Liquid Hydrogen Infrastructure Analysis

Guillaume Petitpas, A.J. Simon,
Julio Moreno-Blanco, Salvador M. Aceves
Lawrence Livermore National Laboratory
Livermore, CA

LLNL-PRES-749854

Project ID#: PD135

DOE Hydrogen and Fuel Cells Annual Merit Review, Washington D.C.
June 13th, 2018

Overview

Timeline and Budget

- Start date: January 2017
- End date: September 2018
- % Complete: 95%

- FY17 DOE funding: $140k
- FY18 DOE funding: $50k
- Total DOE Funds Received to date: $190k

Barriers

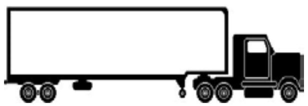
- A. Lack of Hydrogen and Infrastructure Options Analysis
- C. Reliability and Costs of Hydrogen Pumping

Partners/Collaborators

- Project lead: LLNL
- Linde: LH_2 pump operation & maintenance, LH_2 delivery
- Argonne National Lab: H_2 infrastructure
- Strategic Analyses: ECH costs

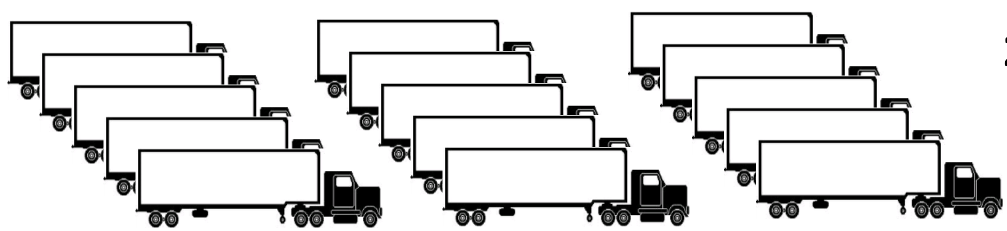
Relevance : Liquid hydrogen (LH_2) has many benefits for the hydrogen infrastructure, especially at large scale(s)

- High density LH_2 allows minimum volume & mass per kg H_2, thus *minimum* cost
- High capacity per truck & short transfer times *minimize* delivery logistics/scheduling
- *Low* potential burst energy: 20 K and <6 bar vs. 300 K and >200 bar
- LH_2 pumps provide *high* throughputs at *low* dispensing costs
- High density of LH_2 can be transferred to compact onboard solutions (cryo/cold)



4,300 kg H_2 capacity
$167/kg
LH_2

800 kg H_2 capacity
$783/kg
350 bar, composite



250 kg H_2 capacity
$1000/kg
190 bar, steel

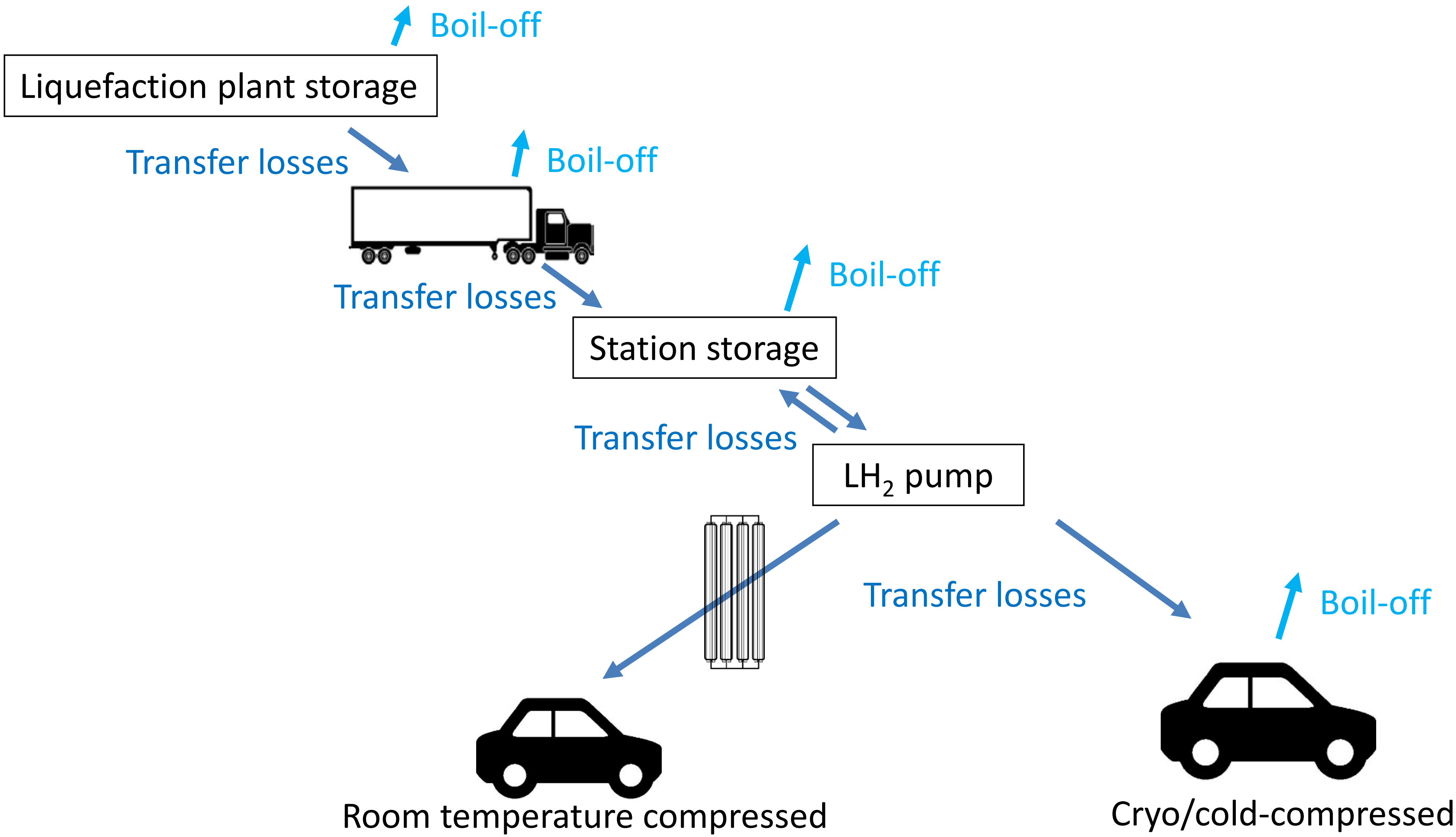
From Reddi *et al*, 2015

Challenges for LH_2:

- High cost of liquefaction (~3 X compression)
- Refueling station integration (setback distances limitations)
- Transfer and boil-off losses

Goal of effort: better understand/quantify losses along LH_2 pathway

Approach : Simulate LH_2 pathway using a thermodynamic model to estimate, then mitigate, transfer & boil-off losses



Transfer and boil-off losses occur all along the LH_2 pathway

Approach : Simulate LH_2 pathway using a thermodynamic model to estimate, then mitigate, transfer and boil-off losses

Task 1 : Simulate boil-off losses from the liquefaction plant to car dispensing

- ✓ Build/adapt thermodynamic model with real gas EOS and 2 phases for LH_2 pathway
- ✓ Evaluate optimal conditions that would minimize boil-off
- ✓ Propose improvements to existing procedures/setups

Task 2: Simulate on-board losses for cryo-compressed vehicles (CcH2)

