III.15 Cryo-Compressed Pathway Analysis (2016)

A.J. Simon
Lawrence Livermore National Laboratory (LLNL)
7000 East Avenue
Livermore, CA 94550
Phone: (925) 422-9862
Email: simon19@llnl.gov

DOE Manager: Erika Gupta
Phone: (202) 586-3152
Email: Erika.Gupta@ee.doe.gov

Project Start Date: October 1, 2015
Project End Date: Project continuation and direction determined annually by DOE

Overall Objectives

- Quantify the techno-economic performance of cryo-compressed hydrogen (CcH2) pathways.

Fiscal Year (FY) 2016 Objectives

- Develop well-to-wheels cost estimates for CcH2 pathways.
- Develop well-to-wheels emissions estimates for CcH2 pathways.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Delivery and Systems Analysis sections of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan.

Hydrogen Delivery

(C) Lack of Hydrogen/Carrier and Infrastructure Options Analysis

(G) Reliability and Costs of Liquid Hydrogen Pumping

Systems Analysis

(A) Future Market Behavior

Technical Targets

This project is conducting systems analyses of the CcH2 delivery pathway. Insights gained from these analyses will be applied to inform hydrogen delivery technology development toward meeting the DOE hydrogen delivery targets.

- Delivery costs associated with centralized hydrogen production: $2/gge
- Liquid hydrogen pumps uninstalled capital costs: $650,000
- Liquid hydrogen pumps specific energy: 0.5 kWh/kg

FY 2016 Accomplishments

- Incorporated physics-based estimates of boil-off losses into the liquid hydrogen delivery chain which are applicable to both the CcH2 pathway as well as the liquid–compressed–gas pathway.
- Identified and remediated hydrogen loss mechanisms from delivery to LLNL's cryo-compressed testing facility.
- Estimated well-to-wheels costs of hydrogen to be $7.85/kg, and costs of driving to be $0.44/mi under well-defined assumptions.
- Estimated well-to-wheels CO_2 emissions of hydrogen to be 280 g CO_2/mi under similar assumptions.

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INTRODUCTION

Several different pathways for delivering hydrogen to vehicles are under development at DOE and beyond. The cost, environmental impact, and safety of hydrogen are all affected by how hydrogen is transported from its production site and delivered to vehicle platforms. Tradeoffs between different delivery pathways can be analyzed using techno-economic models of hydrogen delivery. The results of these analyses inform researchers, policymakers and other stakeholders of the potential benefits of improved hydrogen delivery technology.

Cryo-compressed hydrogen is defined as cold liquid hydrogen (20–40 K), delivered to the vehicle at high pressures (300–900 bar). Potential advantages of CcH2 include very high volumetric and gravimetric energy density, and innate compatibility with efficient liquid hydrogen delivery to filling stations. Potential tradeoffs include the energy consumed in liquefaction and compression, and the possibility of hydrogen losses to the atmosphere through boil-off of liquid hydrogen in storage, transport or transfer. The objective of this project is to generate estimates of the costs and environmental impacts of the CcH2 fueling pathway, informed by a fundamental understanding of the behavior of cryogenic and cryo-compressed systems, and by recent experience with such systems at LLNL's cryo-compressed test facility.

APPROACH

The Hydrogen Delivery Systems Analysis Model (HDSAM), an Excel-based calculation tool developed by Argonne National Laboratory, is the platform on which this analysis was performed. Two major pieces of analysis were integrated with HDSAM to achieve results: physics-based estimates of hydrogen boil-off and other losses throughout the delivery chain and parameterized well-to-wheels calculations of costs and emissions for the entire enterprise.

Hydrogen can be lost from the delivery pathway through several mechanisms: (1) leak-related losses at the liquefier and terminal, (2) boil-off from the transportation trailer from heat infiltration in transit, (3) venting of the vapor-space in low pressure cryogenic vessels at filling stations, (4) venting from the trailer during de-pressurization after unloading at a filling station, (5) boil-off from steady-state heat infiltration into the cryogenic components of a filling station (tank, lines, pump, etc.), and (6) boil-off from the heat deposited by running the pump during dispensing. In this project, HDSAM was extended to estimate most of these losses from known or measurable quantities in operating prototype systems.

