Holistic Fuel Cell Electric Vehicle/Hydrogen Station Optimization Model

Cooperative Research and Development Final Report

CRADA Number: CRD-18-00745

NREL Technical Contact: Michael Peters

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
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Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5700-79223
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Cooperative Research and Development Final Report

Report Date: February 18, 2021

In accordance with requirements set forth in the terms of the CRADA agreement, this document is the CRADA final report, including a list of subject inventions, to be forwarded to the DOE Office of Scientific and Technical Information as part of the commitment to the public to demonstrate results of federally funded research.

Parties to the Agreement: Alliance for Sustainable Energy, LLC; UChicago Argonne, LLC; National Technology & Engineering Solutions of Sandia, LLC; Frontier Energy, Inc.

CRADA Number: CRD-18-00745

CRADA Title: Holistic Fuel Cell Electric Vehicle/Hydrogen Station Optimization Model

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Sponsoring DOE Program Office(s):

Office of Energy Efficiency and Renewable Energy (EERE), Hydrogen and Fuel Cell Technologies (HFCT)

Joint Work Statement Funding Table showing DOE commitment:

Estimated Costs	NREL Shared Resources a/k/a Government In-Kind
Year 1	$105,000.00
TOTALS	$105,000.00

<u>Executive Summary of CRADA Work</u>:

The National Renewable Energy Lab (NREL), Argonne National Lab (ANL), Sandia National Lab (SNL), and Frontier Energy, Inc comprise a team that will perform a review of currently available models that can simulate both a hydrogen station and a fuel cell electric vehicle (FCEV), and whose owners are willing to make them available freely. We will then down select to a single model or model pair, secure agreements for their free use, and validate the resulting model or coupled models. For example, we may evaluate an existing 1-D hydrogen fueling model developed by Kyushu University for the Japanese New Energy and Industrial Technology Development Organization (NEDO). The validation will take place using data from various sources, potentially including the European Joint Research Center (JRC) HyTransfer project, SAE testing performed by Powertech to validate SAE J2601, and whole-station validation using the NREL's Hydrogen Infrastructure Testing and Research Facility (HITRF). The team will make the model and all the validation data open to the public at the end of the project.

<u>Summary of Research Results</u>:

Task 1: Collection of data, literature review, and model evaluation and down select

Description

In this task, the team will collect all available data that may be relevant to the project goals. Data may include detailed second-by-second fueling data, including hydrogen flow rates, pressures, and resulting gas and wall temperatures. These may be available from HyTransfer or the SAE validation tests. The HyTransfer data are at least 3-D partially spatially resolved with respect to the vehicle tanks. The team will conduct a gap analysis of the existing data to determine if there are gaps in the experimental data, and if so, the team will develop a plan for conducting experimental fueling tests to generate the additional data needed.

The team will also obtain a catalog of all existing models that may be appropriate for the project goals. The team will develop, with the expert panel, a set of key model criteria against which the team can judge model applicability. One of these criteria will be the willingness of the model owner to make the model freely available to the public. The team will then downselect to a model or a set of models that can accomplish the project's goals.

Outcome - Successful

The team aggregated light-duty fill data from NREL's hydrogen station, Honda's station in Torrance, CA, and leveraged the publicly available SAE J2601 fill data (http://www.h2protocol.com/). Overall, the project leveraged over 50 unique light-duty fill sequences to serve as validation data for the model. Of particular interest was the vehicle tank pressure and temperature throughout the duration of the fill. Figure 1 shows one of the SAE Validation data sets that NREL analyzed against the developed fueling model.

