Final Scientific/Technical Report

NC State University
Final Scientific/Technical Report
Multi-Decadal Decarbonization Pathways for U.S. Freight Rail
DE-AR0001471

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Public Executive Summary

A-STEP is a first-of-its-kind, integrated, open-source software tool aimed at guiding freight rail decarbonization decision-making. It has tools for studying energy use details for individual trains, networks of trains, battery and hydrogen charging stations, national energy sourcing and pricing, and overall decarbonization costs and environmental impacts. It gives analysts an ability to study the challenges of making such change happen. Completely amenable to analyst specified inputs and parameter values, it can be customized to provide outputs for a wide variety of assumptions about future energy conditions and technological advances. Written in Python, C++, and VB.Net, A-STEP can be implemented on both Windows and Linux-based platforms.

A-STEP comprises five analysis tools. They are:

- RailDecarb: examines the cost and environmental impacts of various decarbonization options and scenarios; for the years 2025 through 2050. It starts from energy pathways and economic forecasts and progresses through traffic assignment, energy intensity analysis, recharging facility assessment, and cost estimation to produce results that can help with decarbonization feasibility assessments. Technological evolution and least-cost capacity expansion form the basis for estimating levelized costs for this energy sourcing transformation, enabling the assessment of benefits and costs for decarbonization options.

- OneTrain: examines the energy consumption, travel time, and other consequences of opting for locomotive technologies other than diesel, including hydrogen, battery, and biodiesel.
- NeTrainSim: studies the energy implications of alternative energy sources in the context of network-level train activities, including the implications of meet-pass phenomena.
- ChargeSta: assesses the sizing and costs of facilities to recharge battery and hydrogen tenders.
- Temoa: examines the nationwide implications of shifting the freight railroad system from the use of diesel fuel to alternate energy sources.

Acknowledgements

Development of A-STEP would not have been possible without the funding provided by ARPA-E under the LOCOMOTIVES program. The authors are indebted to Robert Ledoux and his staff, especially Mirjana Marden and Apoorv Agarwal, for their interest in and support for our efforts. We are also indebted to the project advisory panel that helped guide the effort – Charlie Banks, James Kessler, Gordon Lovegrove, Dana Magliola, Walter Schuchmann, Gerhard Thelen, and especially David Connell, who was so instrumental in helping us obtain locomotive performance data. We must also thank David Humphrey, Jeremy Caldwell, and Brent Castor, of RailInc, who helped us understand car and locomotive movement record keeping; John Gray, of the AAR, who helped us understand how to portray the economics; and Raquel Wright and Judah Lynam, of FRA, who helped us secure very useful information about the rail network and its activity. Of course, the work is ours, and we take responsibility for the quality of our efforts.

The contributors to this effort were PIs George List, Jeremiah Johnson, Eleni Bardaka, Yue Cao, Andreas Hoffrichter, and Hesham Rakha; project team members Ishtiak Ahmed, Kyoungho Ahn, Ahmed Aredah, Christopher Beringer, Jianhe Du, Lynn Harris, Mohamed Hegazi, Rupal Mittal, Aditya Sinha, Tongchuan Wei, and Andreas Weiss; graduate students Ahmad Abdallah, Mehedi Hasnat, Vinson Guov, Derek Jackson, Mehrzad Mehrabipour, and Soumya Sharma; and undergraduates Emily Boldor, Adam Fleischer, Natalie Hackman, Wyat Hamilton, Logan Kemp, Layla Lukas and Owen Martin.

Accomplishments and Objectives

The objective of the A-STEP project was to create a toolset that would be useful for examining decarbonization options for the rail freight industry. That goal has been accomplished.

Several tasks and milestones were laid out in Attachment 3, the Technical Milestones and Deliverables, at the beginning of the project. The actual performance against the stated milestones is summarized here:

Table 1. Key Milestones and Deliverables.

