III.10 Liquid Hydrogen Infrastructure Analysis

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Overall Objectives

- Provide better understanding of losses along the liquid hydrogen pathway (from the liquefaction plant to the fuel cell vehicle) through thermodynamic modeling including real gas equations of state, two-phase behavior, and para–ortho conversion.
- Gather and analyze real-life driving and parking scenarios to infer typical losses for a sample population.
- Study mitigating solutions to reduce boil-off, through improved operation, hardware, upgrade or recovery.

Fiscal Year (FY) 2017 Objectives

- Build simulation platforms for both liquid hydrogen (LH2) transfer from the liquefaction plant to the dispenser (typically low pressure, low temperature) and cryogenic H_2 end-user utilization, i.e., refueling, driving, and parking onboard a fuel cell cryo-compressed vehicle (typically wider ranges of pressure and temperature, into the super-critical regime).
- Verify that the simulation results are consistent with real-life results.
- Propose mitigation strategies.

Technical Barriers

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

(A) Lack of Hydrogen and Infrastructure Options Analysis

(C) Reliability and Costs of Liquid Hydrogen Pumping

Technical Targets

The project addresses the delivery costs targets associated with centralized H_2 production (Table 1).

TABLE 1. Delivery Targets Associated with Centralized H_2 Production

Category	FY 2011 Status	FY 2015 Status	FY 2020 Target	Ultimate Target
Aggregate cost of transport, distribution, and fueling ($/gge)	3.6–4.40	3.35–4.35	2.00	<2.00

gge – gallon gasoline equivalent

No target for H_2 losses or leakage for liquid hydrogen exists, although values <0.5% are mentioned for pipelines and tube trailer terminal truck refueling compressors.

FY 2017 Accomplishments

- Adapted MATLAB code from NASA to model heat and mass transfer phenoma in two-phase systems to simulate boil-off losses when transferring liquid H_2.
- Reviewed the available vehicle utilization scenario and selected data from the Puget Sound Regional Council (named "PSRC-2006") that consist of 298 unique driving–parking scenarios collected between March 2005 and March 2006 in the Puget Sound area, available at: https://www.nrel.gov/transportation/transportationdata/index.cfm.
- Built a refueling–parking–driving thermodynamic model for cryo-compressed vehicles in FORTRAN that includes real gas economies of scale, tank thermal mass, and para–ortho kinetics. It is capable of quantifying boil-off losses over the entire timeframe of a given utilization pattern.

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INTRODUCTION

Liquid hydrogen has many benefits for the hydrogen infrastructure. Its high density allows minimum costs for distribution (e.g., $167/kg H_2 for a liquid trailer vs. $783/kg H_2 for a gaseous trailer), high payload and short transfer times minimize delivery logistics, low temperature and low pressure provides very low potential burst energy, and LH2 pumps can efficiently achieve large throughputs (up to 600 kg/h) with a small footprint (low electricity consumption and compact designs). Those many benefits are the reason why many dispensing stations are using LH2 or considering using it, despite the higher cost of liquefaction.

For example, AC Transit in Oakland uses LH2, and most of the 40 fuel cell forklift refueling stations in the United States are relying on LH2.

Using LH2, however, has a few challenges. Liquefying H_2 is expensive (more than three times the energy of compression to 700 bar), setback distances are more stringent for LH2, and losses along the LH2 pathway (transfer, boil-off) may occur. LH2 losses are not well qualified nor quantified, and more analysis needs to be performed in order to evaluate their impact on the hydrogen economy.

APPROACH

Losses along the LH2 pathway are intrinsic to the utilization of a cryogenic media. They occur when the fluid is transferred between two vessels (liquefaction plant to trailer, trailer to station, station to vehicle, etc.), and when the fluid sits unused for extended periods of time. Those losses can be estimated with good accuracy using thermodynamic models based on conservation of mass and energy, providing the states of the molecules are correctly described. Indeed, the fluid undergoes various changes as it moves along the entire pathway (two-phase transition, supercritical warming, para–ortho conversion) and accurate equations of state and two-phase behavior implementations are essential. The balance of energy during the various dynamics processes then enables to quantify the losses, either through transfer or boil-off.

