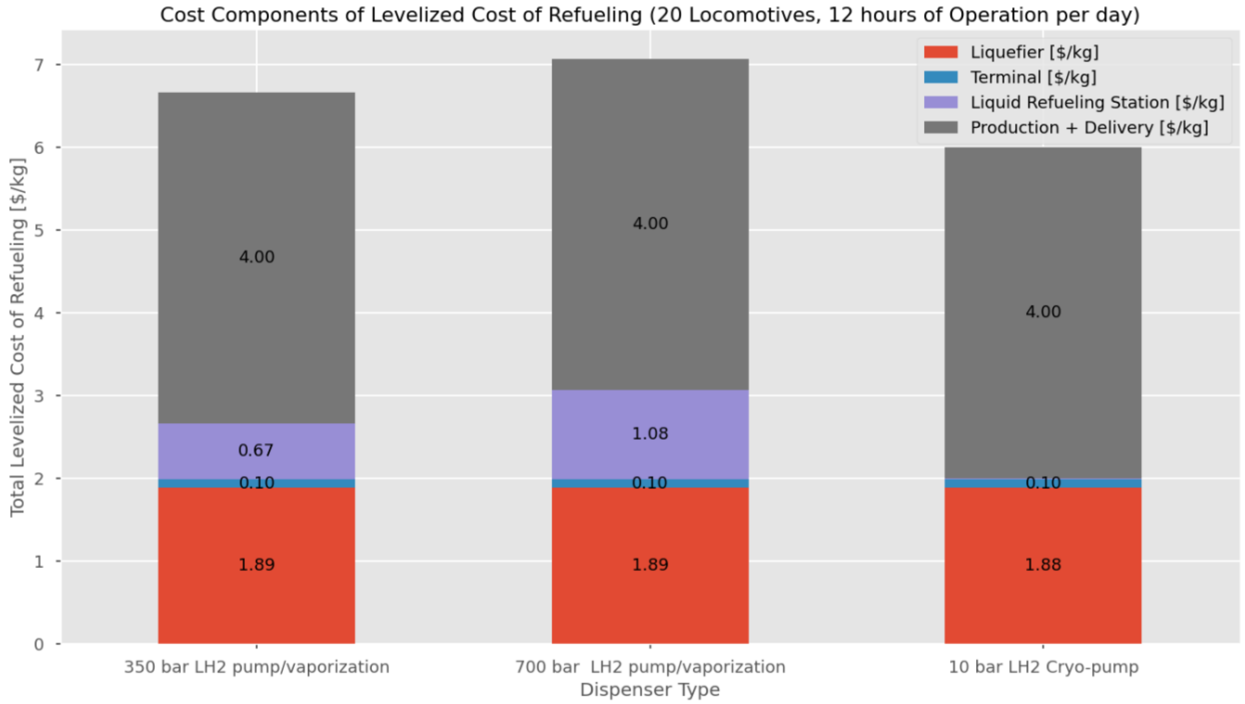
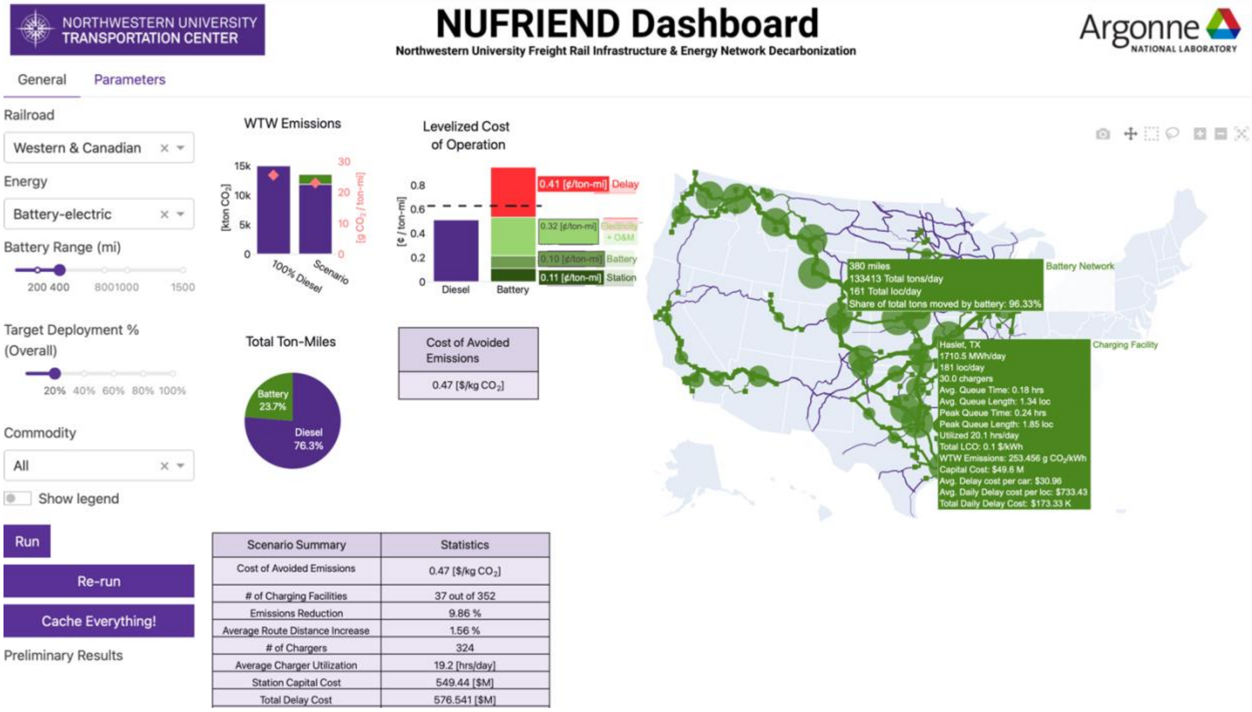


Figure 8 - Cost components of hydrogen locomotive refueling

Section D.4 - Scenario Analysis

To illustrate the functionality of the model, scenario simulation and evaluation results are shown for Western (BNSF, Canadian National, and Canadian Pacific Railways) and Eastern (CSX Transportation, Kansas City Southern, and Norfolk Southern Railways) railroad networks.

Figure 9 shows an example of the NUFRIEND dashboard. It allows users to model different scenarios based on inputs including railroads, energy sources, commodity groups, battery ranges, and target deployment percentages on the left, as well as other specific parameters on a separate pane. In the context of battery-electric and hydrogen deployment, the five-step sequential framework is applied to consider the railroad network and freight traffic, locate and size the charging facilities, route the rail traffic, and estimate the emissions and costs based on LCA and TEA, as outputted in the right. Metrics including WTW emissions, levelized costs of operation (LCO), the proportion of ton-miles served by each energy technology, the cost of avoided emissions, and other detailed operational results are shown. The scenario WTW emissions are the sum of emissions of diesel (blue) and battery/hydrogen (green) routes. The LCO of diesel is the current fuel cost, while the battery-electric LCO is composed of charging facility capital costs, battery capital and O&M cost, and electricity cost and the hydrogen LCO is composed of refueling facility capital costs, energy tender car capital cost, and fuel cost. Above the battery-electric/hydrogen LCO, the scenario average LCO is shown, which includes the cost of diesel refueling needed to serve the segments of the network not covered by battery-electric or hydrogen. Results are also shown down to the facility and track levels with green color denoting coverage of battery-electric or hydrogen technology. Users can hover over them to examine more granular information such as traffic volume, number of chargers or pumps, and station utilization.



Railroad: Western & Canadian

Energy: Battery-electric

Battery Range (mi): 200 400 800 1000 1500

Target Deployment % (Overall): 20% 40% 60% 80% 100%

Commodity: All

☐ Show legend

Cost of Avoided Emissions
0.47 [$/kg CO_2]

Scenario Summary	Statistics
Cost of Avoided Emissions	0.47 [$/kg CO_2]
# of Charging Facilities	37 out of 352
Emissions Reduction	9.86 %
Average Route Distance Increase	1.56 %
# of Chargers	324
Average Charger Utilization	19.2 [hrs/day]
Station Capital Cost	549.44 [$M]
Total Delay Cost	576.541 [$M]

380 miles
133413 Total tons/day
161 Total loc/day
Share of total tons moved by battery: 96.33%

Haslet, TX
1710.5 MWh/day
181 loc/day
30.0 chargers
Avg. Queue Time: 0.18 hrs
Avg. Queue Length: 1.34 loc
Peak Queue Time: 0.24 hrs
Peak Queue Length: 1.85 loc
Utilized 20.1 hrs/day
Total LCO: 0.1 $/kWh
WTW Emissions: 253.456 g CO_2/kWh
Capital Cost: $49.6 M
Avg. Delay cost per car: $30.96
Avg. Daily Delay cost per loc: $733.43
Total Daily Delay Cost: $173.33 K

Figure 9 - NUFRIEND Dashboard Example

This section showcases the functionalities of the dashboard with scenario results for each of the two energy technology categories. Each of the figures show aggregate emissions, cost, and deployment plots, as well as a network map that shows the specific alternative technology deployment. The WTW emissions bar plots show the emissions (in kton CO_2) attributable to diesel (blue) and the alternative technology (green) operations, with the emissions intensity (in g CO_2/ton-mile) of diesel and the deployment scenario in question overlaid (yellow diamond). The levelized cost of operation bar plots show the LCO (in ¢/ton-mile) for diesel and the alternative technology in question. The key cost components are displayed, such as fuel (blue) for diesel, biofuel, e-fuel, and hydrogen; electricity (light blue) for battery; battery and hydrogen fuel tender car costs (orange); and charging/refueling station capital costs (red). The pie chart shows the deployment of the alternative technology as the share of ton-miles captured by diesel (blue) and by the alternative technology (green).