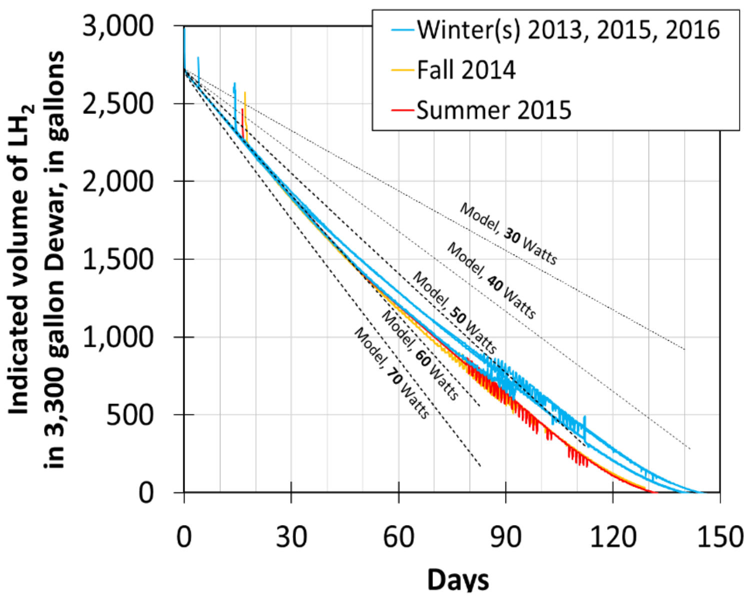
- ✓ Gather real-life driving scenarios (with enough granularity) for a large population
- ✓ Build refueling/parking/driving model for cryo-compressed vehicle, including real gas EOS, tank thermal mass, para/ortho kinetics
- ✓ Quantify boil-off losses on cryo-compressed vehicles

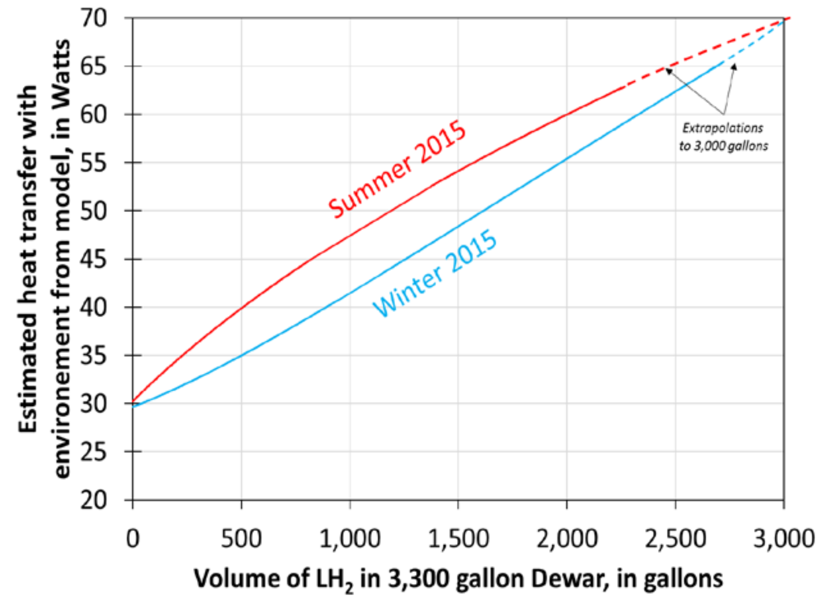
Task 3: Boil-off recovery technologies

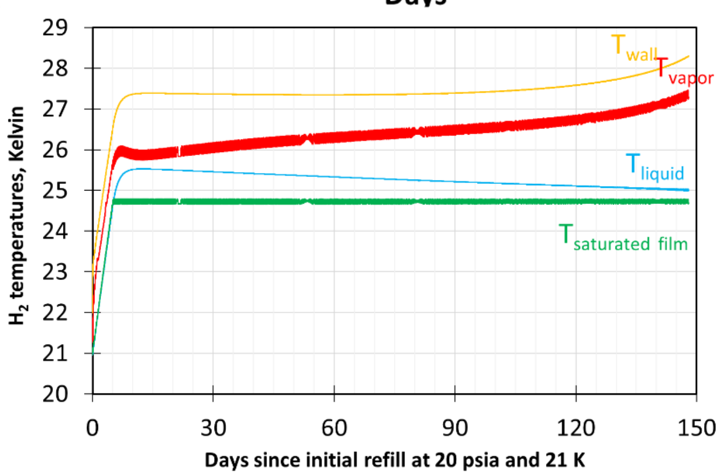
- ✓ Identify the source(s) of most significant boil-off along the LH_2 pathway
- ✓ Review main boil-off recovery options
- Evaluate costs and performances

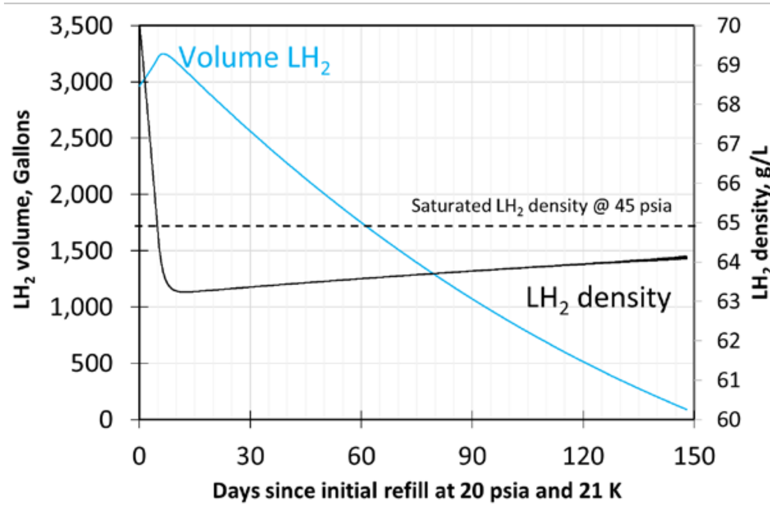
Modeling entire LH_2 pathway enables quantitative understanding

Accomplishments (Task 1): Model results for heat entry only to 3,300 gallon vessel