Two different codes are being implemented. The first simulates the losses when transferring LH2 at low pressure and temperature (<12 bar, <33 K) when the fluid is two phases, which is the condition the fluid is at from its production to its dispensing at the refueling station. The second code simulates the states of the molecules of hydrogen once the fuel is stored onboard the fuel cell vehicle, at pressures and temperatures that can vary over wide ranges (up to 700 bar and room temperature), depending on how the vehicle is refueling and used. Those conditions are generally single phase, and referred to as cryo-compressed or super-critical conditions. The first code is being written in MATLAB, the second in FORTRAN.

RESULTS

A MATLAB code previously developed by NASA to simulate rocket loading was used as the basis of the LH2 transfer model. This code implements complex physical phenomena such as the competition between condensation and evaporation, the convection vs. conduction heat transfer as a function of the relative temperatures on both sides of the saturated film. The code was modified to take into account real gas equations of state, by linking the code to a Refprop sub-routine (.dll). Some semi-empirical relationships, such as between the heat of vaporization and the critical temperature, were also replaced by a Refprop equivalent expression, assumed to be more accurate. Non-constant liquid temperature equations were added in order to simulate a sub-cooled effect. The non-linear solver was modified to enable computation of the boil-off losses during the process. Figure 1 shows an example of an LH2 transfer between a trailer and a 3,300 gal Dewar. The trailer is initially full while the Dewar is initially cold (~20 K) and 1% full. 800 kg of LH2 are transferred in about 37 min, bottom fill only. The boil-off losses from the Dewar occur during the fill and are mostly due to the changes of LH2 volume (total: 14 kg) and the losses from the trailer happen at the end of the fill, when the trailer is depressurized from ~45 psi to 20 psi (total: 14.5 kg). In that calculation, the relief device of the Dewar is set at 30 psi.

Concerning the end-user utilization, the first step consisted in finding reliable inputs for the effort, i.e., vehicle utilization patterns with sufficient resolution over a reasonable time for the simulations. A few databases were investigated, including the Institute for Transportation Studies from University of California, Davis, the Advanced Vehicles and Infrastructure department from Idaho National Laboratory, and the Secure Transportation Data Center from the National Renewable Energy Laboratory. We ended up selecting data from the Puget Sound Regional Council that consist of 298 unique driving–parking scenarios collected between March 2005 and March 2006 in the Puget Sound area. Then, a second code simulating the H_2 thermodynamic states inside the cryo-compressed fuel cell vehicle was written in Fortran. This code needed to be very flexible to accommodate various unique drive–park profiles over extended time (12 mo and over) with very different mass and energy balances depending whether the vehicle was being driven, parked, or refilled. Indeed, under driving conditions,

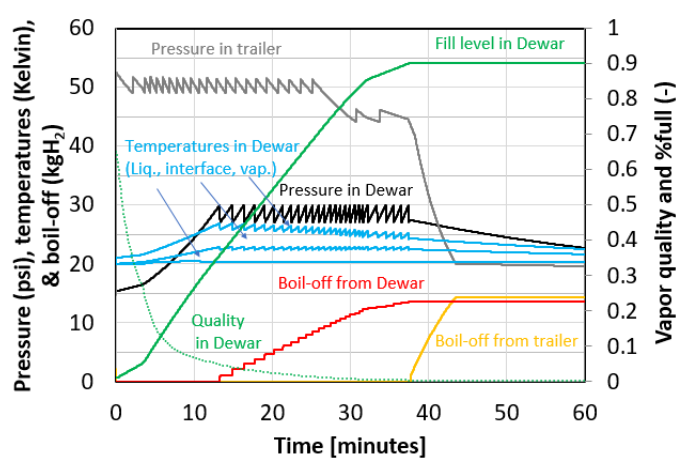

FIGURE 1. Simulation of a liquid fill from a trailer to a 3,300 gal stationary Dewar, computed using the MATLAB code. Pressures in the trailer and Dewar, temperature in the Dewar (liquid, interface, and vapor) and boil-off losses from the trailer and the Dewar are shown on the left axis; vapor quality and fill level in the Dewar are shown on the right axis. See text for details.