Section D.4.1 - Battery-Electric and Hydrogen

Figure 10 and Figure 11 show an example (hypothetical) deployment of a 400-mile range battery-electric locomotive technology for Western and Eastern railroads, respectively, needed to serve approximately 50% of their ton-mileage. Western rail networks are in general more expansive and require more charging facilities compared to Eastern railroads (57 vs 21). This also leads to difficulties in connecting the whole network and affects the overall cost of avoided emissions. The emissions and costs associated with battery-electric technologies are highly dependent on those of the electric grid and therefore sensitive towards the locations of the charging facilities. To reduce emissions by one kilogram of CO_2, it costs Western railroads \$0.11 and Eastern railroads \$0.09 under the examined deployment scenario.

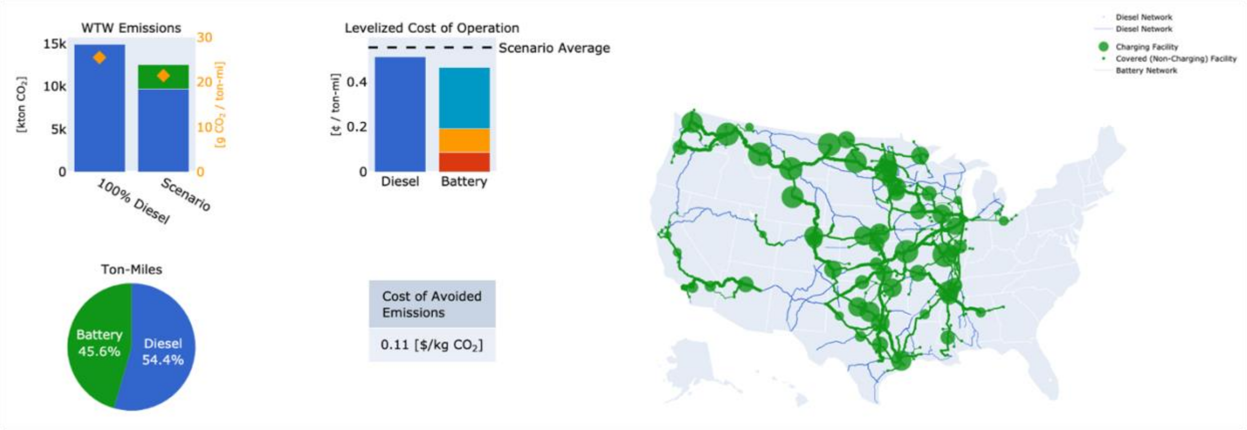


Figure 10 - Example of Battery-Electric Deployment for Western Railroads

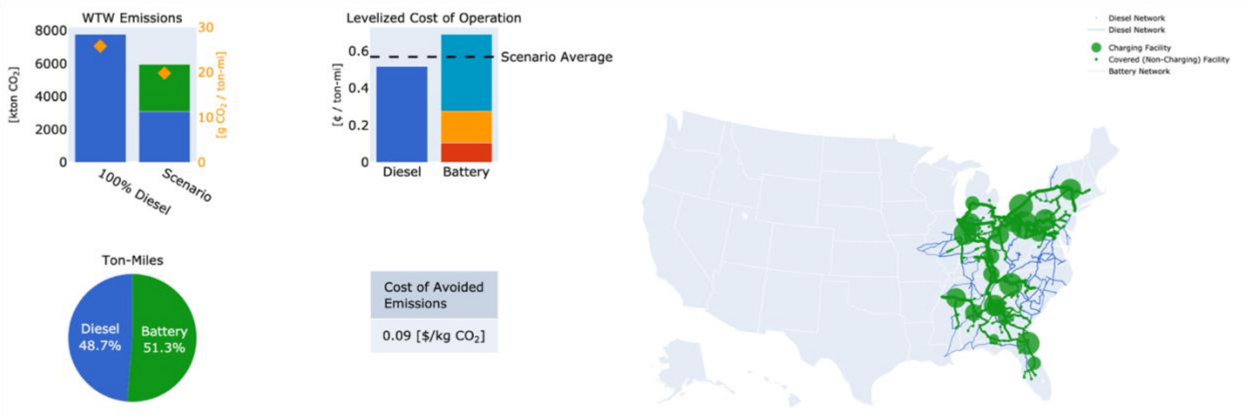


Figure 11 - Example of Battery-Electric Deployment for Eastern Railroads

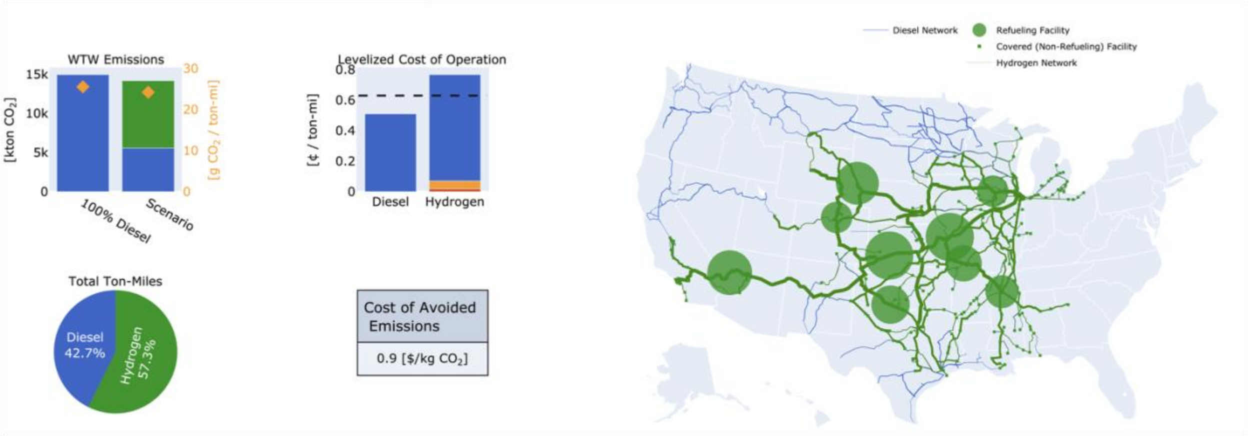


Figure 12 and Figure 13 show a corresponding example deployment of a hydrogen locomotive technology (with an approximate 1000-mile range) for Western and Eastern railroads, respectively, needed to serve approximately 55% of their ton-mileage. Though Western rail networks are in general more expansive than Eastern rail networks, the long range of this hydrogen locomotive diminishes the number of required refueling facilities compared to the battery case (9 for Western vs 3 for Eastern). Most notably, hydrogen locomotive operations are not considerably cleaner than diesel operations, as hydrogen fuel is primarily produced through natural gas reforming. Furthermore, liquid hydrogen fuel exhibits high costs, due to the energy intensive process of onsite liquefaction. The relatively low emissions reductions and high incremental costs lead to high costs of avoided emissions. To reduce emissions by one kilogram of CO_2 through hydrogen operations, it costs Western railroads \$0.9 and Eastern railroads \$1.05 under the examined deployment scenario. More environmentally friendly (e.g., solar, renewable, nuclear powered) and economical processes for hydrogen production would be required to help hydrogen decarbonize the rail freight sector.