Tasks	Milestones and Deliverables
Task 1: Single Train Performance Simulation (TPS)	**M1.1: Compile single train data for ten major alignments**: Complete data and information about 1) the track geometry for at least 10 alignments that will be used for model development, alignments with significant grades and curves, as in the lines on the west side of the Rocky Mountains, 2) fuel consumption data for one or more of those alignments, and 3) data for the energy delivery technologies to be explored. **Actual Performance**: We collected machine-readable track charts and employee timetables for nearly 20 alignments. Machine-readable datasets were created, and they are available for download on the publicly accessible A-STEP website which can be found easily using web search engines. We also obtained information about locomotive types, fuel consumption and performance. **M1.2: Test scenarios for single train defined**. The scenarios for validation are identified and they represent a wide range of operating conditions including extreme scenarios. **Actual Performance**: Ten test scenarios were ultimately developed. One was a hypothetical 200-mile-long alignment with varying grades and curvature and one significant crest. The other nine are nearly 700 miles long and have grades and curves that are typical of the nine Temoa regions. **M1.3: Performance metrics for single train**. Identify target performance metrics. These may include computational performance (i.e., hardware specifications, computing cost, and solution time) as well as solution quality (e.g., the estimates of the time- and location-based power demand and energy consumption, including all losses and regenerative braking) of trains operating over the alignments selected for model development. As an example, if battery technology were the energy source, this would mean the time- and location-based power 1) applied at the wheels, 2) delivered to the traction motors, 3) drawn from the battery, and 4) supplied by the battery. **Actual Performance**: Our most important metric became the second-by-second values of resistance, tractive effort, acceleration, speed, and power for the train and its locomotives and cars. Of greater interest, and used as well, were metrics derived from this information like total energy consumption, the PDFs / CDFs of power demand, and travel times. Moreover, based on these metrics, the trailing tonnage, and the length of the alignment, levelized metrics can also be obtained like KWH/GTMFuel consumption data for nearly 1000 trains traversing specific alignments was obtained from the Union Pacific Railroad. These data were used to check the energy consumption predictions of the model. **M1.4: Complete single train design report**. The document on the plan for model development data, and details about the methods to be used to model train control

Tasks	Milestones and Deliverables
	and energy power delivery is submitted for PD approval. **Actual Performance**: The single train tool, called OneTrain, was created and a document describing it was prepared, submitted, and approved. **M1.5: Go/No-Go: Functioning single train model and documentation report**. The single train model and its data and methods, including the integration of train control and energy power delivery is complete. Performance metric defined in M1.3 assessment validated through module testing scenarios defined in M1.2. **Actual Performance**: The Go/No-Go decision was affirmative. The project continued to progress to closure.
Task 2: Multi-Train Network Simulation	**M2.1: Compile and document multi-train data**. The data and information assembled for developing the network-level macroscopic simulation model. **Actual Performance**: Electronic copies of track charts and employee timetables were collected for nearly 20 alignments. From these "pdfs", machine-readable datasets were created. Information was also obtained about locomotive types, fuel consumption and performance. This information can be found in the OneTrain Excel workbook. All this information is available for download on the publicly accessible A-STEP website which can be found easily using web search engines. **M2.2: Test scenarios for multi-train defined**. The scenarios for validation are identified and they represent a wide range of operating conditions including extreme scenarios. **Actual Performance**: Ten test scenarios were ultimately developed. One was a hypothetical 200-mile-long alignment with varying grades and curvature and one significant crest. The other nine are nearly 700 miles long and have grades and curves that are typical of the nine Temoa regions. **M2.3: Performance metrics for multi-train**. Identify target performance metrics. These may include computational performance (i.e., hardware specifications, computing cost, and solution time) as well as solution quality such as the time- and location-based power demand for all trains operating in a region (at the spatial resolution of the Temoa – see Task 4). If the technology being considered were hydrogen fuel cells, this would mean the time-based power demand seen by all the fuel cells in a given region. **Actual Performance**: Fuel consumption data for nearly 1000 trains traversing specific alignments was obtained from the Union Pacific Railroad. This data was used to check the energy consumption predictions of the model. **M2.4: Complete multi-train network design report**. The data sources and methods to be used to model a multi-train network, considering train departures, train movement, longitudinal train motion, and resolution. **Actual Performance**: The multi-train tool, called NeTrainSim was created; a report was prepared, submitted, and accepted.