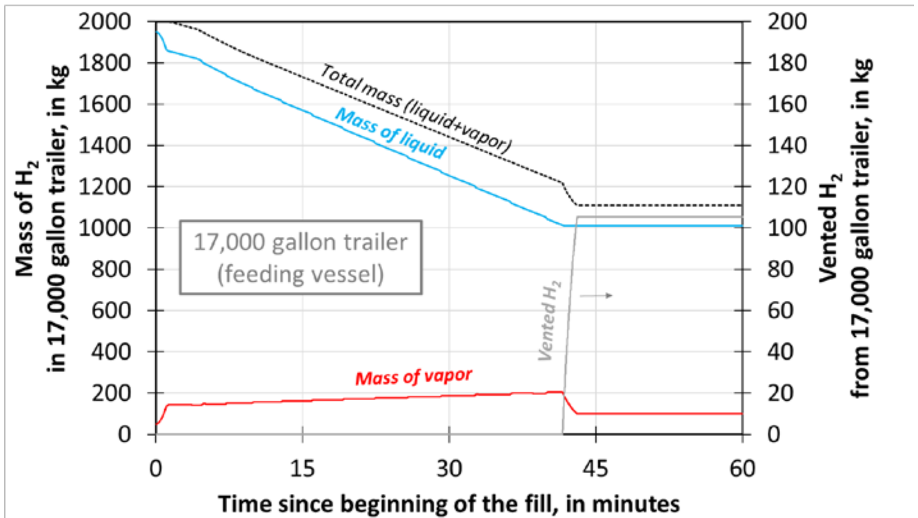


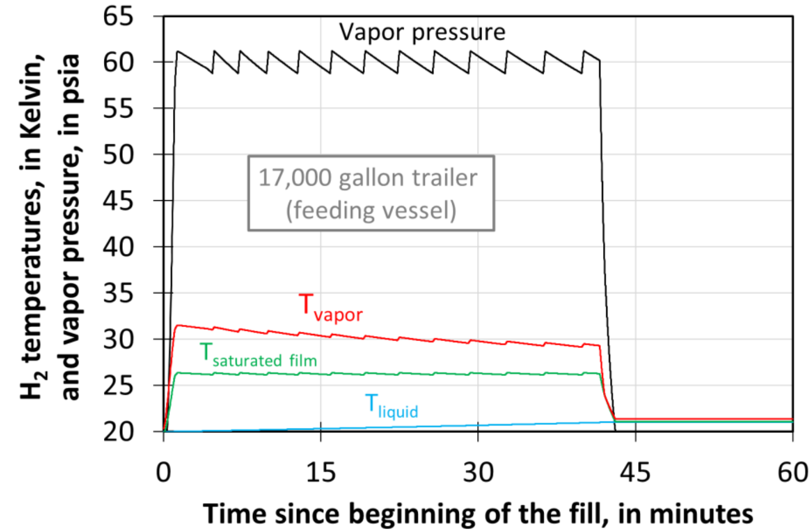


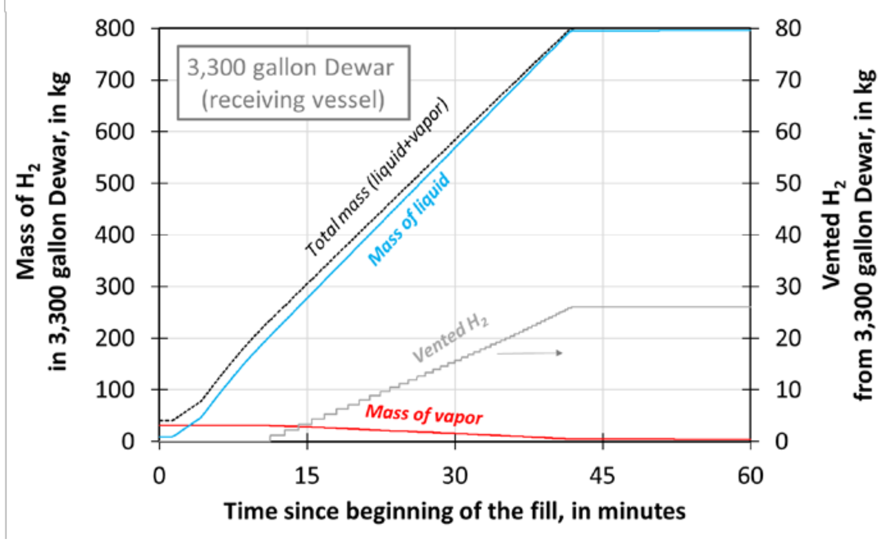


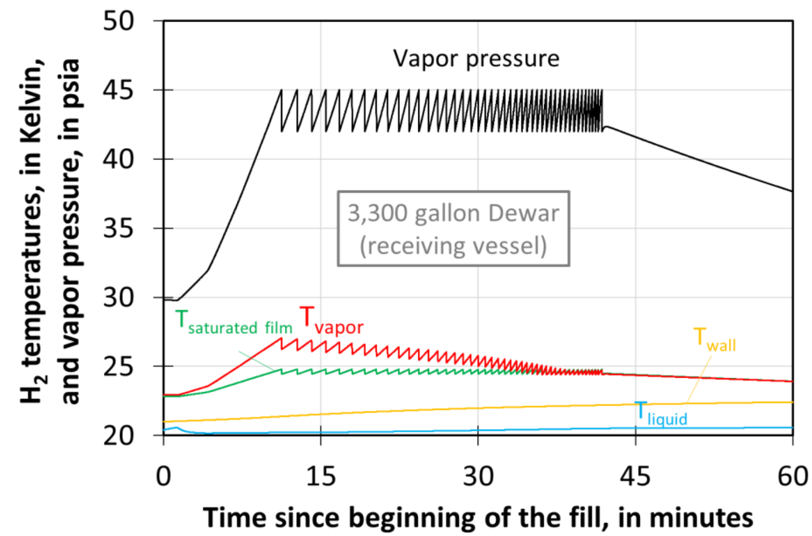
Model enables to estimate heat transfer profile & LH_2 density

Accomplishments (Task 1): Built *m*odel for liquid transfer from LH_2 trailer to stationary vessel (bottom fill)



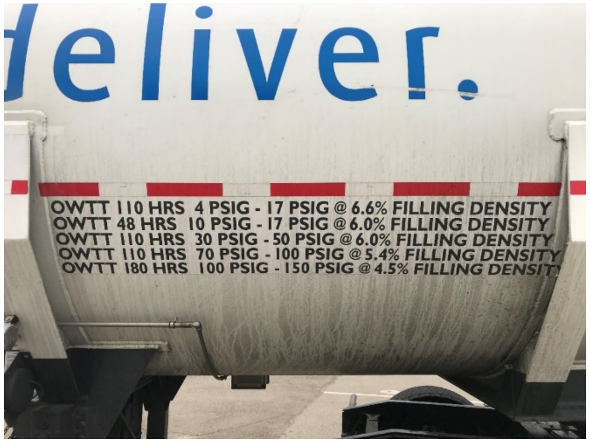




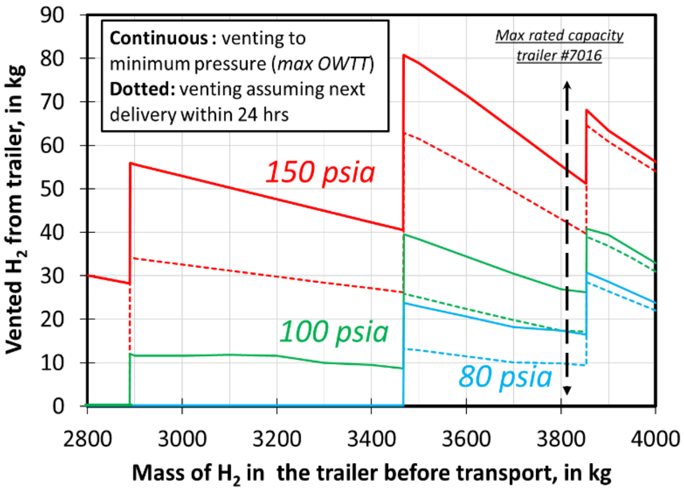


Model enables to estimate temperature and loss variations

Accomplishments (Task 1): Analysis of Code of Federal Regulations shows that minimal to no venting from trailer is necessary.



Picture of Linde LH_2 trailer (side)



CFR title 49 §177.840(i) stipulates that maximum required on-road pressure is a function of time until next delivery, which depends on vapor pressure and LH_2 level.

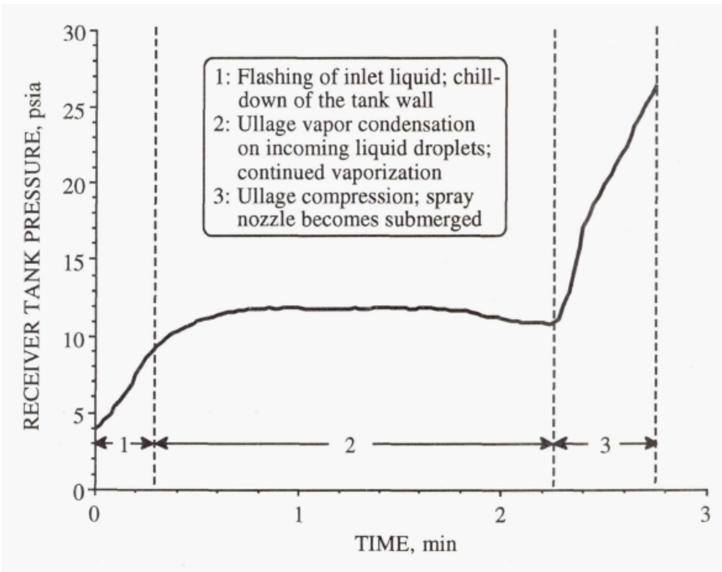
Therefore, if travel time is short enough *or* pressure is low enough *or* LH_2 level is low enough, **NO** venting is necessary.