Also integrated with HDSAM are estimates of the non-delivery components of a hydrogen enterprise that contribute to the total lifecycle cost and environmental impact of CcH2 delivery. Such components include vehicle cost, hydrogen production cost, greenhouse gas (GHG) emissions from hydrogen production, etc. Standardized calculations were used to integrate the delivery-specific costs and emissions (based on the above physics-based refinements) with parameterized estimates of non-delivery factors to estimate top-line results such as the cost and GHG emissions per mile driven on CcH2.

RESULTS

The objective of this project was to generate analyses of the total cost and GHG of driving a fuel cell electric vehicle fueled through a CcH2 delivery chain. That objective was realized by extending and exercising the HDSAM model over a range of assumptions relevant to CcH2 delivery.

Figure 1 depicts *potential* hydrogen losses from boil-off through the delivery chain. The large fraction of hydrogen lost to boil-off in this specific scenario is representative of early market conditions and low technology levels. This scenario is used for illustrative purposes because each loss mechanism is clearly visible; it is not representative of a realistic large-scale deployment of CcH2 technology.

Engineering estimates of steady-state heat transfer ($Q = kA\Delta T/L$) into the various vessels and piping were used to calculate individual boil-off rates ($m = Q/h_{fg}$) that would occur if those vessels were held at constant temperature and pressure. Calculated losses include venting during trailer transport (assuming typical trailer dewar configurations), venting due to onsite storage at service stations, and venting due to heat infiltration into the pump-vessel and associated piping at service stations.

Losses associated with pumping, and losses avoided by pumping were also estimated through basic thermodynamic analysis. It was assumed that a certain fraction of the mechanical energy used by the pump would end up in the hydrogen (due to the mechanical inefficiency of the

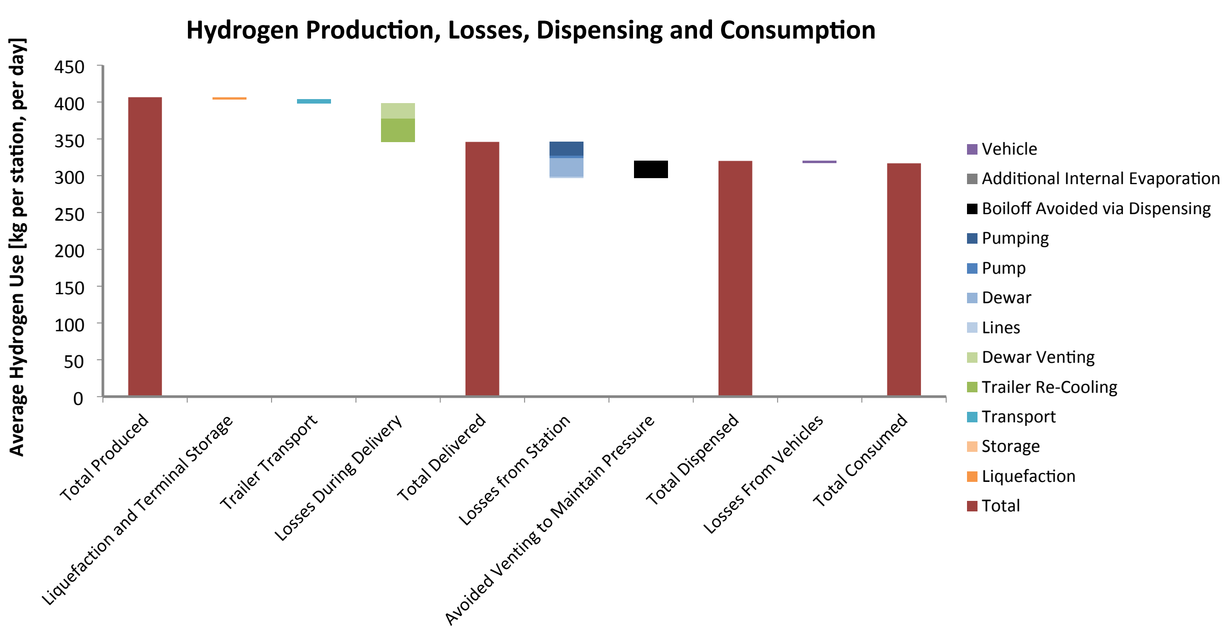

FIGURE 1. Waterfall chart depicting all potential loss (venting and boil-off) mechanisms along the CcH2 delivery pathway

