Optimizing the Heisenberg Vortex Tube for Hydrogen Cooling

Presenting: Jacob Leachman (WSU)
Co-PIs: Konstantin Matveev & Jeffrey McMahon (WSU), Tim Cortes & Sacheverel Eldrid (Plug Power)
Project Assistants: Carl Bunge, Greg Wallace, Jeevake Attapattu (WSU)

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DOE Project Award #DE-EE0008429

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Project Goal:

Establish, via experimentation, atomistic simulations, and Computational Fluid Dynamics, that the Heisenberg Vortex Tube (HVT) can improve the following cryogenic hydrogen systems:

1. Liquid hydrogen pump volumetric efficiency by 20% through vapor separation and subcooling.
2. **Liquid hydrogen storage tank boil-off losses by 20% through thermal vapor shielding (TVS).**
3. Supercritical hydrogen expansion by increasing isentropic efficiency from 31% between 40-50 K to greater than 40%.
### Project Overview

**Timeline:**
- Start: 1/23/2019
- BY1 extended through 9/30/2020
- End: 9/30/2021

**Barriers Addressed:**
1. Reliability & cost of LH₂ pumping
2. High cost & low efficiency of liquefaction
3. Other fueling site/terminal operations

**Budget:**
- Total: $2,372.2k
  - Federal Share: $1,897.8k
  - Cost Share: $474.4k
  - BY1 Expenditures: $965k
  - BY2 Expenditures: $180k
  - Total DOE Spent: $901k

**Partners:**
- Project Lead: Jacob Leachman (WSU)
- Co-PIs: Konstantin Matveev and Jeffrey McMahon (WSU), Tim Cortes and Sacheverel Eldrid (Plug Power)
- Partner Organizations: Washington State University, Plug Power
Relevance & Impact

- Plug Power is the largest single user of liquid hydrogen (LH$_2$) dispensing >27 tons/day. However, LH$_2$ utilization ranges between 93-75%. The barrier to increased utilization is boil-off/venting losses from liquid hydrogen storage facilities. Cryocooler technology cannot yet mitigate this boiloff in a cost-effective manner.

- The Heisenberg Vortex Tube (HVT) is a WSU patented technology utilizing pressurized fluid power for separation into hot and cold streams with no moving parts. The hot stream is exposed to catalyst on the periphery to drive endothermic para-orthohydrogen conversion. This has the potential to address the following DOE HFTO barriers:
  1. Improving LH$_2$ pumping performance by precooling the liquid prior to pumping.
  2. Improving the cost and efficiency of liquefaction through improved ortho-para catalysis.
  3. Improving LH$_2$ utilization for other fueling site/terminal operations.
Approach: Para-orthohydrogen conversion

- Para-orthohydrogen conversion is the largest phase change of any material at cryogenic temperatures and the vortex tube is the first concept to utilize for primary cooling.
Approach: Experimental results from BY1

- Completed tests (21 total) in three different configurations to analyze catalyst sensitivity to swirl. Inlet temperature 46-52 K results shown in figure.

Traditional HVT: 10 tests varying T, ΔP, catalyzed & non.

Straight flow: 1 test varying flow rate catalyzed.

Swirl flow: 3 tests varying flow rate catalyzed.
Approach: Thermal Vapor Shielding

- Temperature stratification within LH2 tanks leads to increased pressure and boil-off. Plug Power utilizes Boil-off-Gas (BOG) compressors to reduce the tank pressure. However, the capacity, cost, and power requirements of BOGs are a limiting factor.

- Para-orthohydrogen conversion to equilibrium within the vapor ullage (<77 K) of a storage tank increases the energy removed from the tank by the BOG compressor up to 35%, thereby increasing utilization by reducing hydrogen vents with no additional input power required.

- We are designing a finned HVT with internal twister to maximize conversion while minimizing ΔP.
Approach:

- **Objective 1**: Refurbish the Cryocatalysis Hydrogen Experiment Facility (CHEF) for supercritical hydrogen measurements.

- **Objective 2**: Produce an optimal HVT designed with an experimentally verified Computational Fluid Dynamics (CFD) model, atomistic simulations of the catalyst performance, and 3D metal printing.