For a system operating at up 80 psia (typically, LH_2 pump), no venting is required most of the time, per code

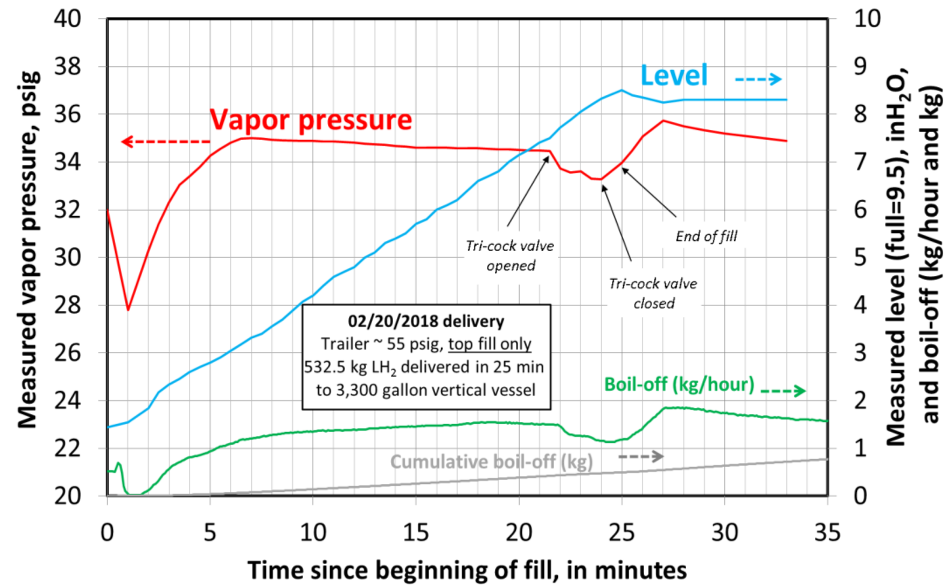
For a system operating at larger pressure (typically, compressors), a maximum of 10 kg venting may be needed if trailer delivers a small load when full.

If <24 hours between 2 LH_2 deliveries, and > 350 kg is delivered at up to 80 psia, NO venting necessary

Accomplishments (Task 1): Top filling a LH_2 vessel enables minimal boil-off losses from receiving vessel during transfer



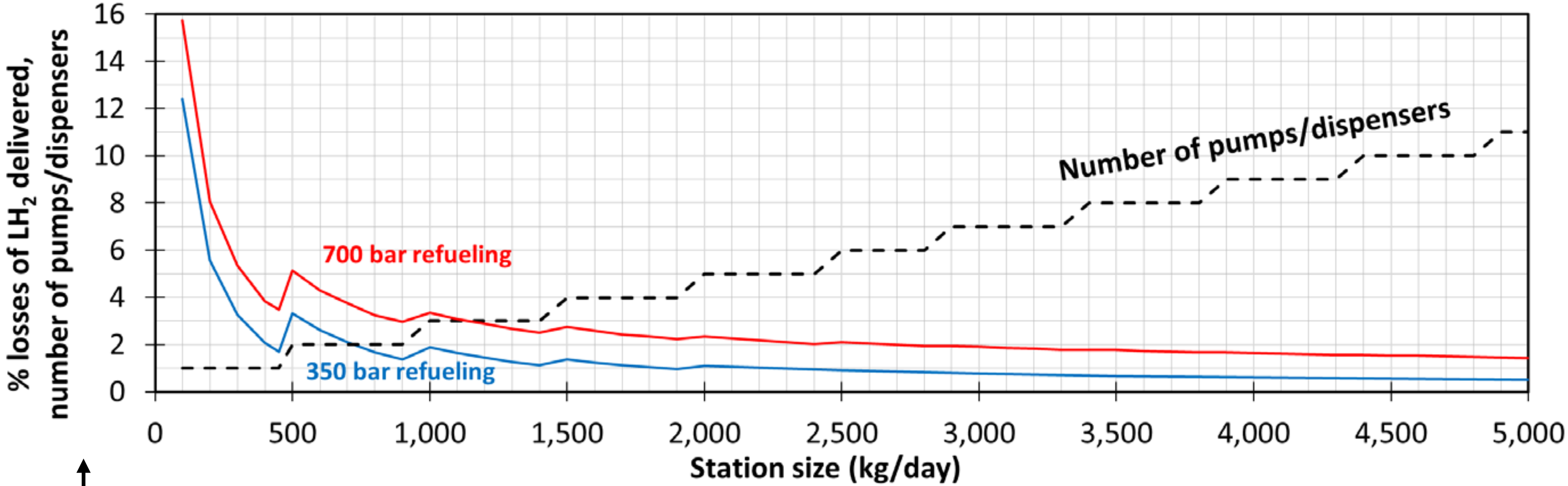
Results from NASA LRC (Ohio), Moran and Chato

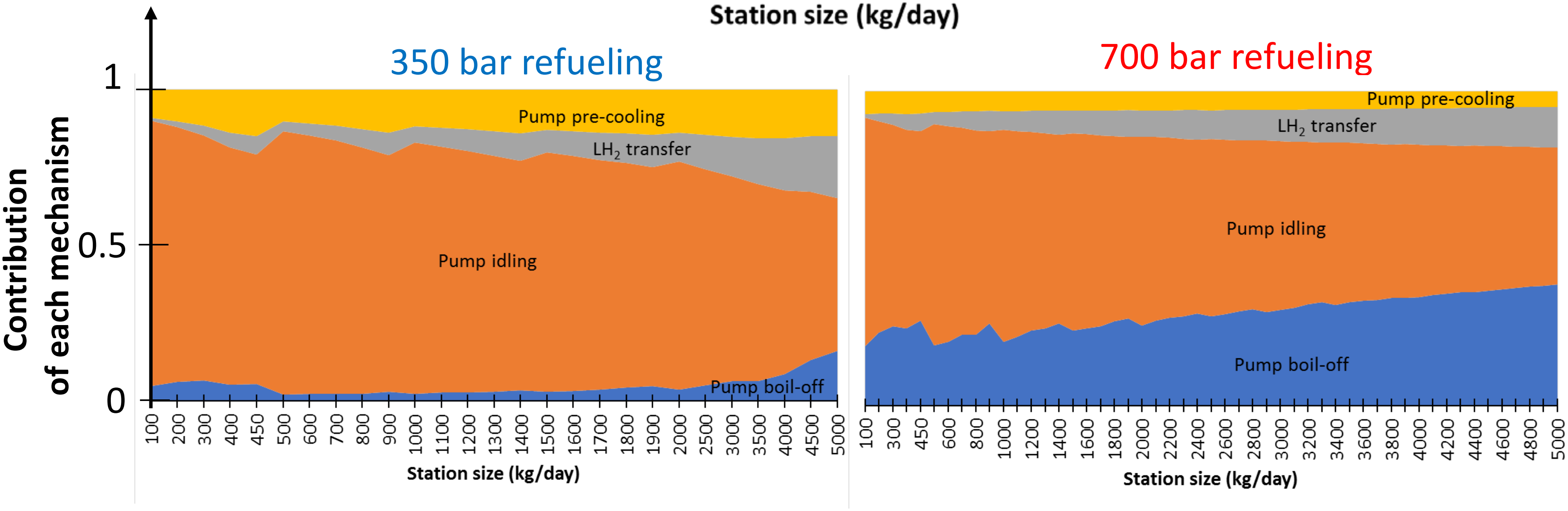


Experimental measurements from LLNL

Using top fill only, less than 1 kg of boil-off for a 532 kg LH_2 delivery over 25 minutes was measured (2 kg/hr peak boil-off flow)