Tasks	Milestones and Deliverables
	M2.5: Functioning network model and documentation report. The completed network model, its data and methods are complete. Performance metric defined in M2.3 assessment validated through module testing scenarios defined in M2.2. **Actual Performance**: The model was created along with a documentation report. Both can be downloaded from a publicly accessible website that can be found and accessed easily using web search engines.
Task 3: Infrastructure Requirements	**M3.1: Complete infrastructure requirements design report**. Details on the data sources and methods used to determine the infrastructure requirements with proper consideration to both on-board and stationary requirements. **Actual Performance**: A tool was developed for sizing charging stations for both battery and hydrogen tenders. The design report for preparing this tool was prepared, submitted, and approved. **M3.2: Complete infrastructure requirements documentation report**. Infrastructure requirements module, including the technical specifications for on-board power electronics, energy storage, and stationary storage of energy carriers. A large-scale model describing the power electronics interfaced charging and grid systems is developed. Various DC-DC and AC-DC power electronic converters are modeled along with wiring and cooling requirements both onboard and wayside. Discharge rates and their associated voltage/current dynamics are quantified. The model provides information on grid support and stability analysis. For the chemical refueling infrastructure, production, storage, dispensing, and possible infrastructure for delivery are considered. The model uses realistic train operation profiles and charging/refueling siting locations. **Actual Performance**: The infrastructure requirements tool was developed, and a document describing it was prepared, submitted, and approved.
Task 4: Decarbonization Energy Pathways	**M4.1 Complete energy system design report**. An inventory of energy system data and a description of the energy system model with particular attention to the planned integration of the freight decarbonization pathways. **Actual Performance**: Temoa, the previously developed tool for analyzing nationwide, temporal energy flows, was used as the basis for a tool that could be used to look at energy flows in the national energy distribution system. A design report that described Temoa was prepared, submitted, and approved. **M4.2 Complete energy system documentation report**. The data and methods used in the energy system model and the relevant results by scenario, including spatially and temporally resolved renewable energy resources, average and marginal electricity emissions factors and prices, and location and capacity of stationary storage, and rail-related greenhouse gas emissions are reported. The model determines the optimal sizing of components and their associated cost. It estimates the marginal emissions

Tasks	Milestones and Deliverables
	avoided by running motive power on distributed, renewable energy rather than from the broader energy system. **Actual Performance**: This document was prepared, submitted, and approved.
Task 5: Probabilistic Cost Modeling	**M5.1 Complete cost modeling design report**. An inventory of data and methods to be used in the cost modeling, accounting for motive power technology, energy consumption, infrastructure, and operations reported. **Actual Performance**: A costing module was prepared as part of the RailDecarb tool. A document describing how that module would be created was prepared, submitted, and approved. **M5.2 Complete cost modeling documentation report**. This report will present the data and methods to be used in the probabilistic cost model, with details on the treatment and impact of uncertainty and interpretation of the results to inform cost targets and the most relevant drivers of the total cost reported. The cost model will meet ARPA-E requirements for the quantification of costs related to items such as 1) technological development, 2) modification of the locomotive fleet, 3) modifications to the rail system to accommodate the demand scenarios (e.g.., changes to locomotive and freight car fleet sizes, temporally and spatially adjusted levels of freight service, and expansion/ contraction of the network infrastructure), and 3) creation and operation of the energy delivery system. Regarding the latter, it will capture the costs of energy storage, fuel and energy acquisition, non-fuel O&M, and logistical modifications. Simple industry accepted unit costs (e.g., $$ per track mile, per freight car, or per basic locomotive) will be used to assess any costs of modifying the rail system to accommodate the projected service demands. It will report total and levelized costs (e.g., per ton-mile or per car-mile). It will quantify the cost-effectiveness of decarbonization. It will account for policies, such as carbon taxes or fees, that might incentivize decarbonization. **Actual Performance**: The costing module was created, and a document describing it was prepared, submitted, and approved.
Task 6: Freight Demand Modeling	**M6.1 Complete freight demand scenarios design report**. The data sources and econometric methods used to create freight demand models under a range of future scenarios which consider ranges of economic growth, alternative trucking technologies, and fuel prices. **Actual Performance**: A module for creating freight demand scenarios was created and integrated into the RailDecarb tool. This document described how that module would be created. The document was prepared, submitted, and approved. **M6.2 Determine at least six freight demand scenarios documentation report**. The data and methods used to construct the freight demand module, the output of the examined scenarios and sensitivities, and the results of back-casted demand and validation. At least six scenarios, on the cost of rail transport for different ES systems,