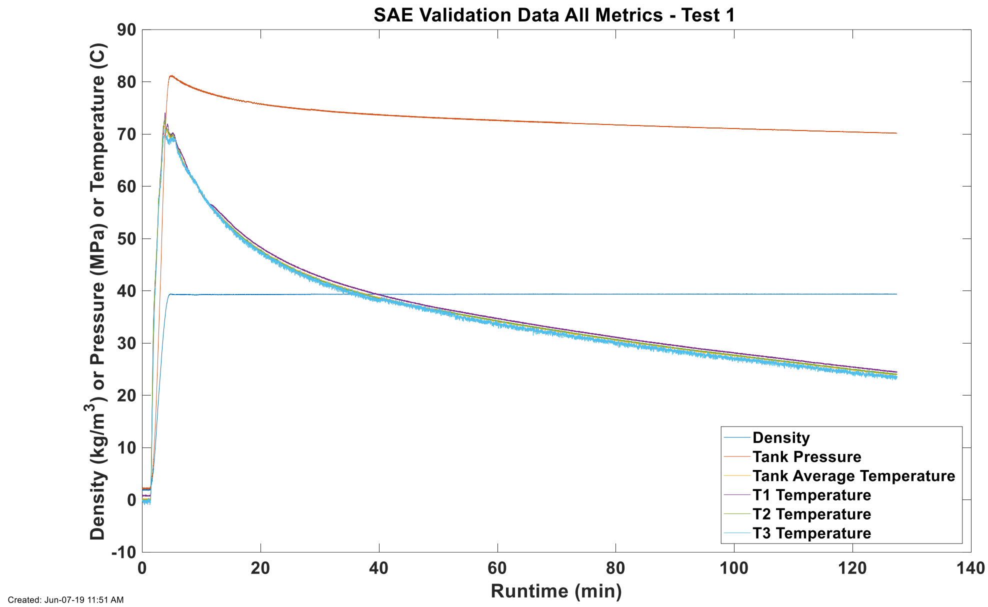


Figure 1 - SAE Fill Data Example

The project team considered a number of different available vehicle tank models including one at Sandia National Laboratories and one commonly used in EU hydrogen projects. Ultimately, the team decided to partner with Kyushu University on their vehicle tank model and NREL would develop the station component model in-house. The decision to go with Kyushu University's model stemmed from the ease of integration at NREL, the models existing capability and acceptance, and a continued goal of strengthening international collaboration between research institutions in the hydrogen space. The collaboration with Kyushu led to a software license agreement (LIC-19-356) for NREL to use Kyushu's Hydrogen Refueling Station Dynamic Simulation ("HRS DS") software.

Task 2: Model joining (if necessary)

Description

If the team is unable to attain a single model that can simulate both a station and an FCEV, it may select two independent models. In that case, the team will join them in such a way as to be transparent to the user. This may involve developing an application program interface (API) for both.

Outcome - Successful

The team decided to build the station side model in-house at NREL and obtain the vehicle model from Kyushu University, so this task was necessary. The team successfully integrated the two models onto one platform. The bulk of the computation of the model takes place in MATLAB with the GUI being Python based. Refer to Figure 3 to view the GUI that was developed in Python.

Task 3: Model data validation

Description

Using data retrieved in task 1, the team will perform a series of analytical runs with the selected model to validate its performance against the actual data. These runs will necessarily be limited to the experimental data, which include relevant data inputs from the temperature and pressure measurement points just upstream of the breakaway on the station to the Compressed Hydrogen Storage System (CHSS), as the data do not include the station as a whole.

Outcome - Successful

The team compared the integrated model against available experimental data and reported the accuracy of the model to the industry partner with monthly meetings. This review process led to an improvement feedback loop that allowed the team to continue to push the accuracy of the model. The most essential part of a fueling model of this nature is to ensure the final vehicle tank temperature is accurate. The team focused much of the validation effort on this task. Ultimately, the model showed good agreement with available experimental data – being within ±3.5 Kelvin for all available data sets. Figure 2 shows a comparison of NREL's ending temperature from the model (y-axis) versus the experimental data (x-axis).