constant hydrogen extraction controls the temperature (quasi-adiabatic conditions), while para–ortho conversion at constant density and thermal energy absorption by the wall under external heat entry are the most important phenomena during parking, and finally pump performance (mainly, entropy) determines the final conditions after a refill. The input file was formatted as hourly data over the 12 mo period, with "0" meaning parking and non-zero meaning distance driven during that hour. A separate file was also used to specify the design and operation of the storage system: pressure rating and inner volume; length to diameter ratio; strength and density of the liner and the composite material; performance of the insulation; outside temperature; initial temperature; and pressure, fill pressure, minimum pressure in the vessel, minimum capacity before refilling, pump entropy, and pump ortho fraction. Here again, the equations of state were implemented using Refprop sub-routines. Figure 2 shows a 12-month-long simulation of a driving pattern (here, 63866-2). For those conditions, about 5 kg of losses are computed, over a total of 210 kg H_2 used (21,076 km), i.e., a 2.3% loss over one year.

CONCLUSIONS AND UPCOMING ACTIVITIES

Two separate codes were developed over the funding period, one to simulate the LH2 losses between the production and dispensing and one to simulate boil-off losses on-board a cryo-compressed fuel cell vehicle under real-life utilization patterns. The first code is undergoing verification, while the second code is fully functional, capable of screening through a lot of a vehicle's utilization scenario. The next steps under the current funding are to complete verification of the first code then run the code to identify main sources of losses, then analyze mitigation strategies.

FY 2017 PUBLICATIONS/PRESENTATIONS

1. G. Petitpas and A.J. Simon, "Liquid Hydrogen Pathway Analysis," Hydrogen Delivery Tech Team Meeting, Argonne National Laboratory, March 29, 2017.

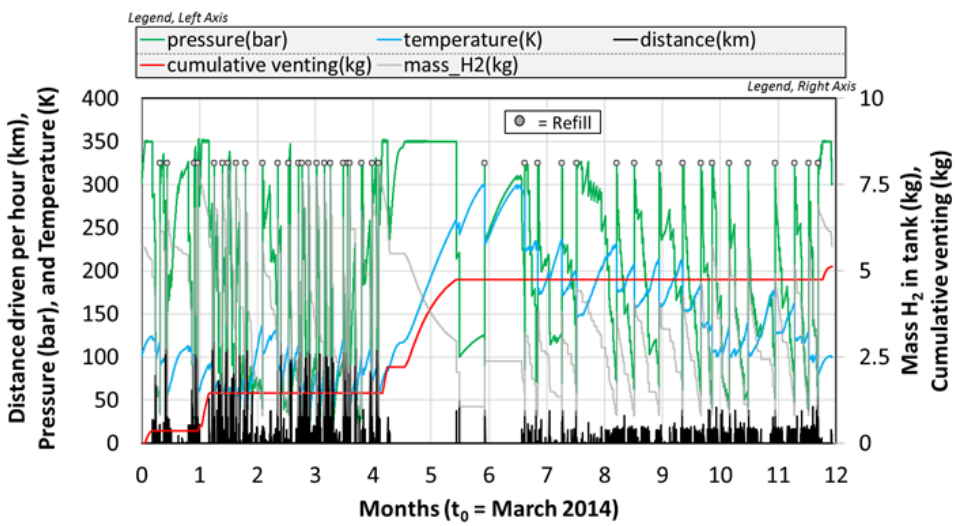

FIGURE 2. One-year-long simulation of the variations of the thermodynamic state of the fuel onboard a cryo-compressed fuel cell vehicle, for driving pattern 63866-2. Results are calculated on an hourly basis. Vehicle is refilled when less than 0.8 kg of usable H_2 is left in the tank, up to 325 bar. Most of the venting losses (see red line, right axis) occur between Months 4 and 6 (July to September) when the vehicle is seldom used (200 km in 2 mo). 210 kg H_2 is used during the 12 months (21,076 km), thus a 2.3% loss.