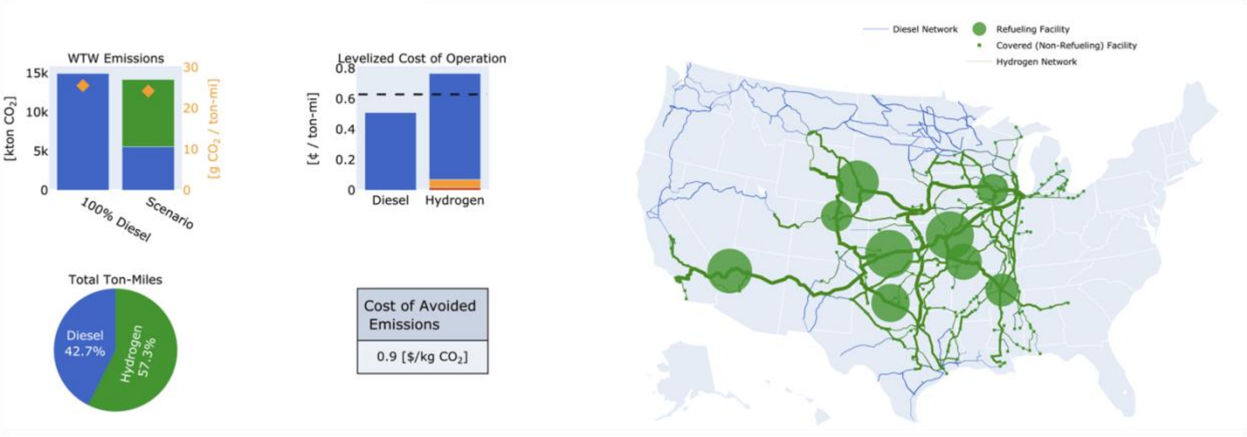


Figure 12 - Example of Hydrogen Deployment for Western Railroads

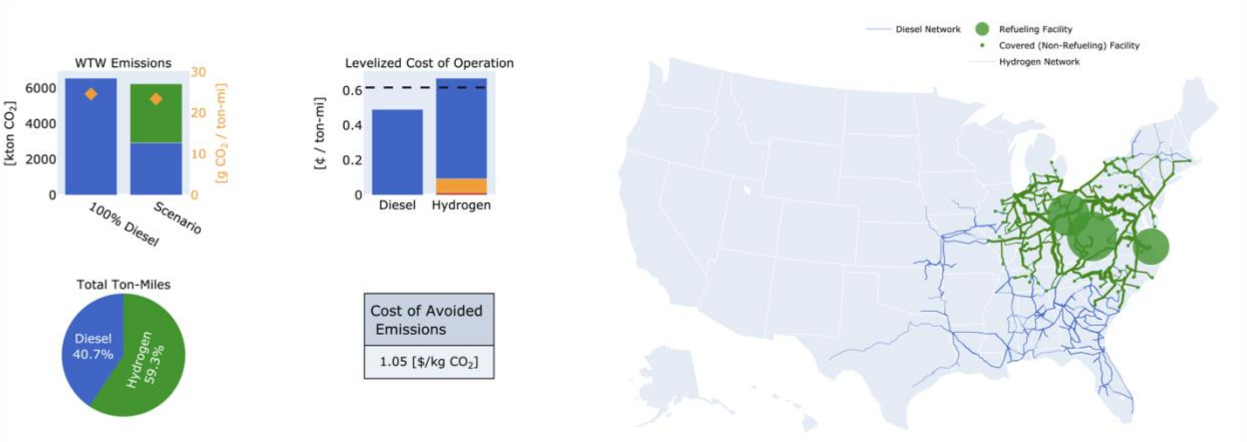


Figure 13 - Example of Hydrogen Deployment for Eastern Railroads

Section D.4.2 - Biofuel and E-fuel

For drop-in fuels such as biofuels and e-fuels, fuel blends are assumed to be applied uniformly across all locomotives on the network. Figure 14 and Figure 15 show the results for 50% deployment of biofuels in Western and Eastern railroads, respectively. This deployment of biodiesels would contribute to a 36% reduction in emissions (for both railroad groups) relative to diesel, with a cost of $0.13 per kilogram of CO2 reduced. Figure 16 and Figure 17 show the results for 50% deployment of e-fuels in Western and Eastern railroads, respectively. As e-fuels are nearly carbon neutral, they would provide a more promising environmental solution than biofuels, albeit at significantly greater cost (nearly double that of conventional diesel). Their deployment in this scenario would contribute to a 50% decrease in carbon emissions at a cost of $0.22 per kilogram of CO2 eliminated.