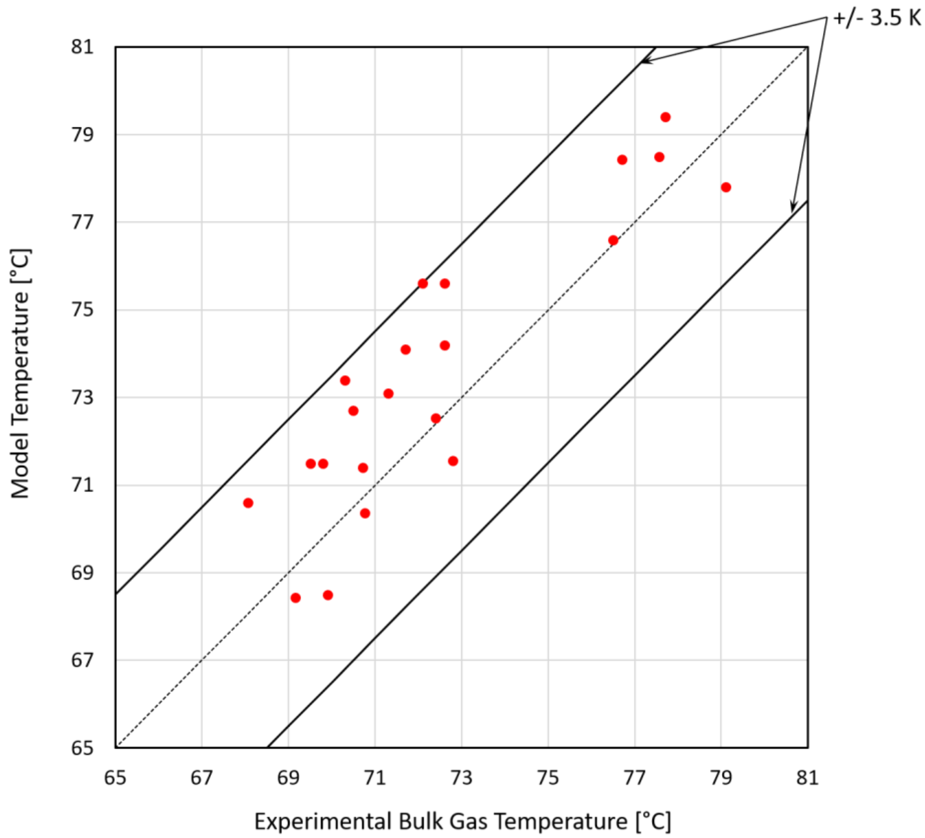


Figure 2 - Experimental Data versus Model

Task 4: Experimental validation

Description

Available data do not include a holistic view of the system from the high-pressure station storage, through various control valves, a hydrogen chiller, dispenser, and hose, and ultimately to the vehicle tank. Because of this fundamental limitation on existing data, the team will utilize the first-in-class capabilities of NREL's HITRF station and vehicle simulator to assess the model from tip to tail. HITRF is the only facility in the U.S. capable of performing this validation. The team will work with the model owner/developer to make necessary adjustments to the data collection needed from the HITRF and/or to the model.

Outcome - Successful

NREL leveraged station data from their own research station, Hydrogen Infrastructure Testing and Research Facility (HITRF), to validate against the model as well. Having the ability to use and generate our own hardware data was beneficial to the project especially when the model was upgraded to include multiple hydrogen tanks. The multiple tank upgrade was integrated as a V2 release of the model and it allowed the team to leverage their own hydrogen vehicle simulator at HITRF to compare results. Figure 3 shows the model GUI with the multiple tank capability. Figure 4 is NREL's light-duty vehicle simulator that was used to make comparisons using multiple hydrogen tanks on the vehicle.