Tasks	Milestones and Deliverables
	and on climate policy, truck automation, economic growth, pipeline infrastructure development, fuel efficiency, and fuel prices will be developed and incorporated in A-STEP to improve practical application. The tool includes expected ranges of price and other attribute values associated with scenarios of high, medium and low economic growth, market penetration of self-driving trucks, fuel price, carbon tax and others, that users can draw from to develop and test multiple scenarios. **Actual Performance**: The demand forecasting module was created and integrated into RailDecarb. A document describing it was prepared, submitted, and approved.
Task 7: Integrated Assessment	**M7.1 Finalize software development and testing plan**. A description of the software development and testing plan to be followed. **Actual Performance**: A document describing how the software would be developed and tested was prepared, submitted, and approved. **M7.2 Complete alpha testing and summarize the results and feedback**. The results from alpha testing: findings, adjustments, refinements, and re-testing results are reported. The Full Roll-out Model (FRM) will include but not be limited to temporal and Temoa-based spatial projections of freight rail system power demand, energy consumption, performance, and cost; freight locomotive fleet composition; trends in source energy consumption, including diesel and other fuels; and supportive ES infrastructure buildout and costs, including manufacturing scale/capacity trends. **Actual Performance**: For alpha testing, the toolset modules were exercised by close associates of the team members, and the team members not involved in software development to ensure that anticipated outputs are provided from the inputs. Enhancements were made and successful closure was reached. **M7.3 Complete beta testing and summarize the results and feedback**. The results from beta testing: findings, adjustments, refinements, and re-testing results are reported. **Actual Performance**: Beta testers beyond those involved in the alpha testing were engaged and the A-STEP team worked with them to review and enhance the capabilities of the toolset. Enhancements were made and successful closure was reached. **M7.4 Complete final technical model documentation**. Detailed documentation for the technical model, data sources and methods, providing users the necessary information for use of the model. **Actual Performance**: The technical documentation for A-STEP was prepared. It can be found on the publicly accessible A-STEP website and can be found easily using web search engines. **M7.5 Integrated modeling suite performance**. Evidence that the module modules are linked and compatible through three case study examples. The representative

Tasks	Milestones and Deliverables
	corridors, train consists, train operational situations (e.g., meet/pass), seasons, time periods, motive power technologies, energy delivery infrastructure requirements, energy mix interactions and lifecycle emissions, and freight demand scenarios that will be the focus of case studies, each of which will progress from 2020 to 2050 in 5-year increments are identified. The timing of new technology introduction, locomotive fleet turn-over, techno-economic risks (e.g., cost growth), potential technological payoffs (reduced emissions), and other factors embodied in the component models that comprise A-STEP are accounted for. **Actual Performance**: The modules that were developed were integrated into five tools: 1) a single train simulator, *OneTrain*; 2) a multi-train (network) simulator, *NeTrainSim*; 3) a charging facility sizing module, *ChargSta;* 4) the power grid interactions and energy supply module, Temoa; and 5) a rail decarbonization analysis procedure, *RailDecarb*. These modules, and a few additional Excel-based supplementary tools, are bundled into a downloadable zip file that can be found on the publicly accessible A-STEP website that can be found easily using web search engines.
Task 8: Technology Transfer and Outreach	**M8.1 Share multi-module design report with Project Advisory Committee (PAC)**. The design reports and a narrative explaining their purpose, scope, and integrative features. Feedback and expressed priorities from the PAC are incorporated into the design reports submitted to ARPA-E. **Actual Performance**: This document was prepared and shared with the PAC. **M8.2 Conduct outreach with the PAC and the railroad industry**. Sharing of our A-STEP work through presentations for the FRA and State Transportation Agencies, and to organizations such as the AAR, AREMA, and the Transportation Research Board (TRB). **Actual Performance**: Throughout the project, briefings were provided to various stakeholder groups, especially at TRB, INFORMS, the UI/UC sponsored 2022 Railroad Environmental Conference, and the 2022 FRA-sponsored decarbonization conference. **M8.3 Report on scenario design and model integration**. A report summarizing the scenarios to be examined and the approach to be used in module integration. **Actual Performance**: This report was prepared, submitted, and approved. **M8.4 Release Open-Source Code**. 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**: The toolset can be downloaded as a zip file. It is also available on a web-accessible Windows server. A ReadMe file guides new users through the process of setting up and

Tasks	Milestones and Deliverables
	running the toolset. A set of example assumptions, that reflect the most current public information are included as default inputs.

For projects involving computer modeling, provide a brief description of the model, key assumptions, how the model was validated, and whether the model and results were presented in peer-reviewed publications.

Project Activities

The project's focus was on developing a toolset that could be used by stakeholders of the freight railroad industry to examine ways in which the industry could be decarbonized. The software for the toolset was developed by a group of nearly a dozen individuals using code developed in Python, C++ and VB.net. The result is a set of five tools that focus on various aspects of the decarbonization problem: 1) *OneTrain*, a single train simulator; 2) *NeTrainSIm*, a multi-train (network) simulator; 3) *ChargSta*, a charging facility sizing module; 4) *Temoa*, a power grid interactions and energy supply module; and 5) *RailDecarb*, a rail decarbonization economic and environmental impact analysis procedure. Along with these modules are a few additional Excel-based supplementary tools, bundled into a downloadable zip file that can be found on the publicly accessible A-STEP website that can be found easily using web search engines.