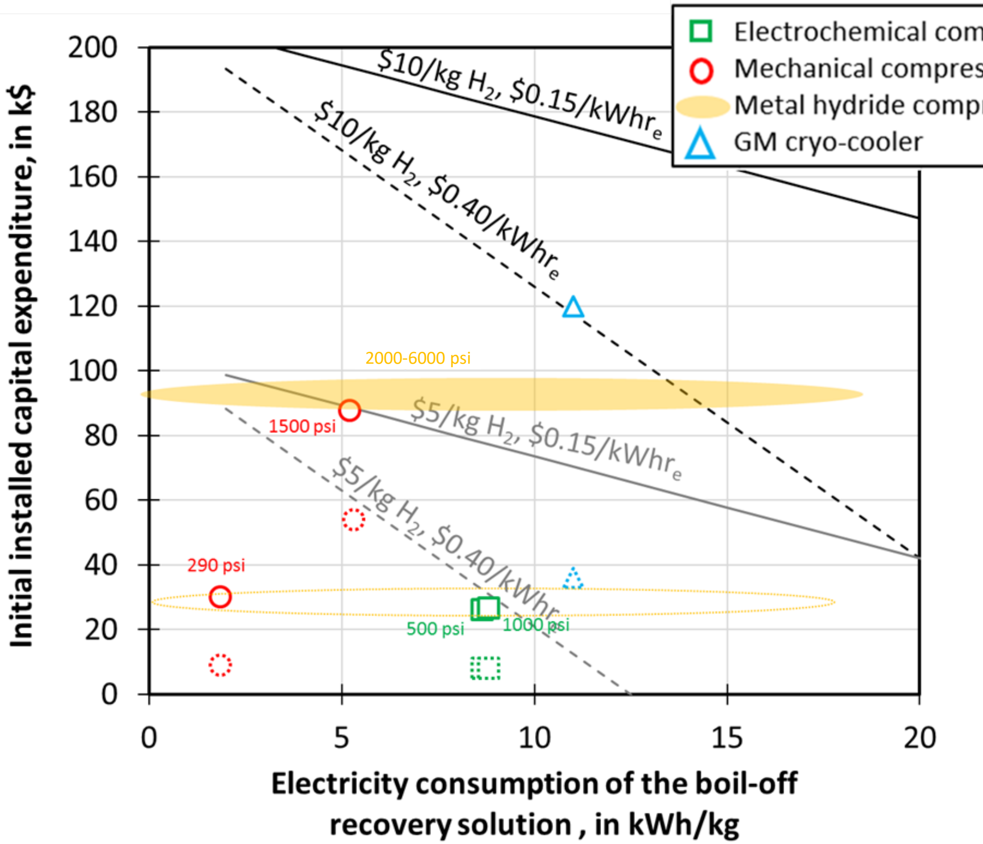
Accomplishments (Task 1): Boil-off loss budget for LH_2 operation





Less than **2%** boil-off losses
for {>2,500 kg/day, 700 bar} and {>1,000 kg/day, 350 bar} HRS

Accomplishments (Task 3): Analysis of boil-off recovery options



Continuous symbols: 2 kg/hr, Dashed: 0.6 kg/hr

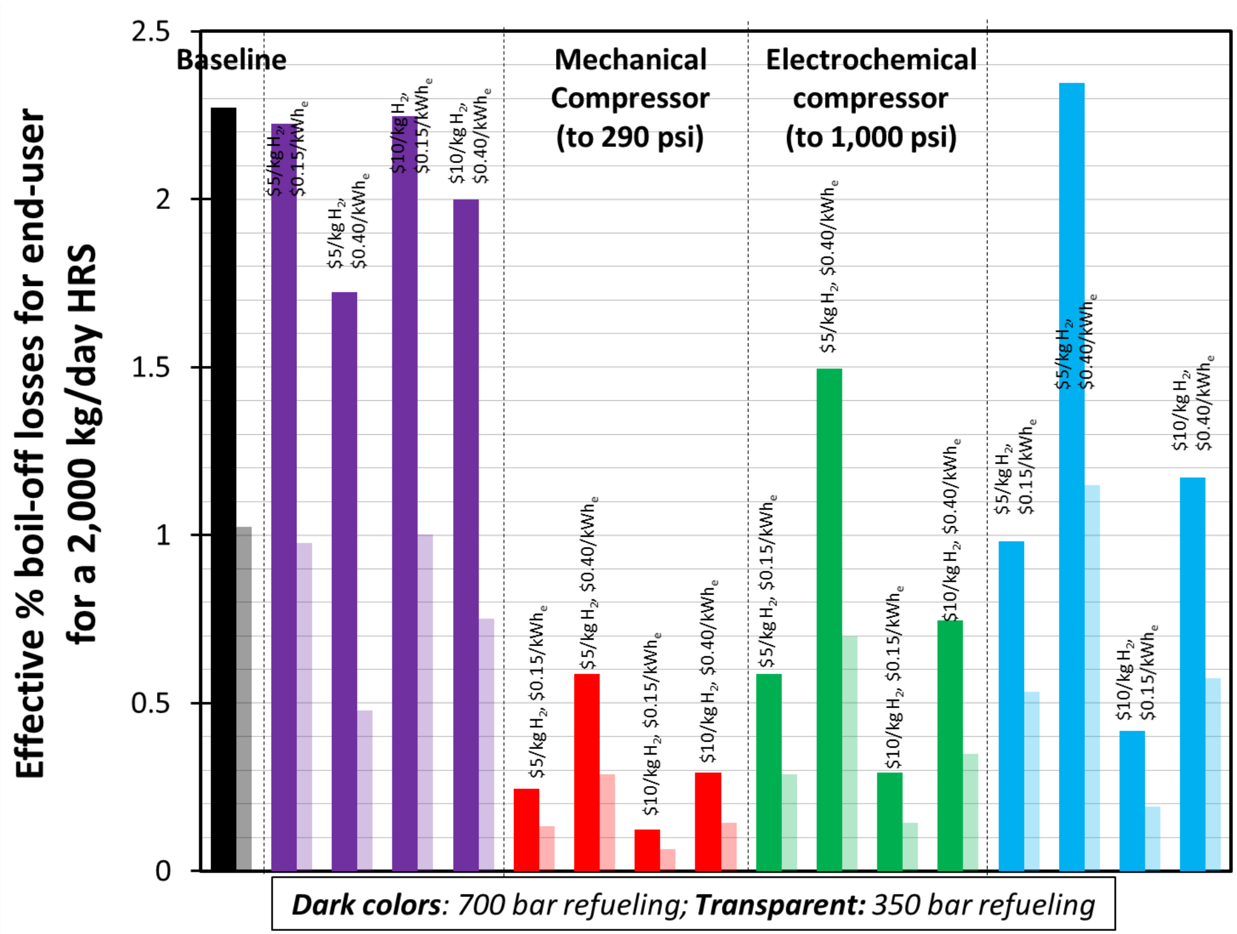
Assumes 5 year pay-back

- All solutions assume recovered H_2 is ultimately sold, at \$5 or \$10/kg.
- For compressors, H_2 could be stored to cascade, in trailer or gas bottles (cost not included in calculations)
- For GM cryo-cooler, vapor H_2 is re-condensed
- Metal-hydride compressors do not use electricity but heat. Also, not well developed for application (more R&D needed to refine costs)

Note: "value" of boil-off recovery solution should be analyzed on a case-per-case basis. Other factors include: footprint, permitting, outlet for gas resale, noise, vibrations, connection to grid...