- **Objective 3**: Verify predicted performance improvements by implementing the HVT in field trials as:
  1. Subcooler to minimize liquid hydrogen pump cavitation,
  2. **Thermal Vapor Shielding (TVS) system for liquid hydrogen storage tanks, and**

Budget Period Year 1—Detailed Calculations of Design and Performance
  Go/No-Go: Performance calculations demonstrate 5% utilization improvement. (Passed)

**Budget Period Year 2—Validating HVT Optimizations and Constructing Field Test Articles**
  Go/No-Go: Experimental performance demonstrating improvements. (Pending)

Budget Period Year 3—Validating Field Test Article Performance
Accomplishments & Progress in BY2

Objective 1: HVT Testing in CHEF

*Task 2.1.1:* Design an experimental test plan and matrix to validate HVT performance relevant to the three planned applications. *Output:* Experimental test plan and matrix to guide CHEF testing. (1 month)

*Task 2.1.2:* HVT testing to complete experimental test matrix. *Output:* Experimental measurements of HVT performance in applications directly relevant to Plug Power. (12 months)

*Task 2.1.3:* Detailed uncertainty analysis of the experimental data points. *Output:* Uncertainty analysis per ASTM E2586 standard. Analysis will consider the bias error and random error of the experimental measurements through both propagation of instrument calibration precisions and repeated system level tests. Journal publication describing analysis will be submitted for peer review. (4 months)
Task 2.1.1 & 2.1.2: Experimental Test Matrix

- We are constructing modified HVTs with twisted tape inserts to maintain swirl over longer distances.

- Following test matrix includes 9 conditions with smooth, rifled, & twisted tape HVT geometries @ 50 K.
Task 2.1.3: Uncertainty Analysis

• All data analyzed per ASTM E2586-18 uncertainty standard
  • All data is normal in distribution and a 95% confidence interval is used to determine the random uncertainty:
    \[ \bar{x} \pm t_{1-\frac{\alpha}{2}, df} \frac{s}{\sqrt{n}} \]
  • Systematic error is added via Root-Sum-Square method:
    \[ u_{c,\text{sensor}}(y) = \sqrt{u_{\text{systematic}}^2 + u_{\text{random}}^2} \]
  • For Raman data, baseline noise (without laser on) is used for systematic error in full width at half maximum parameter \( \gamma \). Total area for each peak is:
    \[ A_{\text{ortho}} = \int_{-\infty}^{\infty} I_{\text{ortho}} \frac{\gamma_{\text{ortho}}^2}{(x-x_{\text{ortho}})^2 + \gamma_{\text{ortho}}^2} \]
    \[ A_{\text{para}} = \int_{-\infty}^{\infty} I_{\text{para}} \frac{\gamma_{\text{para}}^2}{(x-x_{\text{para}})^2 + \gamma_{\text{para}}^2} \]

Where \( I \) is peak height, \( x \) is specific spectrum location, and \( x_{\text{para}} \) is location of para peak, and \( x_{\text{ortho}} \) is the location of the ortho peak.

Validated first continuous flow Raman spectroscopy system for measuring para-orthohydrogen compositions. Measured 49.9% orthohydrogen at 120 mW power in above preliminary plot. Overall uncertainties estimated at ±2.7%. Could be applied for improved liquefier operation.
Accomplishments & Progress in BY2

Objective 2: CFD & Atomistic Optimization of HVT

Task 2.2.1: Use computer aided drafting code, atomistic simulations, and CFD optimal designs to 3D print HVTs for specific applications. Output: Optimized HVTs test articles to be implemented in CHEF. (6 months)

Task 2.2.2: Use atomistic simulations to optimize catalyst surface coating and have applied to HVT. Output: Catalyzed HVT articles to be implemented in CHEF. (6 months)

Task 2.2.3: Validate atomistic and CFD optimums with HVT data from CHEF. Output: Journal publication submitted for peer review. (11 months)
Task 2.2.1: Apply CFD to applications

- Two tubes of 1.26 m and 4 m lengths (mixed regime: vortical and straight flow); T_{in} = 55 K, PR = 1.25