pump) and that some fraction of that energy would heat the low-pressure fluid in which the pump is immersed. This deposited energy would evaporate some of the stored liquid hydrogen. On the other hand, hydrogen dispensed during pump operation is removed from the system; and some of the remaining liquid hydrogen must be evaporated to maintain constant volume (again, assuming constant temperature and pressure operation). The black bar labeled "Avoided Venting to Maintain Pressure" reflects the logic that hydrogen may be vented if vaporization exceeds dispensing demand, and that no venting would occur (and heat would be admitted to maintain pressure) when dispensing demand exceeds heat infiltration.

Losses during liquefaction were estimated to be 0.5% of hydrogen liquefied based on industry experience. This estimate may be refined in future analyses. Losses from CcH2 tanks on vehicles were estimated to be 1% fleetwide. This crude estimate may also be refined in the future, as it depends on wide variations in drive cycles (a regularly driven vehicle will vent no hydrogen from a CcH2 tank, while a long-dormant vehicle could vent a significant fraction of its tank capacity in certain, rare circumstances).

Losses during delivery were estimated under both best-case and worst-case scenarios. LLNL has taken several deliveries of liquid hydrogen to the (relatively small – 800 kg) dewar associated with its onsite CcH2 test facility. LLNL personnel have observed significant venting of hydrogen associated with two phases of the delivery process in this premarket setting: (1) venting from the dewar during transfer of hydrogen from the trailer to the dewar, and (2) venting of hydrogen from the trailer after the transfer is complete and before the trailer leaves the site.

In a best-case scenario, no hydrogen would be vented during delivery because cold hydrogen from the trailer "collapses" the warm hydrogen vapor that builds up at the top of the dewar, and adequate management of heat transfer and mixing within the trailer can be used to control pressure excursions. In a worst-case scenario (which has been observed), the dewar is filled from the bottom, displacing (and venting) the cool, dense hydrogen vapor at the top of the dewar. Additionally, the trailer is brought to full thermodynamic equilibrium during transfer (effectively warming the liquid hydrogen to pressurize it), and then is vented and well mixed to bring the entire volume back to a cold "over-the-road" low pressure. Such a procedure can cause over 10% of delivered hydrogen to be lost, as depicted by the green bars in Figure 1.

After performing this analysis, LLNL personnel worked with our hydrogen supplier to minimize delivery losses by top-filling the dewar and minimally heating the trailer for pressurization. This was an unexpected benefit of the analysis and is a positive outcome for both DOE and LLNL.

Figure 2 depicts an analysis of delivery costs. The costs depicted do include the loss of hydrogen throughout the delivery chain, but do not include the production cost of the hydrogen that is dispensed. The early market scenario depicted assumes a relatively small station (with a design capacity of 400 kg/d and an average dispensing rate of 320 kg/d). The modified HDSAM analysis shows that the largest fraction of CcH2 delivery costs are associated with liquefaction; and the terminal and trucking costs are a small fraction of the overall delivery cost. Station capital and labor are also major contributors to delivery costs, while station energy consumption (some of which is associated with cryo-compression) is not.

Not explicitly depicted is the capital cost of the cryopump itself; that cost is part of the station capital cost. In this specific scenario, the estimated capital cost of $225,000 per pump, installed, represents ~27% of the capital cost of the station, or $0.29/kg of hydrogen dispensed (6% of