Mechanical and electrochemical compressors seem to make most economical sense, although other factors should be considered

Accomplishments (Task 3): Boil-off recovery options would enable lower effective boil-off



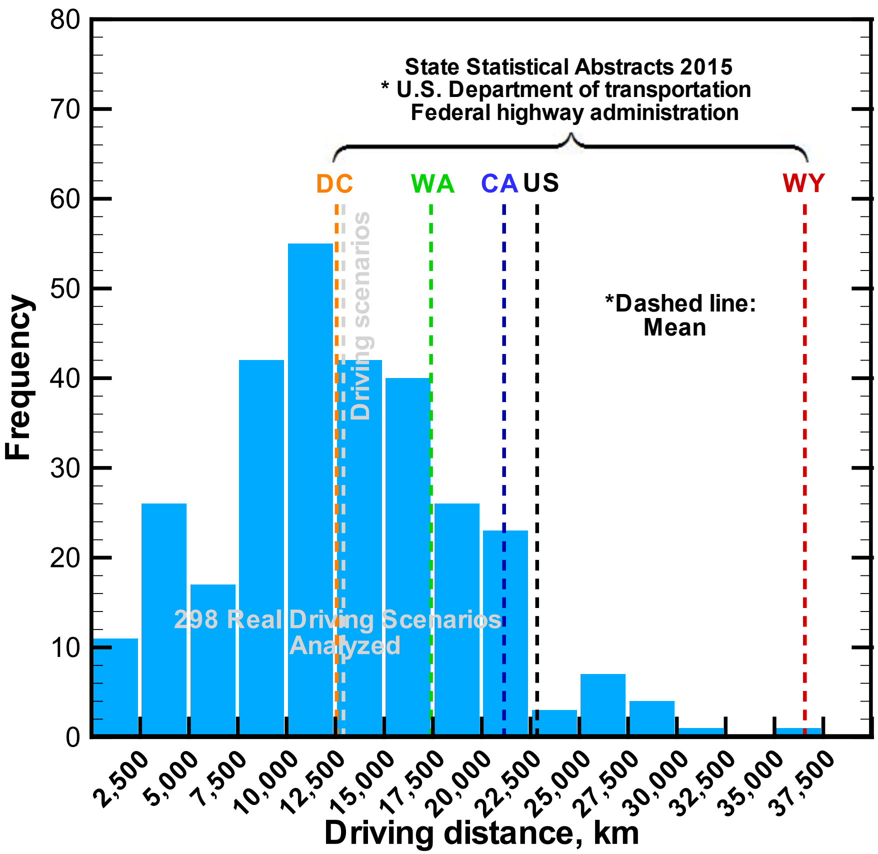
Assumptions:

- Only expenses: electricity & maintenance (5% CAPEX/yr)
- Effective boil-off assumes all H_2 is captured and sold (except for FC)
- Additional expenses are expressed on a kgH_2 basis

Note: "value" of boil-off recovery solution should be analyzed on a case-per-case basis. Other factors include: footprint, permitting, outlet for gas resale, noise, vibrations, connection to grid…

Boil-off recovery solutions may reduce extra cost to end-user, from **2.2%** to less than **1%** (at 700 bar)

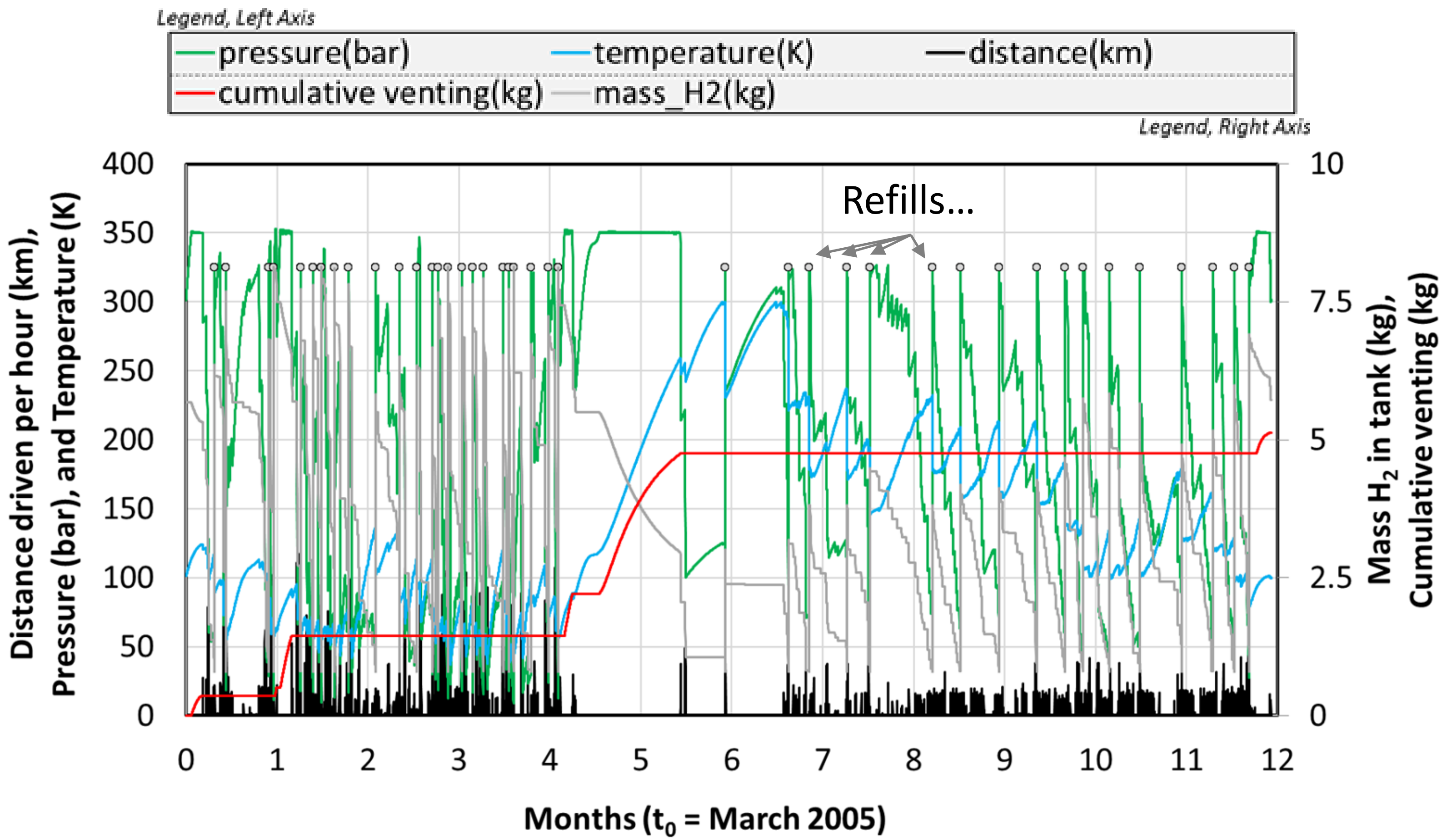
Accomplishments (Task 2) : A set of real usage data for light duty vehicles was used to estimate boil-off losses from a CcH2 population



- Data from a 2004-2006 study by Puget Sound Regional Council, downloaded from : https://www.nrel.gov/transportation/secure-transportation-data.html
- 434 participants, 298 “usable” driving scenarios
- Driving distance recorded as a function of time of the day, over one full year (March 2005 to March 2006)
- Sample population drives significantly less than average (mean=12,500 km over 1 year, US mean is 23,700 km), similar to state with lowest driving (D.C.)