<table>
<thead>
<tr>
<th>Dimensions</th>
<th>Material</th>
<th>Fins</th>
<th>Cooling Power</th>
<th>Ortho out</th>
<th>T out</th>
<th>Flow rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>126 cm x 12 mm</td>
<td>Aluminum</td>
<td>Yes</td>
<td>61.4 W</td>
<td>9.5%</td>
<td>51.3 K</td>
<td>1.9 g/s</td>
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<tr>
<td>400 cm x 8 mm</td>
<td>Aluminum</td>
<td>Yes</td>
<td>87 W</td>
<td>21.9%</td>
<td>52.8 K</td>
<td>0.64 g/s</td>
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<tr>
<td>12 m long</td>
<td>Aluminum</td>
<td>Yes</td>
<td>~180 W</td>
<td></td>
<td></td>
<td>~0.6 g/s</td>
</tr>
</tbody>
</table>

- We’ve used our validated CFD code to show that ~180 W of cooling power can be achieved from 12 m long HVTs in a 55 K ullage space, which is one possible Plug Power application scenario.
Task 2.2.2: Atomistic Simulation of Catalysis

- Full quantum Monte-Carlo code implemented.
- Determined parameters most sensitive to catalysis.
- Determined optimum temperature for adsorption.
- Determined optimum temperature for desorption.
- Other variables are unbounded.
Task 2.2.3: Validate Theory with HVT Data

- Optimization system utilizes quantum simulations to create catalysis lookup tables for CFD. The CFD results are then compared with the original experimental measurements of net para-orthohydrogen conversion.

Final comparisons experiment and theory at Plug Power operating conditions coming later in BY2.

- Example:

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Outputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet T</td>
<td>Inlet P</td>
</tr>
<tr>
<td>53.7 K</td>
<td>56.6 psia</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physics</th>
<th>CFD</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ave. temperature</td>
<td>Inlet O-P fraction</td>
<td>Inlet, outlet temperatures</td>
</tr>
<tr>
<td>O-P fraction per area</td>
<td>Inlet temperature</td>
<td>Inlet, outlet O-P concentrations</td>
</tr>
<tr>
<td>Infinitesimal net conversion</td>
<td>Infinitesimal density</td>
<td>Net Conversion</td>
</tr>
</tbody>
</table>

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Accomplishments & Progress in BY2

Objective 3: Design HVT Field Trials

**Task 2.3.1:** Complete final, detailed design review of field test articles and submit drawings for procurement. *Output:* Work orders to produce field test articles. (3 months)

**Task 2.3.2:** Develop field testing and implementation plans for three applications. *Output:* Plans and procedures for implementing and testing field test articles. (6 months)

**Task 2.3.3:** Assembly and implementation of field test articles. *Output:* Field test articles ready for implementation and testing. (3 months)
Task 2.3.1: Design Field Test Articles

- Although the temperatures in the ullage space are subject to many factors, we've mapped the operational space where utilizing the HVT makes techno-economic sense for Plug Power.

- It is estimated that over 50% of Plug Power sites would benefit from reduced venting afforded by this application.
Task 2.3.2 & 2.3.3: Develop test articles

- We’ve met with component suppliers and have not identified a barrier to developing the test articles.

- We plan to finalize the design and submit for construction in September of 2021 allowing final testing and verification in FY 2022.
Responses to prior reviewer comments

• This project has not previously been reviewed at the AMR.

• Project started in January of 2019 and did not have sufficient materials for review at 2019 AMR.

• COVID-19 canceled 2020 AMR and BY1 was extended through September of 2020 due to procurement dilemmas.
Collaboration and Coordination

- Washington State University (WSU) is the prime grant awardee and responsible for Objectives 1 & 2.
- Plug Power is a sub-awardee and responsible for Objective 3.
- WSU and Plug Power meet virtually every other week to discuss project progress and monthly with a DOE program representative.
Remaining Challenges and Barriers

- In addition to completion of the proposed project tasks, the following challenges and barriers have been identified during this project:
  1. Experimental data and models of the ullage space temperature within an operational liquid hydrogen tank are not available in the literature nor conveniently measured. This information is needed for accurate techno-economic analysis of the project.
  2. Experimental data and models describing the para-orthohydrogen catalyst longevity and associated degradation mechanisms are not available in the literature nor conveniently measured. This information is needed for accurate life-cycle analysis of the project.
Proposed Future Work

• Our remaining work in FY 2021 includes:
  1. Completing the experimental test matrix at Plug Power operating conditions (WSU).
  2. Comparing the experimental measurements to theoretical predictions to determine design optimums (WSU).
  3. Finalizing the design and sending out for construction (Plug Power).
  • Go/No-Go: HVT optimization is complete and shows an isentropic efficiency of 40% (Passed September 2020)

• Our planned work for FY 2022* includes:
  1. Complete experimental testing on HVT degradation mechanisms to attempt life-cycle assessment (WSU).
  2. Model field test conditions (including ullage space temperature) for comparison to experimental results (WSU).