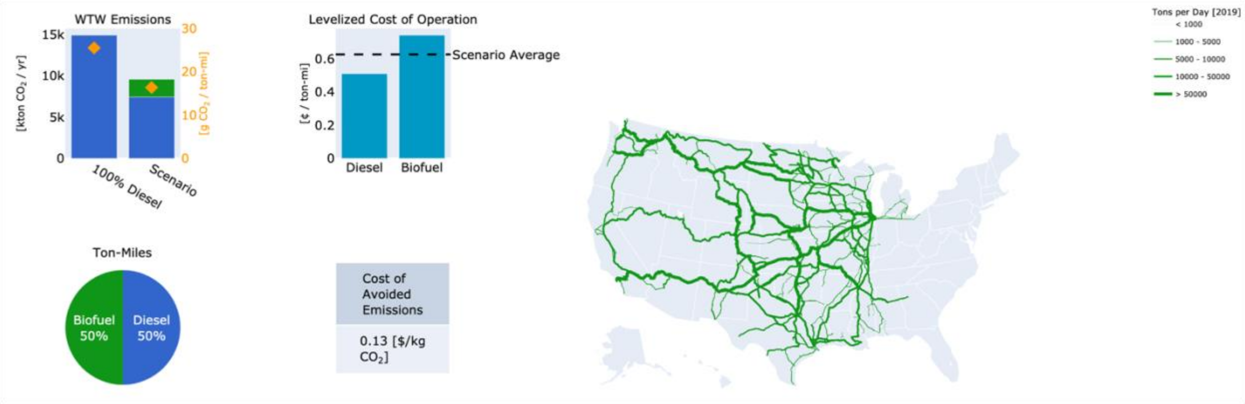


Figure 14 - Example of 50% Biodiesel Deployment for Western Railroads

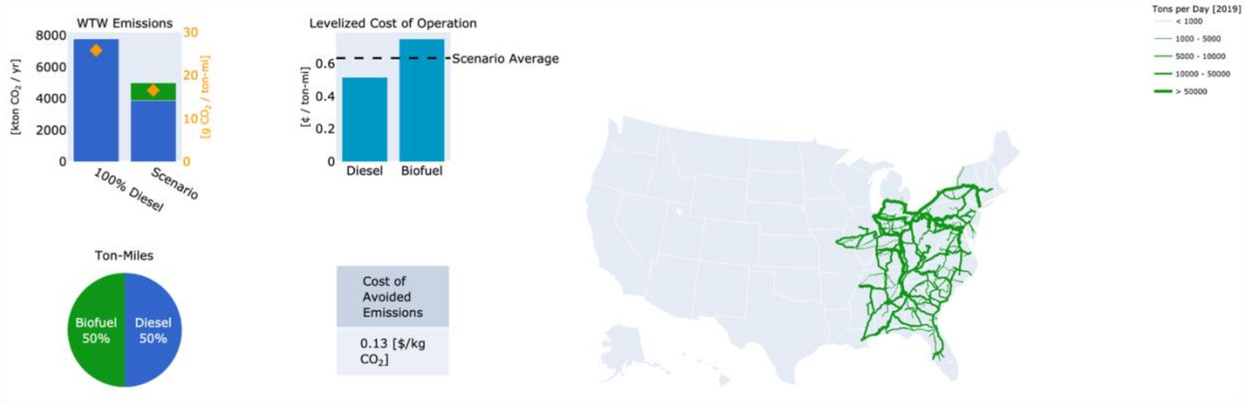


Figure 15 - Example of 50% Biodiesel Deployment for Eastern Railroads

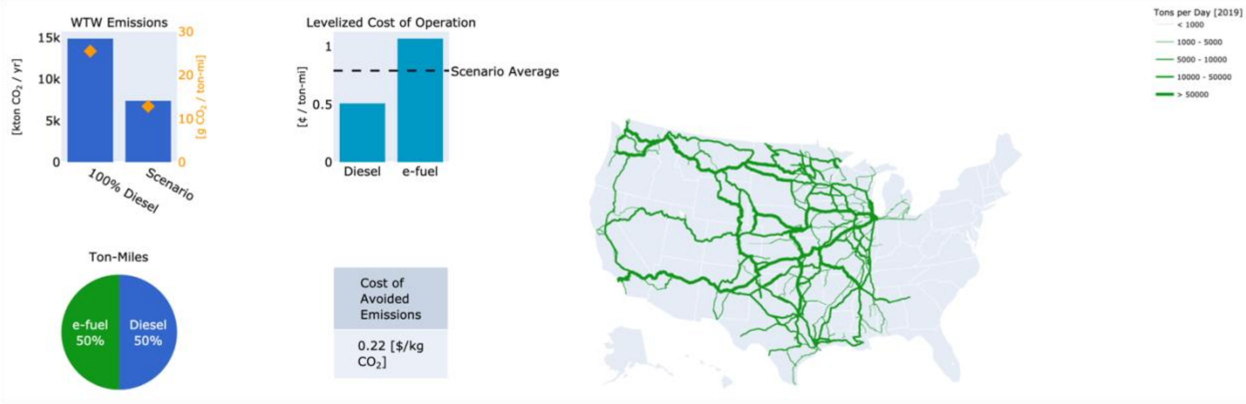


Figure 16 - Example of 50% E-fuel Deployment for Western Railroads

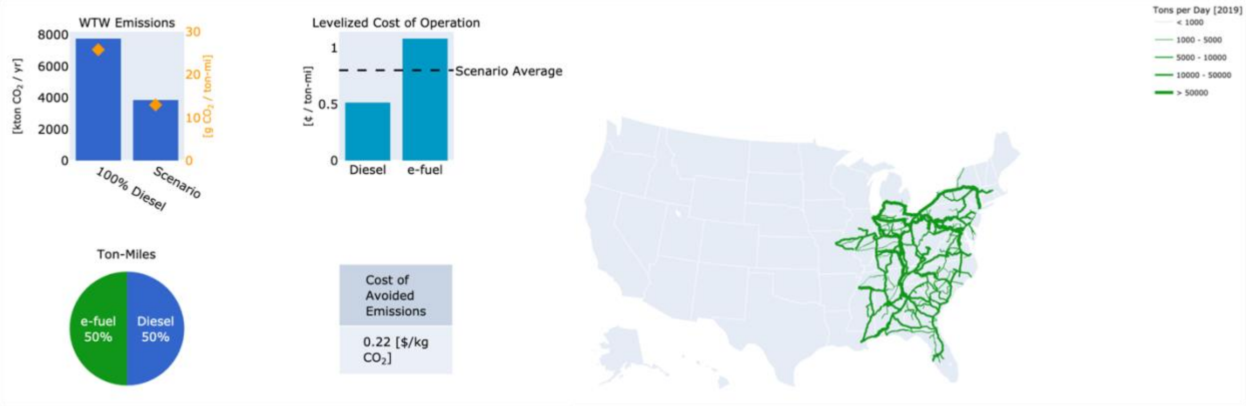


Figure 17 - Example of 50% E-fuel Deployment for Eastern Railroads

Section D.5 - Scenario Comparison

This section evaluates the optimization and simulation results of the battery-electric deployments, demonstrating the framework’s potential in analyzing and comparing across scenarios.

Section D.5.1 - Deployment Percentage

A key functionality of our framework implemented in the dashboard allows users to input different deployment percentages to simulate, optimize, and evaluate different intermediate stages of a technology’s roll-out.

Figure 18-Figure 20 show the results for Eastern railroads under (approximately) 30%, 50%, and 100% target deployments. As the deployment percentages increase, the network coverage increases drastically, with the number of facilities growing from 12, through 21 to 167 at 100%. This highlights the high number of facilities required to serve the “last miles” of the rail network. While emissions decrease rather proportionally with the extent of the roll-out, the initial LCO at 30% deployment is considerably high, due to starting costs on capital infrastructure projects. Higher deployment percentages enable economies of scale to reduce the costs of avoided emissions from \$0.17/kg CO$_2$ at 30% to \$0.09/kg CO$_2$ at 50%.

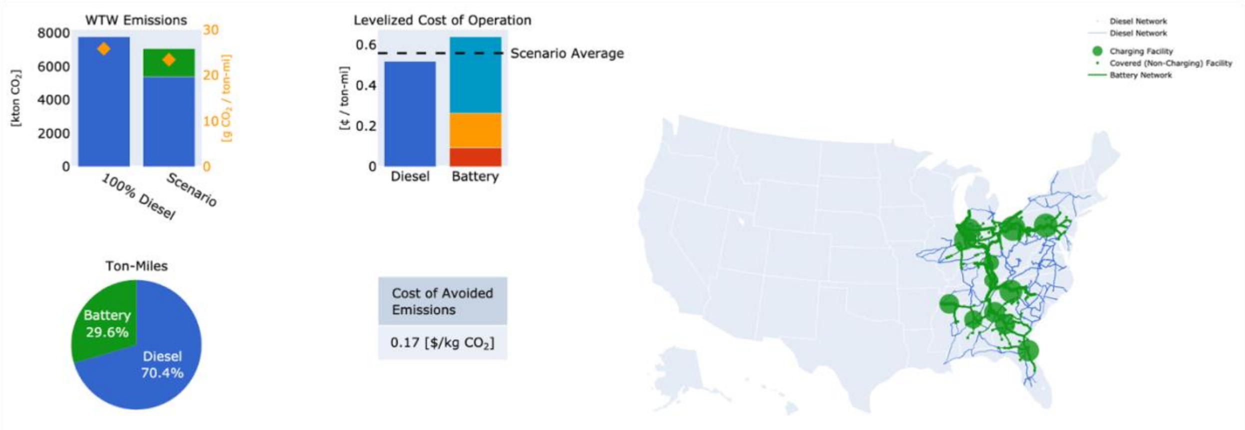


Figure 18 - Results for Eastern Railroads with 30% Target Deployment Percentage

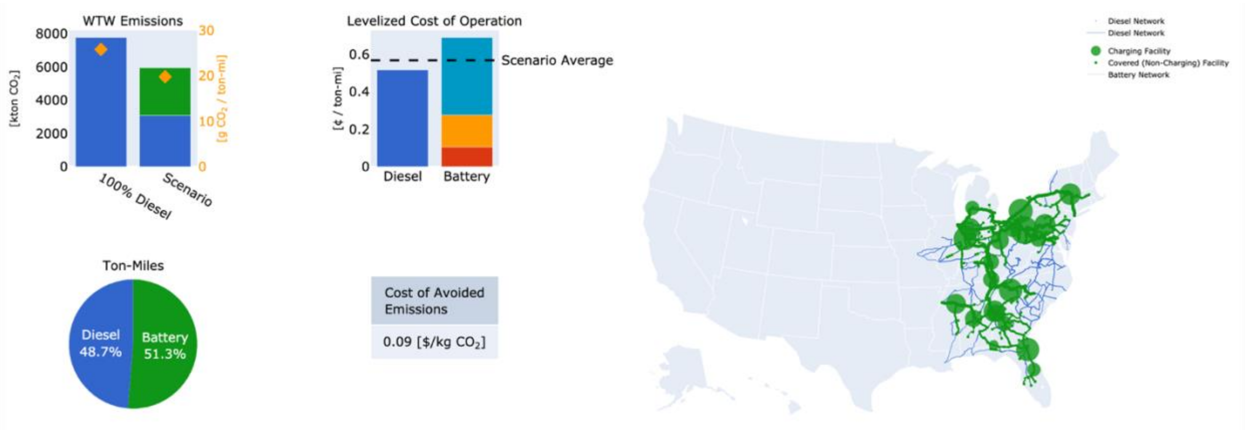


Figure 19 - Results for Eastern Railroads with 50% Target Deployment Percentage

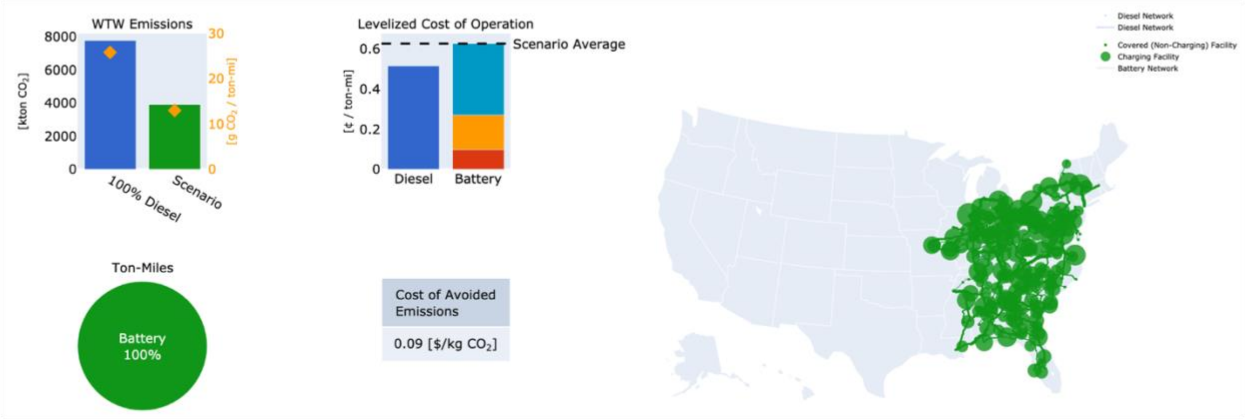


Figure 20 - Results for Eastern Railroads with 100% Target Deployment Percentage

Section D.5.2 - Range

In the context of battery-electric deployment, locomotive range affects both the economics and environmental performance of a particular scenario.