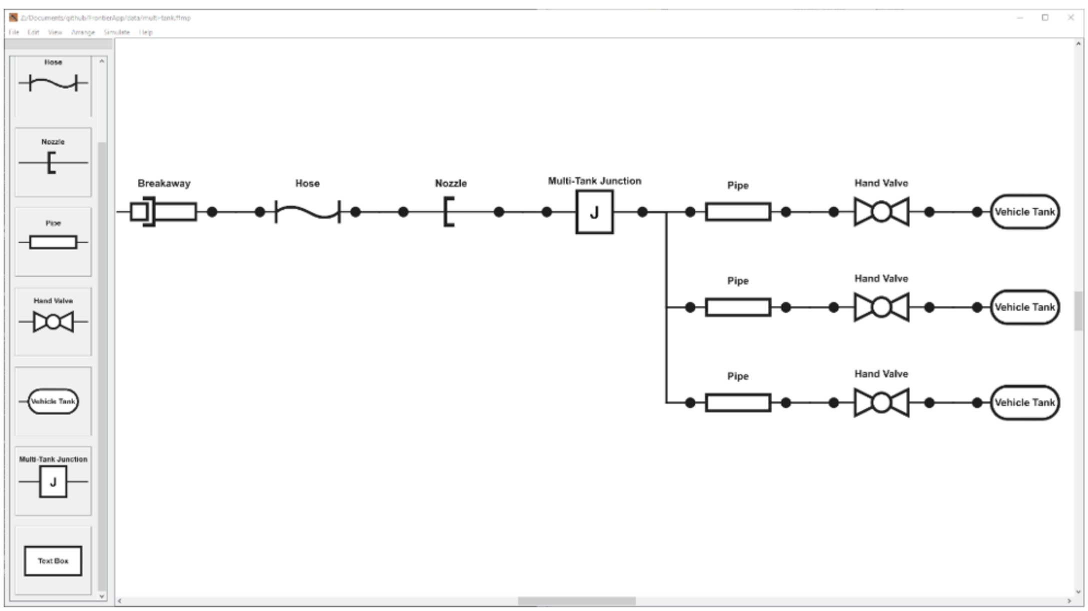
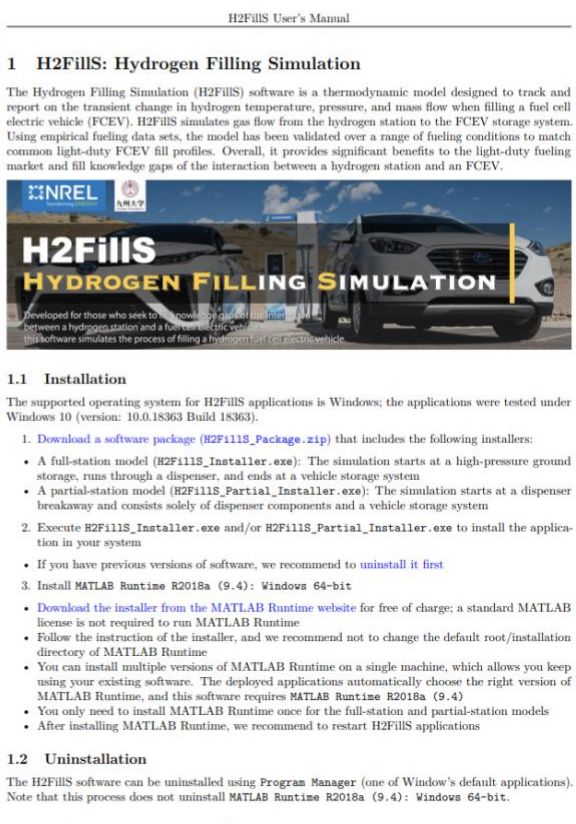


Figure 3 - Multiple Tank Configuration within the NREL Model

Figure 4 - NREL's Light-duty Hydrogen Vehicle Simulator at HITRF



H2FillS User's Manual

1 H2FillS: Hydrogen Filling Simulation

The Hydrogen Filling Simulation (H2FillS) software is a thermodynamic model designed to track and report on the transient change in hydrogen temperature, pressure, and mass flow when filling a fuel cell electric vehicle (FCEV). H2FillS simulates gas flow from the hydrogen station to the FCEV storage system. Using empirical fueling data sets, the model has been validated over a range of fueling conditions to match common light-duty FCEV fill profiles. Overall, it provides significant benefits to the light-duty fueling market and fill knowledge gaps of the interaction between a hydrogen station and an FCEV.

1.1 Installation

The supported operating system for H2FillS applications is Windows; the applications were tested under Windows 10 (version: 10.0.18363 Build 18363).

1. Download a software package (`H2FillS_Package.zip`) that includes the following installers:

- A full-station model (`H2FillS_Installer.exe`): The simulation starts at a high-pressure ground storage, runs through a dispenser, and ends at a vehicle storage system
- A partial-station model (`H2FillS_Partial_Installer.exe`): The simulation starts at a dispenser breakaway and consists solely of dispenser components and a vehicle storage system

2. Execute `H2FillS_Installer.exe` and/or `H2FillS_Partial_Installer.exe` to install the application in your system

- If you have previous versions of software, we recommend to uninstall it first

3. Install `MATLAB Runtime R2018a (9.4): Windows 64-bit`

- Download the installer from the MATLAB Runtime website for free of charge; a standard MATLAB license is not required to run MATLAB Runtime
- Follow the instruction of the installer, and we recommend not to change the default root/installation directory of MATLAB Runtime
- You can install multiple versions of MATLAB Runtime on a single machine, which allows you keep using your existing software. The deployed applications automatically choose the right version of MATLAB Runtime, and this software requires `MATLAB Runtime R2018a (9.4)`
- You only need to install MATLAB Runtime once for the full-station and partial-station models
- After installing MATLAB Runtime, we recommend to restart H2FillS applications

1.2 Uninstallation

The H2FillS software can be uninstalled using `Program Manager` (one of Window's default applications). Note that this process does not uninstall `MATLAB Runtime R2018a (9.4): Windows 64-bit`.