* Any proposed future work is subject to change based on funding levels.
Since January of 2019 our team has:

- Retrofitted the Cryocatalysis Hydrogen Experiment Facility (CHEF) for 70 bar measurements, a cycle time less than 2 days, and the first continuous flow cryogenic Raman spectroscopy system for para-orthohydrogen analysis; subsequently allowing over 35 tests in various flow configurations.

- Developed a computational analysis system that utilizes full atomistic simulations of para-orthohydrogen catalysis to create lookup tables for computation fluid dynamics (CFD) simulations. These results have been validated by experiment and used to optimize the HVT for a Plug Power application.

- Designed a novel HVT-based heat exchanger to reduce the ullage temperature within Plug Power liquid hydrogen tanks. The HVT has the potential to increase Boil-off-Gas (BOG) compressor capacity 35% with no moving parts or additional power requirements. We’ve determined this application could reduce venting and benefit over 50% of Plug Power sites. We are finalizing a design for production.
Technical backup and additional information
Technology Transfer & Publication Activities

**Patents:**

**Peer-Reviewed Publications:**
## Progress towards DOE Targets & Milestones

<table>
<thead>
<tr>
<th>Task #</th>
<th>Task Title</th>
<th>Milestone Type</th>
<th>Milestone Number*</th>
<th>Milestone Description</th>
<th>Milestone Verification Process</th>
<th>Anticipated Start Date</th>
<th>Anticipated Quarter</th>
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</thead>
<tbody>
<tr>
<td>2.3.1</td>
<td>Complete Detailed Design Review</td>
<td>Milestone</td>
<td>2.1</td>
<td>Complete detailed design review with drawings.</td>
<td>Send slides of final designs for production to PM.</td>
<td>13</td>
<td>5</td>
</tr>
<tr>
<td>2.2.1</td>
<td>Finalize Optimal CFD and catalyst design for production</td>
<td>Milestone</td>
<td>2.2</td>
<td>Show the optimal CFD design, atomistic simulation and send out for 3D printing and catalyst deposition.</td>
<td>Send slides of CFD optimal analysis, atomistic simulation, and design drawings to PM.</td>
<td>13</td>
<td>6</td>
</tr>
<tr>
<td>2.3.3</td>
<td>Assembly of Field Test Articles</td>
<td>Milestone</td>
<td>2.3</td>
<td>Assemble Scaled Field Test articles and prepare for implementation</td>
<td>Send slides of field test article construction to PM</td>
<td>17</td>
<td>7</td>
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<tr>
<td></td>
<td>Go/No-Go Decision Point</td>
<td>Go/No-Go</td>
<td>2</td>
<td>HVT optimization is complete and shows an isentropic efficiency of 40%.</td>
<td>Send draft of article on HVT performance for publication to PM. HVT achieves isentropic efficiency of 40%.</td>
<td>24</td>
<td>8</td>
</tr>
</tbody>
</table>
Task 1.1.1: Design CHEF Retrofit

- Completed Operational Readiness Review of CHEF
  - Helium cooldown test indicates 5.8x faster performance than previous system
  - 2-day cycle time is achieved
  - Welds are certified per ASME B31.12 to 124 bar (with FOS > 3)
  - Safety plan reviewed by H2 Safety Panel
Task 1.1.2: CHEF renovation complete

- Experiment upgrade is complete
  - Number of connections in vacuum chamber reduced from 103 to 63
    - All weld or VCR type
    - Indium-Cu seal on optic lenses
  - All components are helium leak tight
    - Internals are leak-tight to 17.3K
    - 4.2e-7 torr vacuum level
  - Control box complete with H2 sensor (and E-stop) controlled purge valve
  - 1kW Fuel cell backup power installed for safety systems
Task 1.2.1: Implement CFD