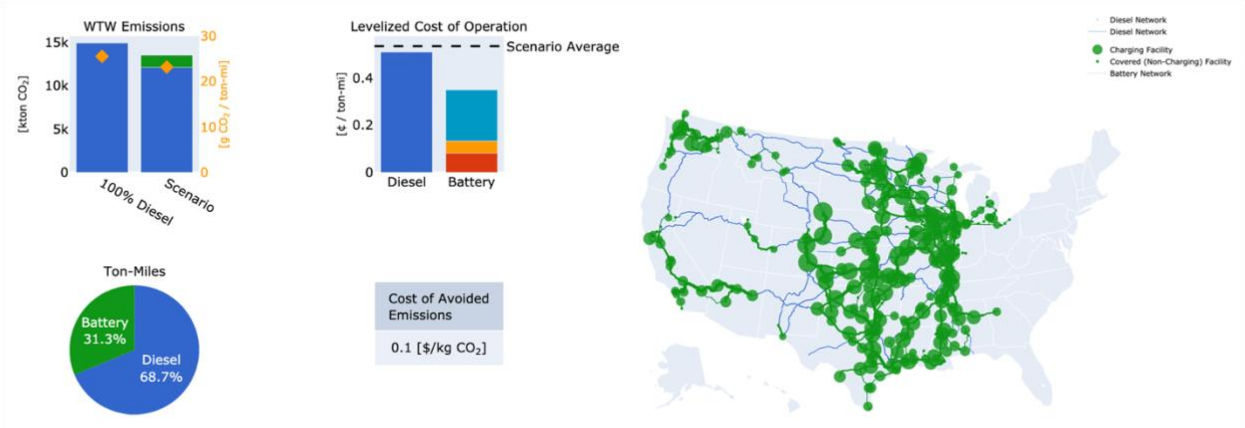


Figure 21-Figure 23 illustrate the key trade-off associated with locomotive range. Increasing the locomotive range increases the energy storage capacity per locomotive and thus increases the total battery purchase and operating costs. However, an increase in locomotive range allows for greater reach and fewer charging stations to be deployed, reducing the total facility capital costs, while increasing the network penetration of service that can be provided. This trade-off is illustrated by the costs of avoided emissions which are \$0.10/kg CO$_2$ at 200-mile range, \$0.11/kg CO$_2$ at 400-mile range, and \$0.06/kg CO$_2$ at 800-mile range. The stark decrease in the cost of avoided emissions between the 400-mile and 800-mile range cases comes from the consolidation of freight along key corridors that allows emissions reductions to go from 16% with 400-mile range locomotives to 46% with 800-mile range locomotives. Furthermore, locomotives with longer ranges (e.g., 800 miles) can significantly reduce emissions, as they can be used to decarbonize more energy intensive commodities (i.e., intermodal) that are typically shipped over long distances. Note that with locomotives with a 200-mile range, though a 50% target deployment level was set, only 31% of ton-miles could be served by battery-electric locomotives, due to the insufficient range on the expansive Western railroad network. The flexibility of the range parameter supports the sensitivity analysis of optimal technology range values.

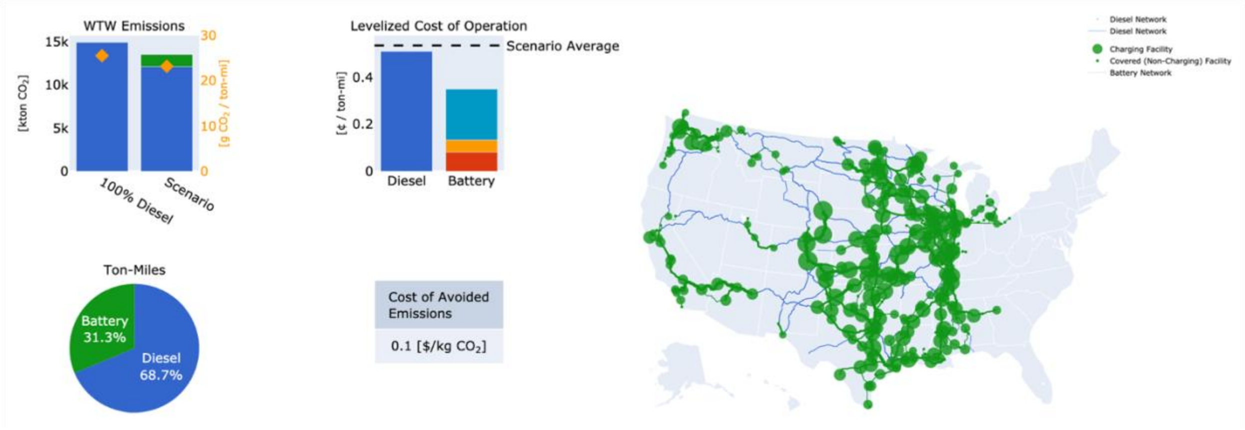


Figure 21 - Results for Western Railroads with 200-mile Range

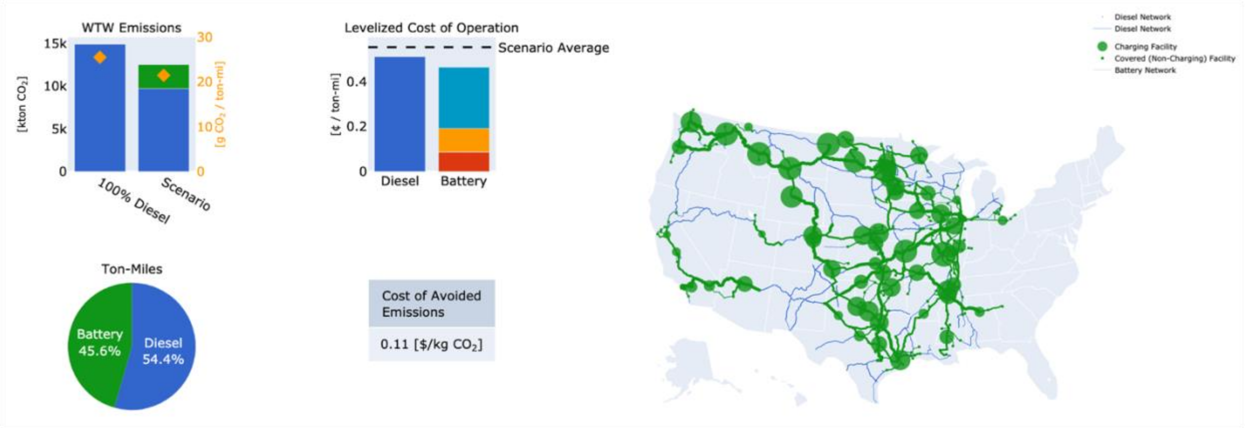


Figure 22 - Results for Western Railroads with 400-mile Range

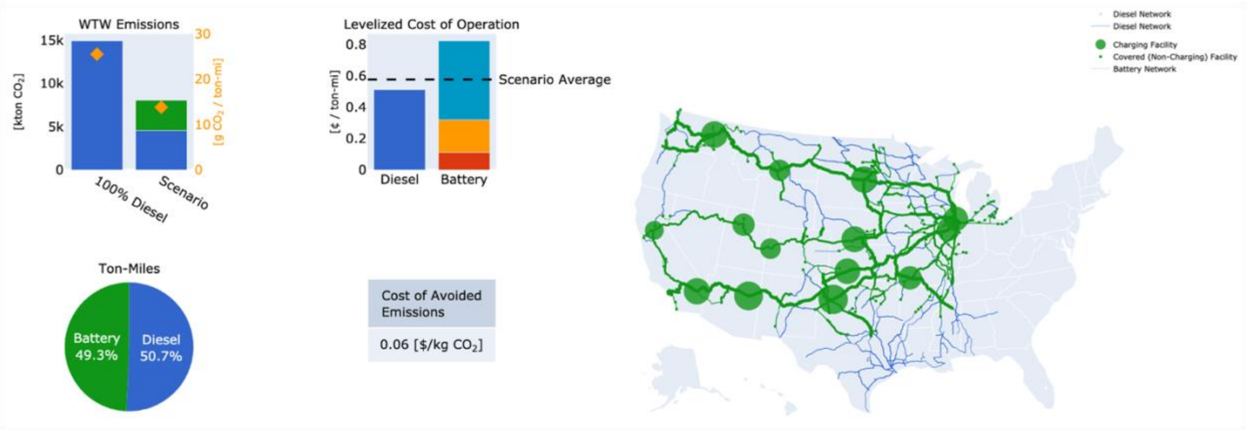


Figure 23 - Results for Western Railroads with 800-mile Range

Section D.6 - Measurement of Operational Impacts

This section provides numerical results and analysis of the operational performance metrics that were used to evaluate scenarios, namely delay times and costs and commodity-specific deployment differences.