Mean data is 12,500 km/year, ~ lowest driving among 50 states, thus ***extremely conservative*** data to estimate boil-off

Accomplishments (Task 2): A FORTRAN code was built to simulate park/drive/fill with real gas EOS (REFPROP V9.1) & para/ortho kinetics

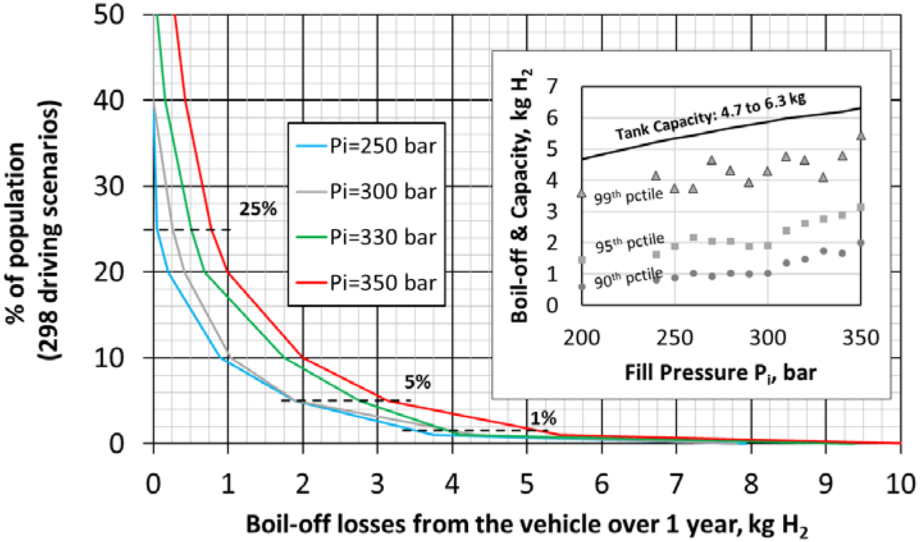


Example of driving scenario # 63866-2

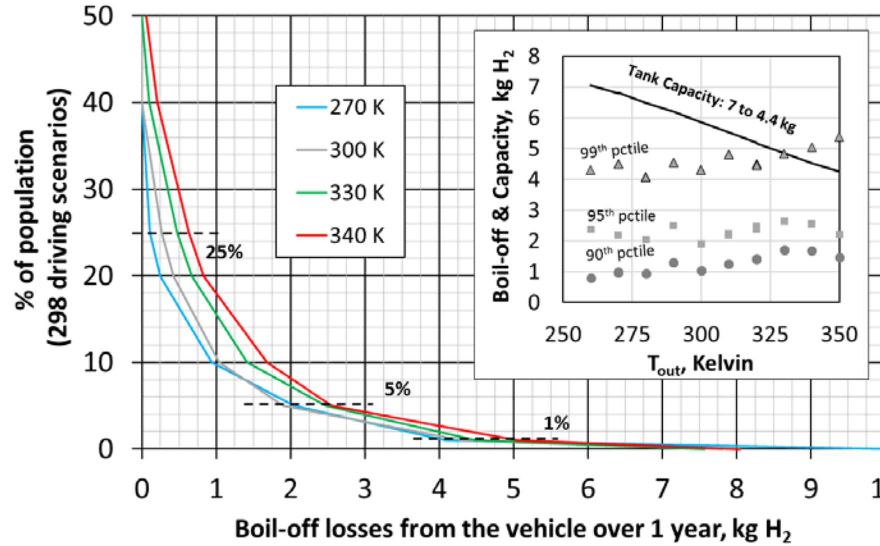
Assumptions: refill when 1 kg H_2 left, 60 mile/kgH_2…

Each scenario could be simulated as a function of many parameters (volume, L/D, outside temp, initial T, P and X_{ortho} , …)

Accomplishments (Task 2): Ensemble results were obtained, providing statistics on expected boil-off losses for a CcH2 population



Influence fill pressure (for a 350 bar tank)



Influence outside temperature

Average boil-off per driver and per year: 0.34 kg, i.e. 0.25% of all hydrogen used

Using very conservative inputs (=little driving),
50% of CcH2 population would experience no boil-off losses,
1% of population would see > 5 kg boil-off/year

AMR 2018 feedbacks from reviewers

Weaknesses include the limited commercial viability of the onboard LH2/CCH2approach. … Many assumptions are being made regarding parking and conditions under which the cars are used. Customers will cover the entire spectrum of usage options (not just some kind of average usage) and will need to understand the effects of all these extremes. Data from real drivers are used. Ideally, hourly varying outside conditions should be used, but that information was not available. Instead, various values for a constant outside temperature can be simulated.

There does not appear to be any prioritization of the loss mechanisms or their mitigation. First step was to identify, then prioritization & mitigation were based on losses relative importance.

The project should show how industrial gas companies can adopt the analysis and what market effects, such as low-cost energy, lead to such large amounts of boil-off. Market effect out of scope, engineering/thermodynamic analysis only.

The activity faced initialization issues that are apparently not fully resolved. The subtle differences between thermodynamics and heat transfer are poorly communicated and minimized, as are the behavioral differences between American and European drivers. Project almost over. Goal was not to simulate American vs. European drivers; although user-agnostic…

There is an unclear degree of focus on LH2supply chain losses versus cryo-compressed park/drive/fill pattern analysis. It was not clear to us either, hence the need for building accurate simulation tools. Now we believe LH2 supply chain losses (pump utilization) need more focused.

More vision and physical action are needed regarding how to demonstrate the concept to prove the theoretical work. Model validation is complicated due to limited experimental data.

Collaborations with Industry Leaders

- **Linde:** Very cooperative, sharing detailed information, interpreting and sharing data from multiple pumps, and on LH_2 deliveries.

Special acknowledgements to Martin Bruecklmeier, Wilfried Reese, Kyle McKeown, Erik Tudbury.

- **Praxair:** Sharing data on LH_2 plant operation. Visit of Ontario (CA) plant.

Special acknowledgement to Al Burgunder.

Risks/Challenges for FY18 milestones, Future work

- ***Challenge: need adequate simulation tool for top fill***
  - **Challenge**: our 0D thermodynamic simulation framework can not capture the underlying physics of sprays (boiling heat transfer, droplets interaction…
  - **Solutions** : In the future (beyond scope), a full CFD code should be used, similar to the work performed by Yanzhong Li and Lei Wang from the Xi'an Jiaotong University (Xi'an, China) and the State Key Laboratory of Technologies in Space Cryogenic Propellants (Beijing, China)
- ***Future work up to end of FY18***
  - Publish reports and articles at IJHE
  - Already published:

5 page memo on how DOT regulations apply to trailer venting: https://www.osti.gov/biblio/1424618

2 codes released as open-source: https://github.com/LLNL/LH2Transfer, https://github.com/LLNL/cryoH2vehicle

Any proposed future work is subject to change based on funding levels

Summary: LLNL has developed models to simulate boil-off losses from plant to car for LH_2 pathway, quantified their magnitude & proposed mitigation solutions

Relevance — LH_2 has great benefits for large scale(s) hydrogen deployment (cost, logistics, safety..). Better understanding of losses is necessary

Approach — Simulate losses mechanisms along the LH_2 pathway using real gas EOS and 2 phases, statistics for real-life of park/drive/fill scenarios

FY18 Progress — 2 models constructed and released as open-source
Quantified losses along ENTIRE pathway, including from CcH_2 vehicle (**<2%** up to dispensing for large stations**, 0 to 5%** for 99% of drivers, **0.25%** of hydrogen consumed is boiled away through driving)
Identified potential to reduce/eliminate losses from trailer
Identified main contributors to losses (high P in Dewar, pump)
Analyzed techno-economics of boil-off recovery technologies

Future work — Publish 1 report (60+ pages) and 2 papers (IJHE)
Develop CFD capabilities for modeling top-fill *(beyond scope of the project)*