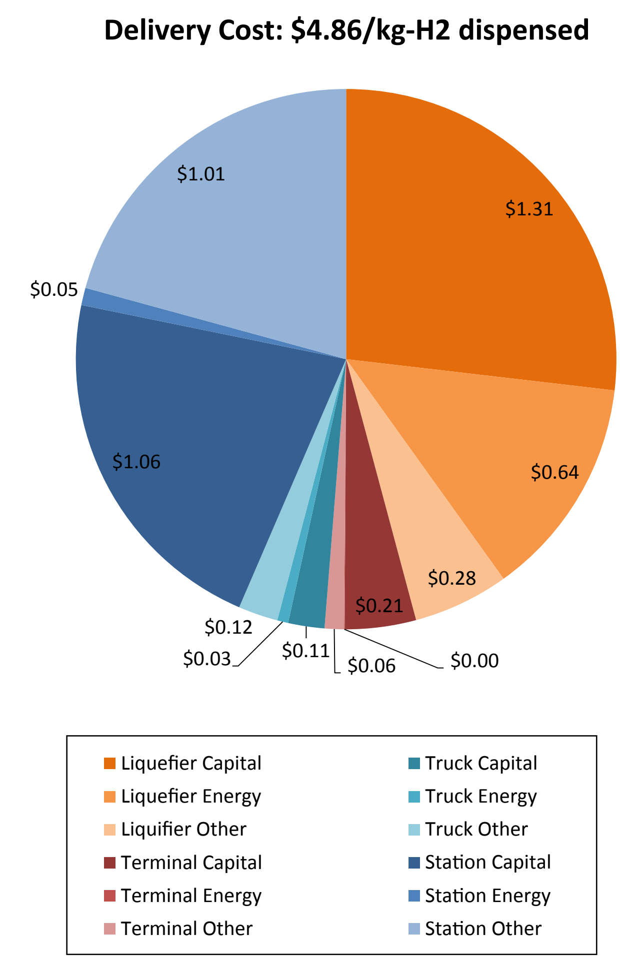

FIGURE 2. Contributions to the total cost of delivery by the major components of the delivery pathway for CcH2. The scenario depicted here is for small, early market stations (designed to dispense up to 400 kg/d) and mature delivery and dispensing technology.

the delivery cost). This cost is a major factor, and should be compared to equipment in other delivery pathways (compressors and chillers in the liquid–compressed–gas pathway, and storage cascades in the compressed gas pathway).

The total GHG emissions of the CcH2 pathway are shown in Figure 3. Production (assumed to be central station steam methane reforming) and liquefaction (assumed to be central and co-located with the terminal) dominate the pathway's total GHG emissions per mile of driving. Diesel-fueled liquid hydrogen trucking, and electricity-driven station operation, are small contributors. In fact, in scenarios where there is significant boil-off or hydrogen venting, eliminating the GHG emissions associated with the production and liquefaction of lost hydrogen can fully offset the GHG emissions from trucking and dispensing.

Multiple sensitivities to pathway parameters were investigated. Figure 4 depicts the sensitivity of hydrogen venting losses (using our observed "worst-case scenario" delivery practices) to station size. In this study, larger stations result in fewer losses because each delivery causes hydrogen venting in proportion to the residual hydrogen in the trailer, and because larger stations have lower surface area-to-volume ratios. Several other sensitivity studies were conducted to investigate the effects of pump cost, pump efficiency and heat transfer coefficients. The modified HDSAM tool is capable of analyzing the effects of almost any cost or performance parameter on hydrogen losses, delivery costs, costs of driving, and GHG emissions.