Section D.6.1 - Delay

In the scenarios that have been analyzed, the time spent charging constitutes the dominant component of the total delay for battery-electric locomotive deployments. This is primarily due to the technological challenges surrounding innovations in charging speeds and battery energy densities. Additionally, freight movements require massive amounts of energy, making the battery capacities larger than those used for passenger vehicles, and are therefore slower to charge. The incremental time associated with queuing, on the other hand, remains relatively small and well bounded. These manageable queuing times are a result of our intuitive approach to size facilities to ensure they can meet peak demand, which gives average daily operations the extra slack needed. With the total average delay time, we can apply estimates of the time-value of freight to capture the economic impact of the delay to operations. These results are shown for an example scenario (a Western railroad with a 400-mile battery locomotive technology, deployed over 80% of total ton-miles) in Figure 24, with the delay costs factored into the levelized cost of operations (LCO) metric. Delay costs constitute 33% of the total levelized cost of operation for this battery technology deployment scenario. However, as we increase the technological range, these delay costs decrease as locomotives need to charge less frequently during their trips. Figure 25 shows the delay costs decrease from 33% to 16% of the levelized cost of operation if battery locomotive ranges are increased from 400 to 800 miles.

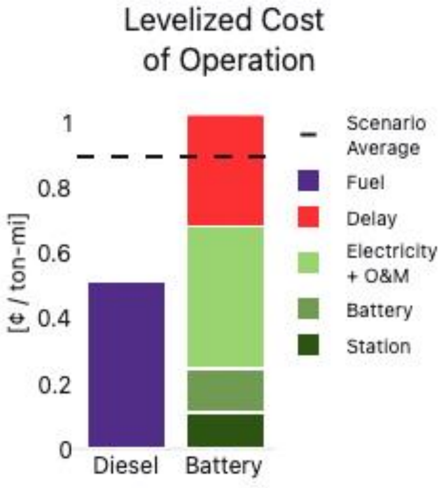


Figure 24 - LCO with delay costs included for a Western railroad with 400-mile range battery locomotives for 80% of total ton-miles.

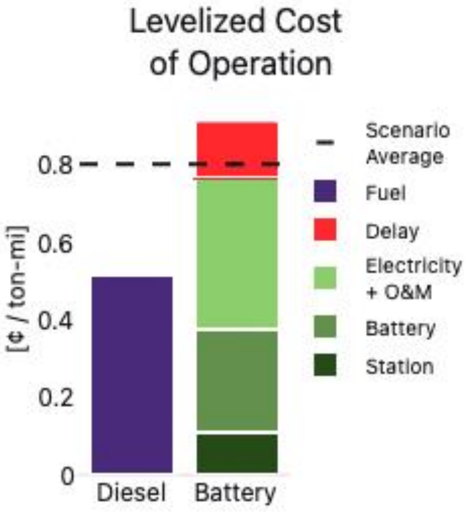


Figure 25 - LCO with delay costs included for a Western railroad with 800-mile range battery locomotives for 80% of total ton-miles.

Section D.7 - Deployment Profiles

Results can be run for a range of desired deployment percentages (alternative technology penetration rate as a percentage of ton-miles captured) to understand its relationship with key components such as emissions reduction potential, cost components, and operational impacts. For example, we can examine the relationship between deployment percentage and emissions reductions as well as between deployment percentage and number of facilities and chargers needed. Due to a “dirty” electric grid, at full deployment, battery-electric locomotives can only reduce emissions by 50% for the scenario shown in Figure 26. Furthermore, the results highlight the difference between the role of chargers and charging facilities—chargers meet energy demand, and thus grow linearly with deployment percentage, while charging facilities serve specific rail corridors, which requires a drastic increase for serving the last-mile routes. Overall, deployment profiles are valuable for enabling stakeholders to better understand the potential impact and implications of deploying alternative technologies, such as battery-electric locomotives, at different levels of penetration.

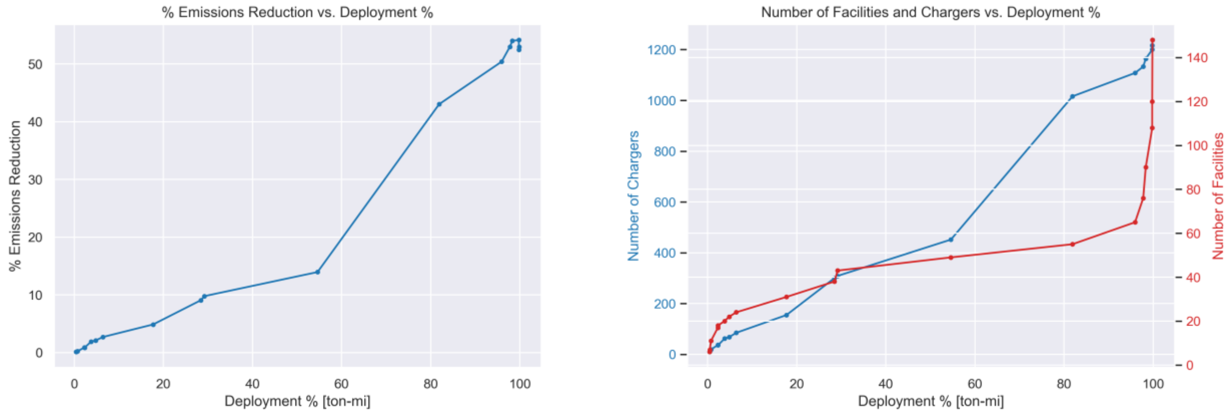


Figure 26 - Results for varying deployment penetration for a Western railroad for battery locomotives with 400-mile ranges on average, assuming a cleaner, but not fully renewable, electric grid

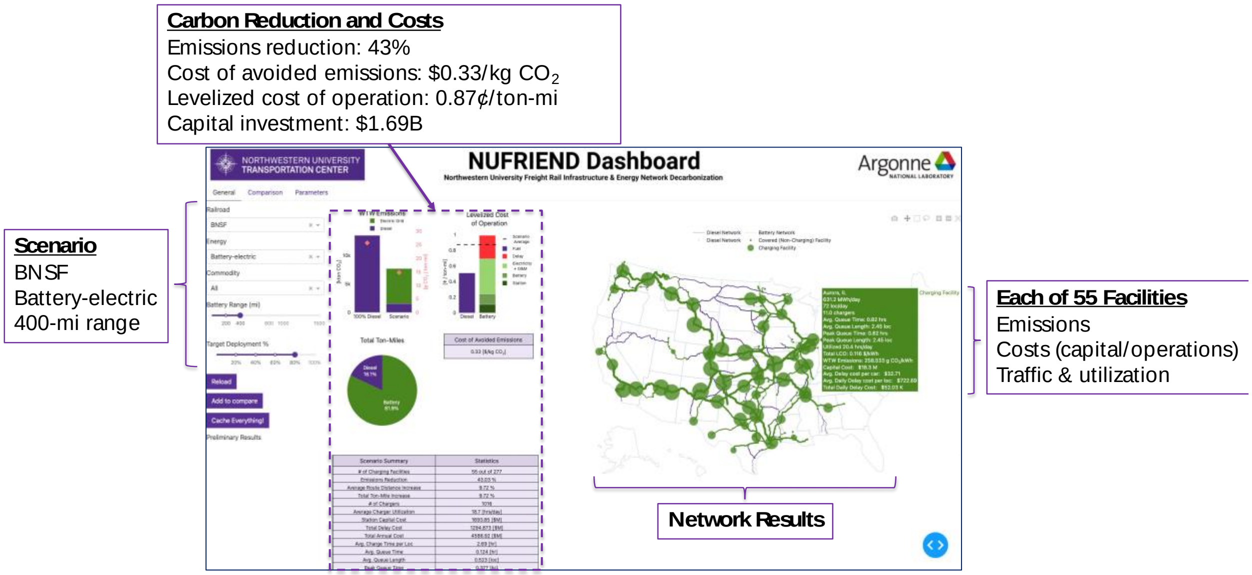
Section E - Project Outputs

NUFRIEND Dashboard

The NUFRIEND Dashboard features many degrees of freedom for the modeling of fuel technology deployment scenarios to capture uncertainty in future conditions:

- All Class I railroad networks
- All primary commodity groups from the AAR
- Any desired deployment percentage (in ton-miles served by the fuel technology)
- Locomotive fuel technologies:
    - Diesel
    - Biofuel
    - E-fuel
    - Battery – variable range
    - Hydrogen – variable range

Figure 27 shows an example of the NUFRIEND dashboard and highlights the information available in each of the charts generated for a particular scenario. Aggregate scenario-wide results are shown on the left-hand side of the dashboard in the bar and pie plots and summary tables. Results are also shown down to the facility and track levels with the green colored network denoting the coverage of the alternative fuel technology. Users can hover over the network components to examine more granular information such as traffic volume, number of chargers, and station utilization.