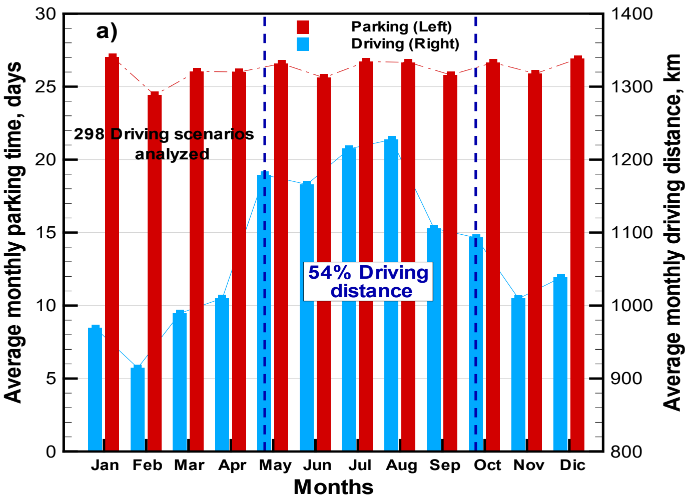
Lawrence Livermore National Laboratory

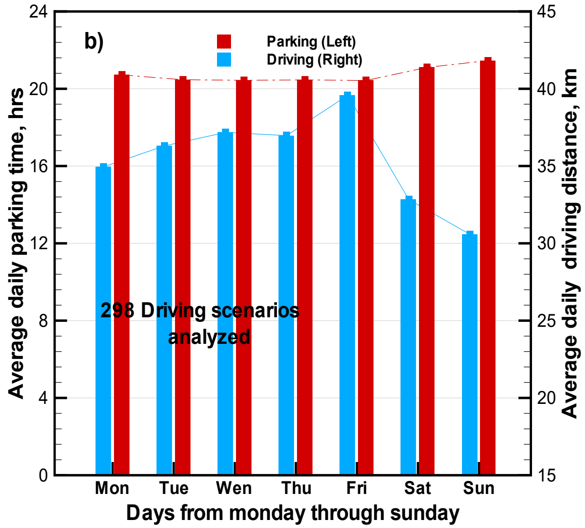
The work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344

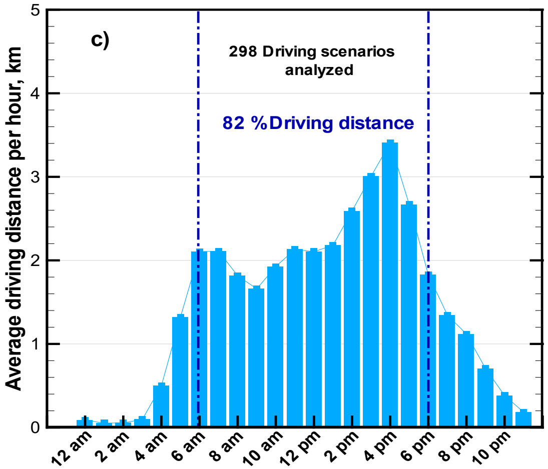
LLNL-PRES-749854

Technical back-up slides

Accomplishments (Task 2): A set of real usage data for LDVs was used to estimate boil-off losses from a CcH2 population





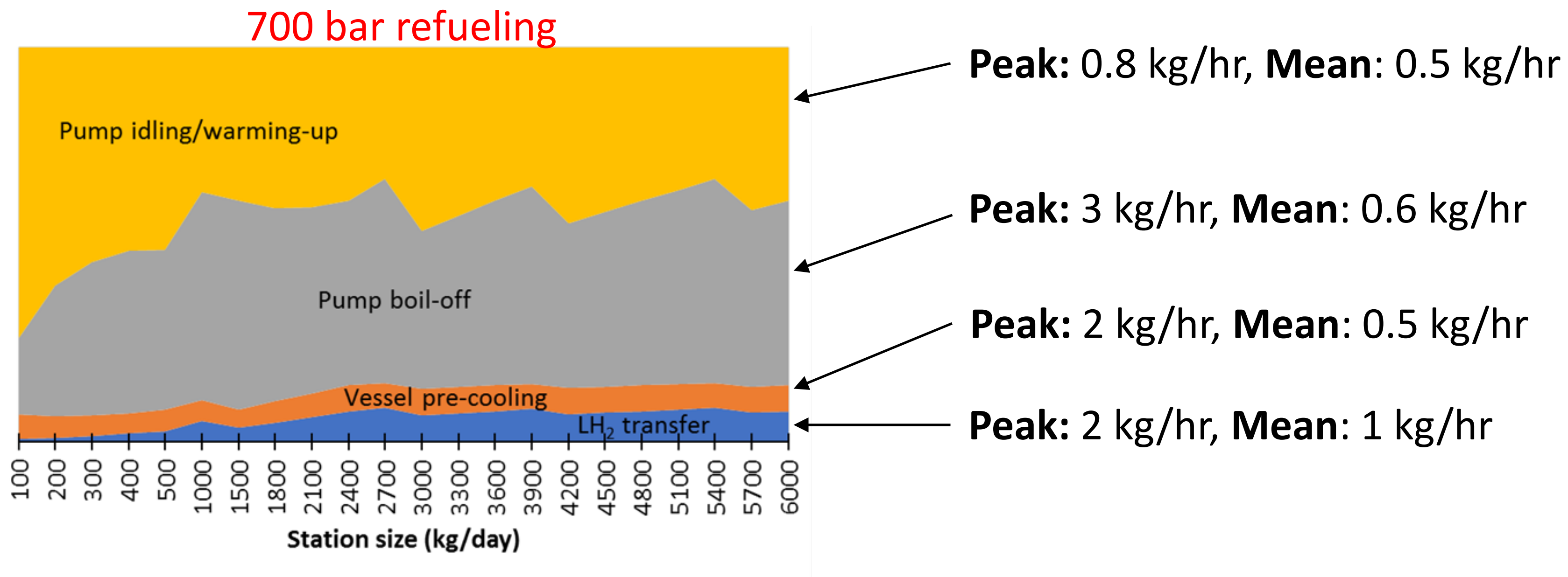


Profiles show similarities with HDSAM…

- More driving in Summer
- More driving on week days, especially Friday
- Throughout the day, peak driving at 6 AM-7 AM and 4-5 PM

Real usage data obtained for a population of 298 unique light-duty vehicles over 1 year exhibit realistic patterns

Accomplishments (Task 3): Mitigation & boil-off recovery approaches



- Better cryogenic design would certainly help reducing first 3 boil-off mechanisms. For example, LH_2 pump is located about 10 meters from main vessel at LLNL

- Better models may help understanding the influence of initial conditions on top fill performance, ultimately reducing LH_2 transfer losses

- If losses can not be further reduced, boil-off recovery solutions may be needed

2-3 kg/hr *peak* venting flow rate needs to be captured for routine LH_2 operations, based on measurements at sub-optimal LLNL setup

Accomplishments (Task 3): Considerations for boil-off recovery approaches…

- Various technologies can be used to recover boil-off losses:

Compressors	**Cryo-coolers**	**Fuel Cell**	**Flaring ?**
(mechanical, electro-chemical, metal hydride)	(Stirling, Gifford-McMahon, pulse-tube)	(net metering, local power provider)	(catalytic burner, …)

- To make sure all boil-off is captured, the solution should be sized for peak flow (2-3 kg/hr), even if it would operate at a lower nominal value (0.6 kg/hr) most of the time…

- What to do with recovered H_2 ?

Feed cascade, if cascade is present…
10 to 60 kg of boil-off may be recovered every day. 1 typical industrial gas bottle holds 0.5 kg H_2

- Recovery makes economic sense only if the associated costs (CAPEX+OPEX) are lower than the cost of the recovered H_2…

- The value of recovery may also lie in easing station permitting