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Figure 5 - User Manual Installation Section

Task 5: Documentation

Description

The team will work with the model owner to develop a comprehensive user's guide to enable the correct use of the model, along with accurate input parameters. The documentation will also include important information on how the model works, along with any assumptions made in its development. A user's guide is important to ensure that the model is used correctly and that the results of the model reflect reality as closely as possible.

Outcome - Successful

As part of this effort the NREL team created a comprehensive user manual for the modeling software. The 35-page User Manual goes through the process of how to use the model, example of how to set parameters, and includes a list of error messages that users can reference to troubleshoot their issues. Figure 5 shows an excerpt from the user manual developed on the project. The full version of the user manual is available to the public and is located here: https://www.nrel.gov/hydrogen/assets/pdfs/h2fills-user-manual.pdf

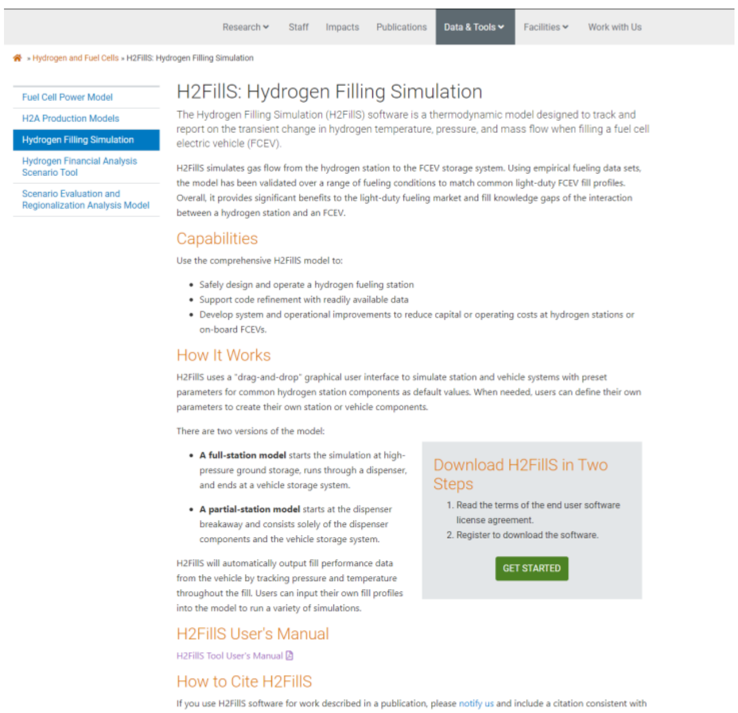

Figure 6 - H2FillS Website

Task 6: Dissemination

Description

The team will make the model and the associated data available to the public through an open-source license. This public disclosure will help prevent any organization from asserting intellectual property rights to the work in an attempt to restrict competition in the field. The team will participate in a series of public webinars, conference presentations, and peer-reviewed papers to disseminate the results.

Outcome – Successful (except for open-source)

The model developed in this project was released to the public on May 15th, 2020 under the name of H2FillS. Figure 6 shows the website as it would look when a user access it. The model is available for download here: https://www.nrel.gov/hydrogen/h2fills.html

The team was not able to obtain approval to make the model open source to the public. The team discussed this aspect with the project partners and ultimately decided it was best to focus on the validation and useability of the model over the open-source aspect. There was also some fear from project partners that if the model were made open source it could be misused/misrepresented in other forums. The model was released as a downloadable executable that is free and only requires free software to operate.

For greater detail on the process and analysis, the researchers are publishing a forthcoming journal article titled:

T. Kuroki, K. Nagasawa, M. Peters, D. Leighton, J. Kurtz, N. Sakoda, M. Monde, Y. Takata. "Thermodynamic Modeling of Hydrogen Fueling Process from High Pressure Storage Tanks to Vehicle Tank."

In the event the article is not accepted by any currently seeking publication in academic or industry journal, it may be published by NREL.