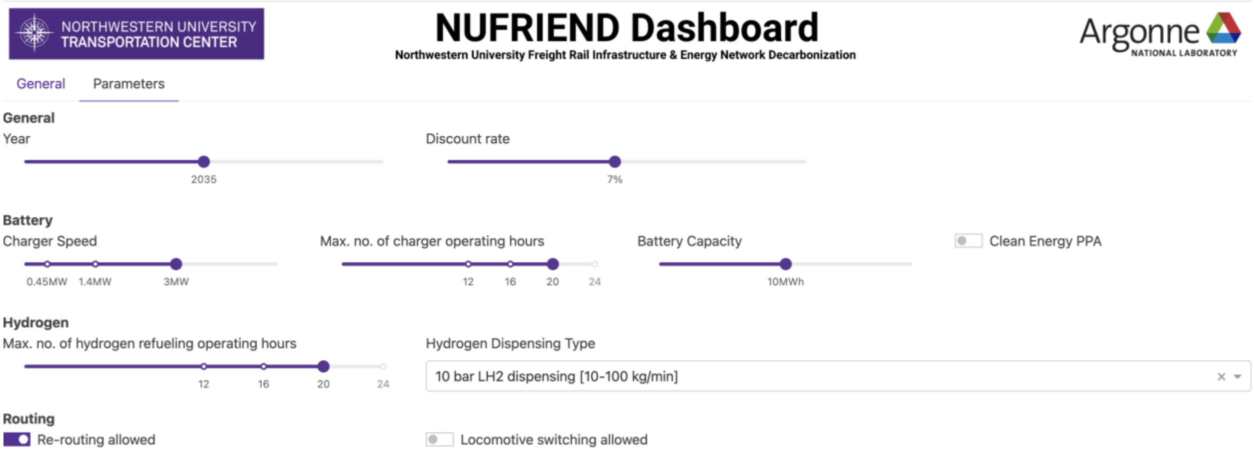
Carbon Reduction and Costs
Emissions reduction: 43%
Cost of avoided emissions: $0.33/kg CO_2
Levelized cost of operation: 0.87¢/ton-mi
Capital investment: $1.69B

Scenario
BNSF
Battery-electric
400-mi range

Each of 55 Facilities
Emissions
Costs (capital/operations)
Traffic & utilization

Network Results

Figure 27 - NUFRIEND Dashboard Example



General
Year: 2035
Discount rate: 7%

Battery
Charger Speed: 0.45MW, 1.4MW, 3MW
Max. no. of charger operating hours: 12, 16, 20, 24
Battery Capacity: 10MWh
○ Clean Energy PPA

Hydrogen
Max. no. of hydrogen refueling operating hours: 12, 16, 20, 24
Hydrogen Dispensing Type: 10 bar LH2 dispensing [10-100 kg/min]

Routing
● Re-routing allowed
○ Locomotive switching allowed

Figure 28 - NUFRIEND Dashboard Parameter Pane

The dashboard enables a high degree of freedom to cater for users’ operation needs. Users can input datasets from their actual operations, including their network map, energy source costs and technological parameter forecasts. Other parameters that allow user modification on the dashboard (Figure 28) include:

- Scenario settings
  - Railroad networks
  - Energy source
  - Energy source-specific settings (e.g., battery range)
  - Primary commodity groups from the AAR
  - Desired deployment percentage (in ton-miles served by the fuel technology)

- General
    - Year
    - Discount rate
- Battery
    - Charger speed
    - Maximum number of charger operating hours
    - Battery capacity
    - Clean Energy PPA
- Hydrogen
    - Maximum number of hydrogen refueling station operating hours
    - Hydrogen dispensing type

Technology-to-Market

With the production of the NUFRIEND framework and dashboard, further initiatives in user engagement and feedback were implemented to refine the fully functioning simulation framework. Apart from the Industry Advisory Board (IAB), whose members represent an important class of end-users for the open-source tool, exploration on partnership with railroads was conducted and noted as valuable follow-on opportunities. Discussions were held with BNSF, UP and CSX regarding using tools in scenario exploration, though they could not be carried out in the initial project period. Discussion was also initiated with a short line railroad representative (Anacostia Rail Holdings) with respect to an extension of the work to short line networks. Continued discussions with the railroads, locomotive OEMs, and railroad executives will prove extremely valuable for any follow-on prospects and continued validation and use of the developed NUFRIEND framework.

Journal Articles

1. Hernandez, Adrian and Ng, Max T.M., C. Siddique, P. L. Durango-Cohen, A. Elgowainy, H. S. Mahmassani, M. Wang, Y. Zhou, (In press) "Evaluation of rail decarbonization alternatives: Framework and application," Transportation Research Record, 2023.

Presentations

Our work has been presented at various conferences throughout the course of the project. Presentations have covered the technical framework, analysis of findings, and live dashboard demonstrations, as listed in Table 4.

Table 4 - List of Presentations

Date	Event
May 23-25, 2022	2022 ARPA-E Summit in Denver, Colorado
Jun 5, 2022	4th International Symposium on Infrastructure Asset Management in Evanston, Illinois
Aug 30, 2022	Meeting with short line railroad (Anacostia) representative
Oct 16, 2022	2022 INFORMS Annual Meeting in Indianapolis, Indiana
Nov 2, 2022	Railroad Environmental Conference in Champaign, Illinois
Nov 16-17, 2022	Northwestern University Transportation Center Business Advisory Council Meeting in Evanston, Illinois

Jan 8-12, 2023	Transportation Research Board 102nd Annual Meeting in Washington, D.C.

Status Reports

Quarterly reports have been submitted to the project sponsor from the start of the project through the effective end date.

Media Reports

A series of informational pieces analyzing several interesting project dimensions (battery-electric range, biofuels vs. e-fuels, deployment profiles, and cost vs. emissions objectives) has been produced and published online.[3] Additionally, to publicize the functionalities and power of the NUFRIEND tool, a 3-minute demonstration video has been produced, capturing the five essential features of the dashboard. The video, which will also be provided for users, can be accessed online.[4] Finally, a user guide for the NUFRIEND Dashboard has been produced and made available for public access.[5]

Collaborations Fostered

To assist with the project's technology-to-market initiatives, the Northwestern University Transportation Center leveraged its existing Business Advisory Council and industry connections to put together an Industry Advisory Board (IAB) for the project, the members of which are shown in Table 5. The IAB members represent individuals across multiple companies and entities that operate in the rail sector, providing valuable perspectives on the challenges and opportunities to decarbonize freight rail. Several group and individual meetings were held with IAB members to gain valuable insights and showcase the dashboard and framework for feedback, to ensure its value for all stakeholders, as shown in Table 5.

Table 5 - Members of Industry Advisory Board

Member	Title	Organization	Information	Meeting
John Gray	Senior VP –Policy & Economics	AAR	Policy; relevant AAR working groups and data	7/15/22, 3/1/22, 12/15/21, 11/10/21
Jamie Helmer	Director Fuel Efficiency	NSC	Alternative fuels and locomotive efficiency	7/15/22
April Kuo	Director - Technology Services	BNSF	Rail Operations and scheduling	/
Adam Longson	VP - Energy	CSXT	Energy source impacts	7/15/22, 11/10/21

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[3] https://www.transportation.northwestern.edu/research/featured-reports/locomotives.html
[4] https://drive.google.com/file/d/1Dx1jz3Y2dil5v-HC94EwBk4utXNnyPcj/view?usp=sharing
[5] https://www.transportation.northwestern.edu/docs/research/featured-reports/nufriend_dashboard_user_guide.pdf

John Lovenburg	VP, Environmental	BNSF	Wabtec battery pilot; Technology deployment considerations	7/15/22, 3/15/22, 2/16/22, 11/10/21
Roger Nober	EVP - Law & Corporate Affairs, CLO	BNSF	Regulations	7/15/22
Mike Swaney	Director, Operations Analytics	BNSF	New energy technology	7/15/22
Barbara W. Wilson	Rail Executive	/	Perspectives of shortline railroad	7/15/22, 11/10/21
Norman Carlson	Vice Chair	Metra	Passenger rail interest	7/15/22, 11/10/21
Scott Remington	VP Operations - M&A	OmniTRAX	Perspectives of shortline railroad	7/15/22

Websites Featuring Project Work Results

The NUFRIEND Dashboard has been made available for public use online.[6] Additionally, information on the project and objectives, informational reports on key findings, a list of related publications, and a user guide and demo video are hosted on a dedicated NUTC webpage.[7] Information on the developed framework and results is also linked on Argonne National Library's GREET model webpage.[8]

Release Open-Source Code

Software code in Python 3.10 of the NUFRIEND dashboard has been published on GitHub with full documentation regarding the workflow and data input and output.[9]

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[6] https://nufriend.transportation.northwestern.edu

[7] https://www.transportation.northwestern.edu/research/featured-reports/locomotives.html

[8] https://greet.es.anl.gov/other.models

[9] https://github.com/maxtmng/nufriend

Section F - References

[1] "Sources of Greenhouse Gas Emissions," U.S. Environmental Protection Agency, 2022. [Online]. Available: https://www.epa.gov/ghgemissions/sources-greenhouse-gas-emissions

[2] "Freight Transportation Energy Use & Environmental Impacts," U.S. Department of Transportation, Bureau of Transportation Statistics, 2019.