- State-of-the-art computational fluid dynamics (CFD) software STAR-CCM+ was chosen for thermofluid simulations
- Two new computer workstations (with 48 and 32 cores) were set up; another 28-core workstation was employed as well
- Computer workstations and CFD software were tested
- As a part of this preparatory work, two vortex tubes of novel geometries were modeled with air at normal temperatures and H2 at cryogenic conditions; optimum geometries were determined; two publications were produced

VT with conical sections for room air

Cyclonic VT for cryogenic H2
Task 1.2.2: 1\textsuperscript{st} 3D Printed Vortex Tube

- Since tests/results in the literature are often incompletely described, we built our own highly-controlled room-T experiment for (1) obtaining detailed data for CFD validation and (2) testing novel-geometry VT prior to deploying them in more expensive cryogenic experiments.

- Novel-shape miniature VT was 3D-printed from titanium alloy (first in the world); and then successfully tested and simulated with CFD.

Mesh-convergence CFD (verification) study

Validation study
Task 1.2.3: Parametric CFD Study

- In CFD studies of three initially proposed HVT applications, significant benefit was identified only in App. # 2 (thermal vapor shielding to reduce boil-off losses)
- A number of parametric simulations were conducted at different operational conditions of HVT ($P_{in} = 100$-$145$ psig, $P_{out} = 25$-$80$ psig, $T_{in} = 40$-$50$ K) using para-ortho conversion rates from initial tests in CHEF
- Isentropic efficiencies above 40% were demonstrated in some configurations in numerical simulations
- High conversion rates in HVT need additional experimental confirmation

Example of temperature field and ortho-H2 distribution from CFD simulations
Task 2.2.1: HVT nozzle optimization

Desire to maximize swirl flow for improved catalysis

~40 configurations tested, with angular momentum (h) compared at x/d=1

Increased angular momentum predicted over standard VT inlets

Experiments needed to validate driving factors in catalysis

4-Inlet Standard
h=0.0020 (g/m-s)

Archimedean Spiral
h=0.0022 (g/m-s)

Divergent
h=0.0026 (g/m-s)
**Task 1.3.1: TVS application justification**

**Objective:** Reduce liquid hydrogen storage tank boil-off losses by 20% through thermal vapor shielding (TVS). **Concept:** Heat exchanger with HVT in vapor or liquid of the tank can reduce tank temperature and pressure.

**Conclusion:** Para-orthohydrogen conversion to equilibrium within the vapor ullage (<77 K) increases the energy removed from the tank by the Boil-off-Gas (BOG) compressor by up to 35%, thereby increasing utilization by reducing hydrogen vents, warranting additional consideration.

Key HVT Metrics:
- Maximize entropy of vent stream
- Minimize thermal mass
- Fast response time
- Low-blockage risk
Task 1.3.2: Design calcs for TVS-HVT

- Maximum temperature in tank vapor ullage is currently unknown. Conducted CFD analysis of simplified tank stratification for estimate.

- Extrapolation from NASA & historical studies\textsuperscript{1,2} indicates max temperature could approach 77 K; tank ullage temperature is highly variable based on tank utilization, warranting further studies outside original scope.

2. https://ntrs.nasa.gov/citations/1979009886

Figure ___: The analysis of the temperature of a cold gas holder as a function of time over the period of 24 hours as influenced by the liquid hydrogen denspense rate (172).
Task 1.3.2: Control Volume & Balances

Start with:

\[
\dot{Q}_{\text{in}} + \dot{W}_{\text{in}} + \sum_{\text{in}} \dot{m} (h + PE + KE) - \sum_{\text{out}} \dot{m} (h + PE + KE) = \frac{dE}{dt}
\]

Simplified:

\[
\dot{Q}_{\text{in}} + \dot{m}_{\text{return}} h_{\text{return}} - \dot{m}_{\text{vent}} h_{\text{vent}} - \dot{m}_{\text{BOG}} h_{\text{BOG}} - \dot{m}_{\text{L}} h_{\text{L}} = \frac{dE}{dt}
\]

Where:

\[
\frac{dE}{dt} = \frac{(m * u)_{L,2} + (m * u)_{G,2} - (m * u)_{L,1} - (m * u)_{G,1}}{t}
\]