Software Record:

H2FillS is tracked with a software record: SWR-19-67

Supplementary Deliverable/Milestones

SNL and ANL to confirm model is working on platforms outside of NREL's internal platform. ANL and SNL to identify model user interface bugs and provide written feedback for task 5 to the NREL team. ANL and SNL to provide a 1 page third-party assessment of validation work completed under task 4

SNL and ANL were successful in their advisory role. They attended all of the monthly meetings and provided valuable feedback to the NREL team. In addition, SNL and ANL were the first to test the model outside of NREL and provided verbal and written feedback to the team that improved the model functionality. The NREL team considers all of these deliverables met and welcomes future collaborations with SNL and ANL in the hydrogen space.

NREL will secure an open-source license for the final model and make publicly available.

See Task 6 Outcome for details

Frontier Energy shall facilitate reviews by stakeholder groups, coordinate and compile recommendations and feedback regarding the models.

Frontier Energy was successful in their role as the project lead. They were able to coordinate reviews and recommendations through the monthly meetings and continued communication throughout the duration of the project. NREL extends a thank you to the Frontier Energy team for their support on this project.

Task 7: Nozzle-Freeze Lock

Description

The team will complete a round of nozzle freeze lock benchmarking per the ISO/DIA 17268 test protocol in a temperature and humidity-controlled environment.

Outcome - Successful

As part of a collaborative effort to understand under what conditions nozzle freeze-lock occurs at commercial hydrogen stations, NREL developed a nozzle freeze-lock test stand (atmospheric chamber) to conduct real world fueling tests at specific ambient temperature and dew point temperature settings. The test stand utilized the existing research-based hydrogen station at the Hydrogen Infrastructure Testing and Research Facility (HITRF). The test points were derived from industry partner collaborations and established codes, standards, and protocols (ISO/DIA 17268 and SAE J2601). Table 1. below details the specific temperature and dew points tested and the figure 7. shows the test stand developed and used for the analysis. Each test point was evaluated over 10 fills or until 2 subsequent freeze events occurred, then the test concluded.

Table 1. Nozzle-Freeze Lock Test Points

Dew Point Temperature (°C) \ Ambient Temperature (°C)	15	25	30	35	38	40	45
13.4	Test 1	Test 2	Test 3	Test 2	Test 3	Test 3	Test 1
20		Test 1	Test 2	Test 2	Test 2	Test 2	
25			Test 1	Test 1	Test 1	Test 1	
30				Test 1	Test 1	Test 1	

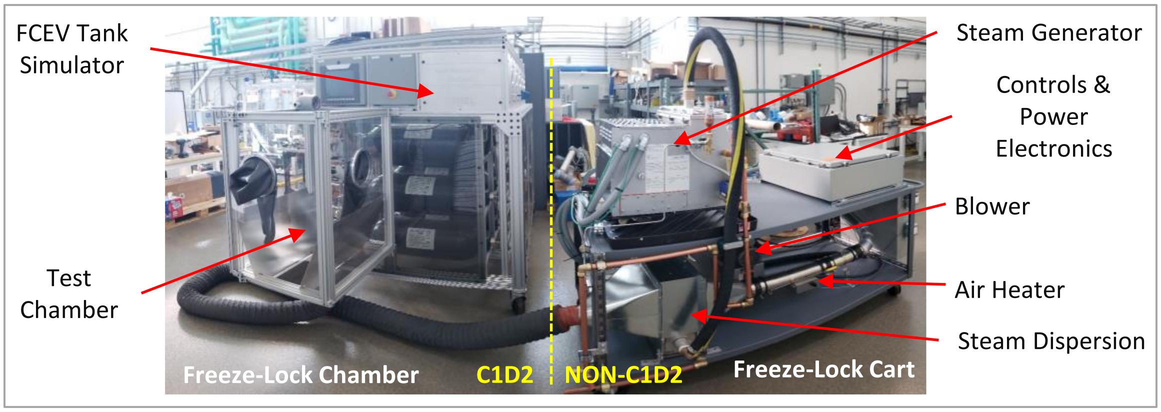

Figure 7. Nozzle Freeze-Lock Test Stand

Over 170 filling events were completed over the range of tests conditions evaluated. The test data was analyzed to help determine if trends existed between temperature, dew point temperature, and fill number. The data indicated that freeze-lock occurrence appears more likely at ambient temperatures of 35°C-40°C, dew point temperature of 20°C-30°C, and between fill numbers 3-6. Figure 8 shows results for freeze-lock occurrence by fill number and figure 9 shows each nozzle-condition occurrence plotted by temperature and dew point event as a fraction of total observed events.