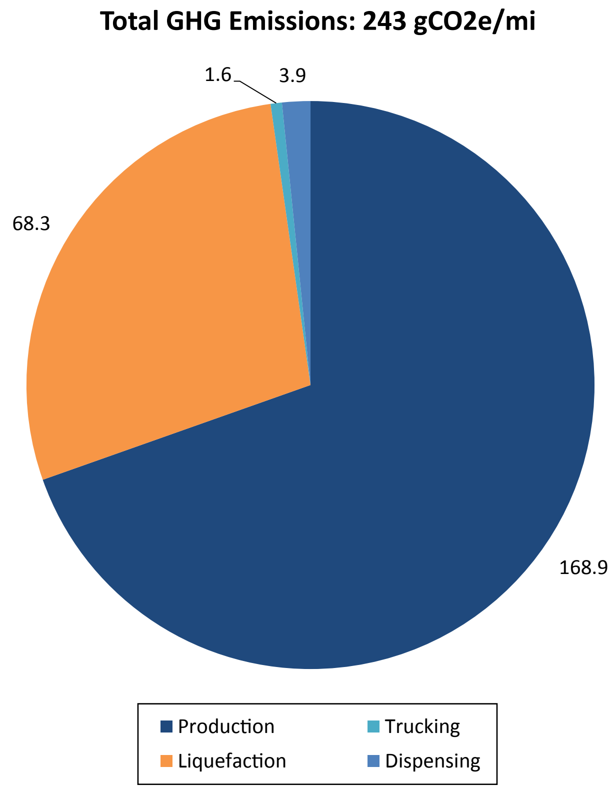

FIGURE 3. Contributions to the total GHG emissions from a light-duty vehicle fueled with CcH2. These results reflect the same scenario as depicted in Figure 3.

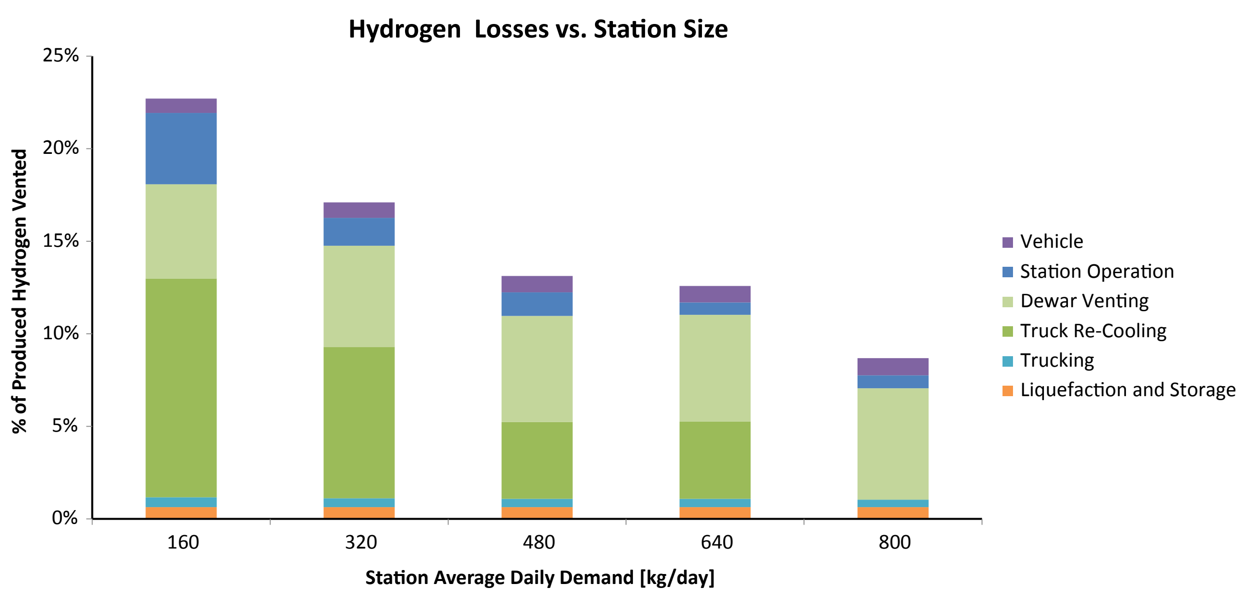

FIGURE 4. Sensitivity of hydrogen boil-off to station size. All parameters except the average station size were held fixed at a low technology level (large heat transfer rates, inefficient delivery practices) to illustrate the potentially compounding effects of observed losses on early markets.

CONCLUSIONS AND FUTURE DIRECTIONS

Top-line estimates of \$5.75/kg H_2 (total cost of hydrogen to the consumer), \$0.41/mi (cost of driving), and 240 g CO_2/mi were generated as representations of a mature CcH2 market, and the sensitivity of these figures to changes in technology cost and performance were thoroughly investigated.

In future years, the thermodynamic analysis of hydrogen transfers will be extended to include best practices of non-equilibrium pressurization of the trailer and dewar. System models will be benchmarked against performance measured at LLNL's CcH2 test facility. The CcH2-specific and generally relevant liquid hydrogen analyses will be formally included in a future version of HDSAM.