[3] "U.S. Transportation Sector Greenhouse Gas Emissions Fast Facts," U.S. Environmental Protection Agency, EPA-420-F-21-049, 2021.

[4] "Freight Rail and Preserving the Environment," American Association of Railroads, 2022.

[5] T. Meyer, "Decarbonizing road freight transportation – A bibliometric and network analysis," *Transp. Res. Part Transp. Environ.*, vol. 89, p. 102619, Dec. 2020, doi: 10.1016/j.trd.2020.102619.

[6] J. Schofer, H. Mahmassani, M. Ng, and B. Johnson, "The U.S. Railroads and COVID-19: Keeping Supply Chains Moving," Northwestern University Transportation Center, May 2021. doi: 10.6084/m9.figshare.14773533.

[7] T. Solomon and N. Singer, "Freight Activity in the U.S Expected to Grow Fifty Percent by 2050," Bureau of Transportation Statistics, 2021. [Online]. Available: https://www.bts.gov/newsroom/freight-activity-us-expected-grow-fifty-percent-2050

[8] "Compilation of State, County, and Local Anti-Idling Regulations," U.S. Environmental Protection Agency, EPA420-B-06–004, 2006. [Online]. Available: https://www.epa.gov/sites/default/files/documents/CompilationofStateIdlingRegulations.pdf

[9] J. Saul, "Amazon and others commit to using zero-carbon shipping fuels by 2040," *Reuters*, 2021. [Online]. Available: https://www.reuters.com/business/sustainable-business/amazon-others-commit-using-zero-carbon-shipping-fuels-by-2040-2021-10-19/

[10] J. B. McCall, "Dieselisation of American Railroads: A case study," *J. Transp. Hist.*, vol. 6, no. 2, pp. 1–17, Sep. 1985, doi: 10.1177/002252668500600201.

[11] "Research & Investments Driving Tomorrow's Sustainable Locomotive Fleet," American Association of Railroads, 2022. [Online]. Available: https://www.aar.org/article/research-investments-driving-tomorrows-sustainable-locomotive-fleet/

[12] "Oppose Rail Electrification and Support Sensible Climate Policy," American Association of Railroads, 2021. [Online]. Available: https://www.aar.org/wp-content/uploads/2020/12/AAR-Electrification-Fact-Sheet.pdf

[13] F. Duffner, M. Wentker, M. Greenwood, and J. Leker, "Battery cost modeling: A review and directions for future research," *Renew. Sustain. Energy Rev.*, vol. 127, p. 109872, Jul. 2020, doi: 10.1016/j.rser.2020.109872.

[14] N. D. Popovich, D. Rajagopal, E. Tasar, and A. Phadke, "Economic, environmental and grid-resilience benefits of converting diesel trains to battery-electric," *Nat. Energy*, vol. 6, no. 11, pp. 1017–1025, Nov. 2021, doi: 10.1038/s41560-021-00915-5.

[15] M. Wang *et al.*, "Summary of Expansions and Updates in GREET® 2021," Argonne National Lab.(ANL), Argonne, IL (United States), 2021.

[16] B. Stephens, "Wabtec's FLXdrive battery-electric locomotive begins revenue tests on BNSF," *Trains*, 2021. [Online]. Available: https://www.trains.com/trn/news-reviews/news-wire/wabtecs-flxdrive-battery-electric-locomotive-begins-revenue-tests-on-bnsf/

[17] B. Jansen, "Progress Rail and Pacific Harbor Line Sign Agreement," Progress Rail, 2020. [Online]. Available:

https://www.progressrail.com/en/Company/News/PressReleases/ProgressRailAndPacificHarborLineSignAgreementForBatteryLocomotive.html

[18] K. South, “Union Pacific Railroad to Assemble World’s Largest Carrier-Owned Battery-Electric Locomotive Fleet,” *Union Pacific News Releases*, 2022. [Online]. Available: https://www.up.com/media/releases/battery-electric-locomotive-nr-220128.htm

[19] M. Luczak, “CP’s Hydrogen Locomotive Powers Up,” *Railway Age*, 2022. [Online]. Available: https://www.railwayage.com/mechanical/locomotives/cps-hydrogen-locomotive-powers-up/

[20] A. J. Scott, “Location-Allocation Systems: A Review,” *Geogr. Anal.*, vol. 2, no. 2, pp. 95–119, Sep. 2010, doi: 10.1111/j.1538-4632.1970.tb00149.x.

[21] M. L. Balinski, “Integer Programming: Methods, Uses, Computation,” p. 62, 1965.

[22] F. M. Vanek and E. K. Morlok, “Improving the energy efficiency of freight in the United States through commodity-based analysis: justification and implementation,” *Transp. Res. Part Transp. Environ.*, vol. 5, no. 1, pp. 11–29, 2000, doi: 10.1016/S1361-9209(99)00021-8.

[23] “Weekly Railroad Traffic,” American Association of Railroads, 2020. [Online]. Available: https://www.aar.org/whats-included-in-weekly-rail-traffic-categories/

[24] F. S. Hillier and G. J. Lieberman, *Introduction to operations research*, 9th ed. 9th ed.New York: McGraw-Hill Higher Education, 2010.

[25] “2019 Annual R-1 Report of Finances and Operations,” Surface Transportation Board, 2020. [Online]. Available: https://www.stb.gov/reports-data/economic-data/

[26] A. Burnham, Z. Lu, M. Wang, and A. Elgowainy, “Regional Emissions Analysis of Light-Duty Battery Electric Vehicles,” *Atmosphere*, vol. 12, no. 11, p. 1482, Nov. 2021, doi: 10.3390/atmos12111482.

[27] E. D. Frank, A. Elgowainy, K. Reddi, and A. Bafana, “Life-cycle analysis of greenhouse gas emissions from hydrogen delivery: A cost-guided analysis,” *Int. J. Hydrog. Energy*, vol. 46, no. 43, pp. 22670–22683, Jun. 2021, doi: 10.1016/j.ijhydene.2021.04.078.

[28] A. H. Lovett, C. T. Dick, and C. P. L. Barkan, “Determining Freight Train Delay Costs on Railroad Lines in North America,” p. 18.

[29] “2019 Carload Waybill Sample Reference Guide.” Surface Transportation Board, 2020.

[30] A. Elgowainy, A. Vyas, M. Biruduganti, and M. Shurland, “Railroad Energy Intensity and Criteria Air Pollutant Emissions,” p. 45, Oct. 2018.

[31] Y. Zhou, “Non-Light-Duty Energy and Greenhouse Gas Emissions Accounting Tool (NEAT): Documentation and User Guide for Updated Domestic Freight Component.” Argonne National Laboratory, 2018.

[32] “Utility Rate Database,” OpenEI. [Online]. Available: https://openei.org/wiki/Utility_Rate_Database

[33] R. S. Isaac, “Fuels and Fuel Technologies for Powering 21st Century Passenger and Freight Rail: Simulation-Based Case Studies in a U.S. Context,” UC Davis, 2020.

[34] J. Kelly *et al.*, “Cradle-to-grave lifecycle analysis of U.S. light-duty vehicle-fuel pathways: a greenhouse gas emissions and economic assessment of current (2020) and future (2030-2035) technologies.” Department of Energy, 2022. [Online]. Available: https://greet.es.anl.gov/publication-c2g_lca_us_ldv

[35] Federal Railroad Administration and Bureau of Transportation Statistics, “North American Rail Network,” 2022. Accessed: Nov. 01, 2021. [Online]. Available: https://www.bts.gov/maps

[36] S. Peterson, “WebTRAGIS: Transportation Routing Analysis Geographic System User’s Manual,” ORNL/TM--2018/856, 1784200, May 2018. doi: 10.2172/1784200.

[37] A. T. Wijayanta, T. Oda, C. W. Purnomo, T. Kashiwagi, and M. Aziz, “Liquid hydrogen, methylcyclohexane, and ammonia as potential hydrogen storage: Comparison review,” *Int. J. Hydrog. Energy*, vol. 44, no. 29, pp. 15026–15044, Jun. 2019, doi: 10.1016/j.ijhydene.2019.04.112.