A summary of freeze-lock testing shows:

- Number of freeze events: 47 of 170 fills (28%)
- Temperature with most frequent freeze events: 35°C (11 events)
- Dew Point Temperature with most frequent freeze events: 30°C (14 events)
- Freeze-Lock Average Time: 27.54 secs
- Longest Event: 108 sec at 36°C and 30°C Dew Point

Understanding the conditions where nozzle freeze-lock occurs will help prevent and mitigate the issue in commercial hydrogen fueling stations. The observed trends help station providers predict days when nozzle freeze-lock might be an issue and implement proactive countermeasures.

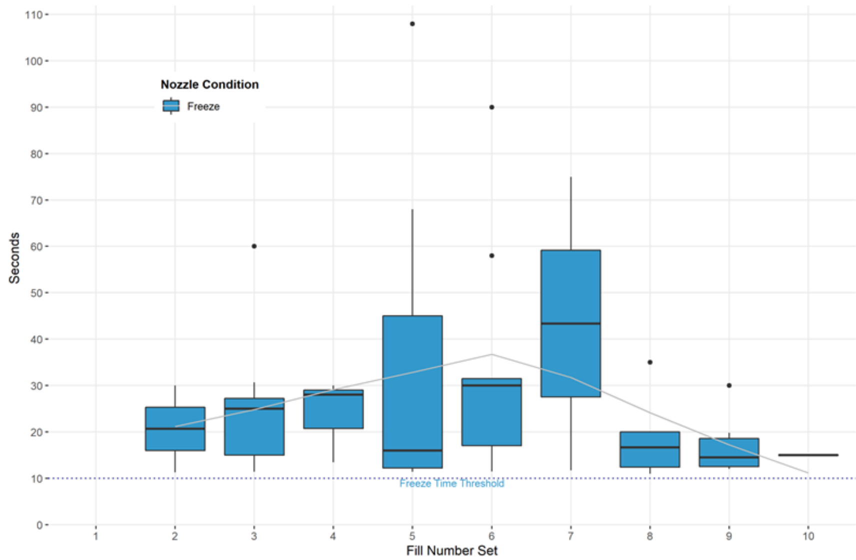

Figure 8. Freeze Condition by Fill Number (Temperature and Dew Point)

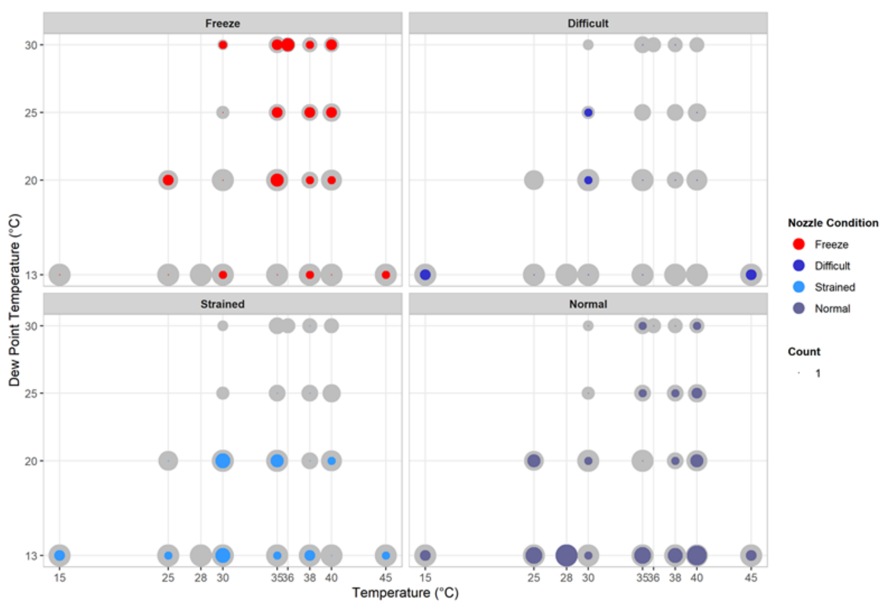

Figure 9. Nozzle Free-Lock Condition by Test Temperature and Dew Point as a Fraction of Total Observed Events

<u>Subject Inventions Listing</u>:

None

<u>ROI #</u>:

None