Project Outputs

A. Journal Articles

D. Jackson, S. Belakaria, Y. Cao, J. R. Doppa and X. Lu, Machine Learning Enabled Design Automation and Multi-Objective Optimization for Electric Transportation Power Systems, *IEEE Transactions on Transportation Electrification* 8:1, 1467-1481 (2022), DOI: 10.1109/TTE.2021.3113958

Ahn, K.; Aredah, A.; Rakha, H.A.; Wei, T.; Frey, H.C., Simple Diesel Train Fuel Consumption Model for Real-Time Train Applications, *Energies* 16, 3555 (2023), DOI: https://doi.org/10.3390/en16083555

Aredaha, A., J. Dua, M. Hegazib, G. List, and H. Rakhaa, Comparative Analysis of Alternative Powertrain Technologies in Freight Trains: A Numerical Examination Towards Sustainable Rail Transport, *Applied Energy*, Vol. 356, February 2024, 122411.

B. Papers

V. Guov, D. Jackson, and Y. Cao, Sizing BESS and On-site Renewable for Battery-electric Freight Rail Fast Charging Station, *2022 IEEE 13th International Symposium on Power Electronics for Distributed Generation Systems* (PEDG), Kiel, Germany Proceedings, Not yet available (2022)

Jordan, K., Sinha, A., Venkatesh, A., Jaramillo, P., Johnson, J.X., Inspecting Decarbonization Pathways in an Open Energy Outlook for the United States, *INFORMS Annual Meeting*, Indianapolis, IN (2022)

George F. List, identifying low cost decarbonization pathways for the rail freight industry is critical to achieve goals of net zero carbon emissions, *INFORMS Annual Meeting*, Indianapolis, IN (2022)

Jordan, K., Sinha, A., Venkatesh, A., Jaramillo, P., Johnson, J.X., The Open Energy Outlook: An open and collaborative modeling effort for decarbonization analysis, *Global Clean Energy Action Forum*, Pittsburgh, PA

V. Guov, D. Jackson, Y. Cao, Sizing BESS and On-site Renewable for Battery-electric Freight Rail Charging Station, *Proceedings: IEEE International Symposium on Power Electronics for Distributed Generation Systems* (PEDG), 1-6 (2022)

List, George, Andreas Hoffrichter, and Lynn Harris, Multi-decadal Decarbonization Pathways for U.S. Freight Rail, Rail Rolling Stock and Motive Power Committee Meeting (AR020), *2023 Transportation Research Board Annual Meeting*, January 9, 2023

Aredah, Ahmed, Karim Fadhloun, Hesham Rakha, and George List, NeTrainSim: A Longitudinal Freight Train Dynamics Simulator for Electric Energy Consumption, paper TRBAM-23-00999, *2023 Transportation Research Board Annual Meeting*, January 10, 2023

Wei, T., Sinha, A., Johnson, J.X., and List, G.F., "Evaluation of Techno-Economical Feasibility and Carbon Intensity of Decarbonization Energy Pathways for U.S. Freight Rail," Poster Presentation No. GC42G-0778, *Proceedings, 2022 American Geophysical Union (AGU) Fall Meeting*, Chicago, IL, December 12-16, 2022.

Ahmed Aredah, Mohamed Hegazi, George List, Hesham Rakha, Comparative Analysis of Alternative Powertrain Technologies in Freight Trains: A Numerical Examination Towards Sustainable Rail Transport, *2024 TRB Annual Meeting,* Washington, DC Conference Proceedings, N/A (2024).

C. Status Reports

Quarterly status reports were provided quarterly to ARPA-E

D. Media Reports

The press releases to date are on the web pages describing A-STEP. The ARPA-E program manager has been apprised of these postings.

https://itre.ncsu.edu/focus/rail/astep/
https://www.ccee.ncsu.edu/news/2023/ccee-researchers-tackle-rail-decarbonization-with-innovative-a-step-software-tool/

E. Invention Disclosures None

F. Patent Applications/Issued Patents None

G. Licensed Technologies None

H. Networks/Collaborations Fostered

Follow-on collaborations with Arizona State University, several Federal research laboratories, and one railroad locomotive equipment supplier

I. Websites Featuring Project Work Results

https://itre.ncsu.edu/focus/rail/astep/
https://www.ccee.ncsu.edu/news/2023/ccee-researchers-tackle-rail-decarbonization-with-innovative-a-step-software-tool/

J. Other Products (e.g. Databases, Physical Collections, Audio/Video, Software, Models, Educational Aids or Curricula, Equipment or Instruments)

None to date

K. Awards, Prizes, and Recognition

None to date

Follow-On Funding

To date, no additional funding has been committed or received from other sources (e.g., private investors, government agencies, nonprofits). We have had several inquiries about using the tool from Federal research labs and railroad product developers.