

Heisenberg Vortex Tube for Cooling and Liquefaction

DOE FCTO Annual Merit Review May 19th-21st 2020

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PROJECT ID: IN015

Washington State University

H
HYdrogen
Properties for
Energy
Research

Overview

Plug Power is the largest single user of liquid hydrogen (LH_2) dispensing 27 tons/day. However, LH_2 utilization ranges between 93-75%.

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

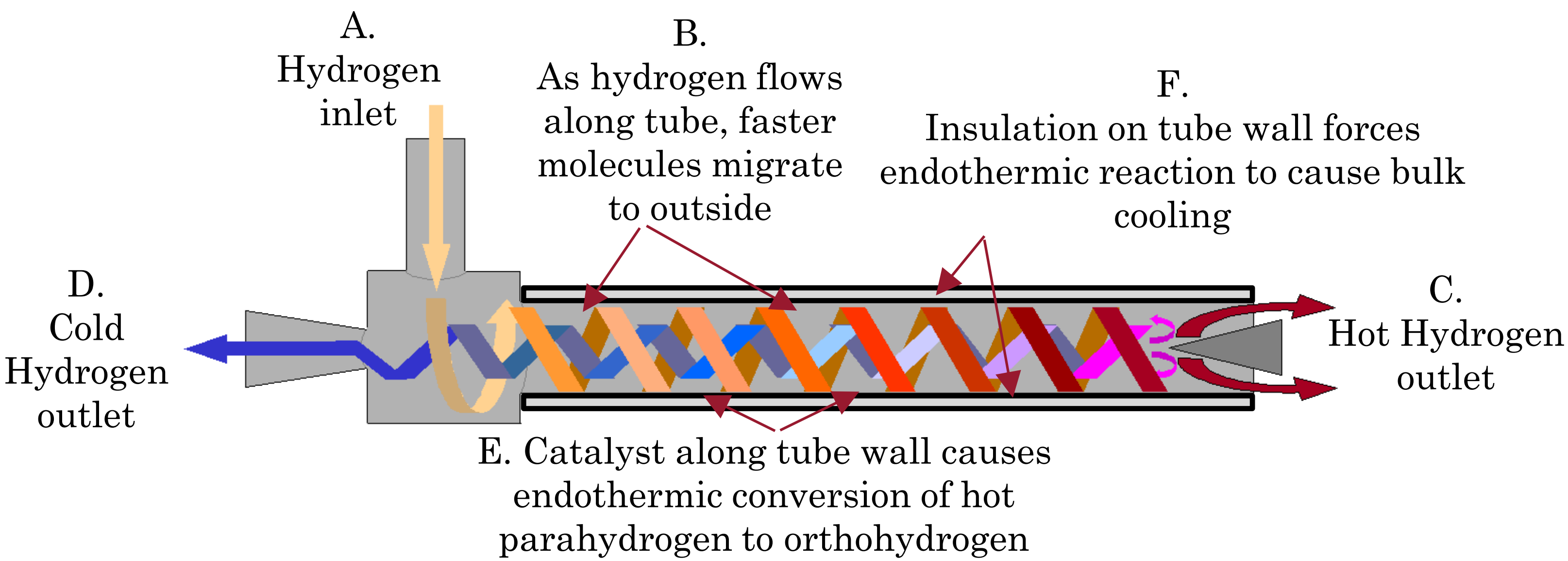
1. Liquid hydrogen pump volumetric efficiency by 20% through vapor separation and subcooling.
2. Liquid hydrogen storage tank boil-off losses by 20% through thermal vapor shielding (TVS).
3. Supercritical hydrogen expansion by increasing isentropic efficiency from 31% between 40-50 K to greater than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

Timeline: Start: 1/23/2019 End: 9/30/2021

Budget: $2,372.2k Federal Share: $1,897.8k Total DOE Spent: $965k

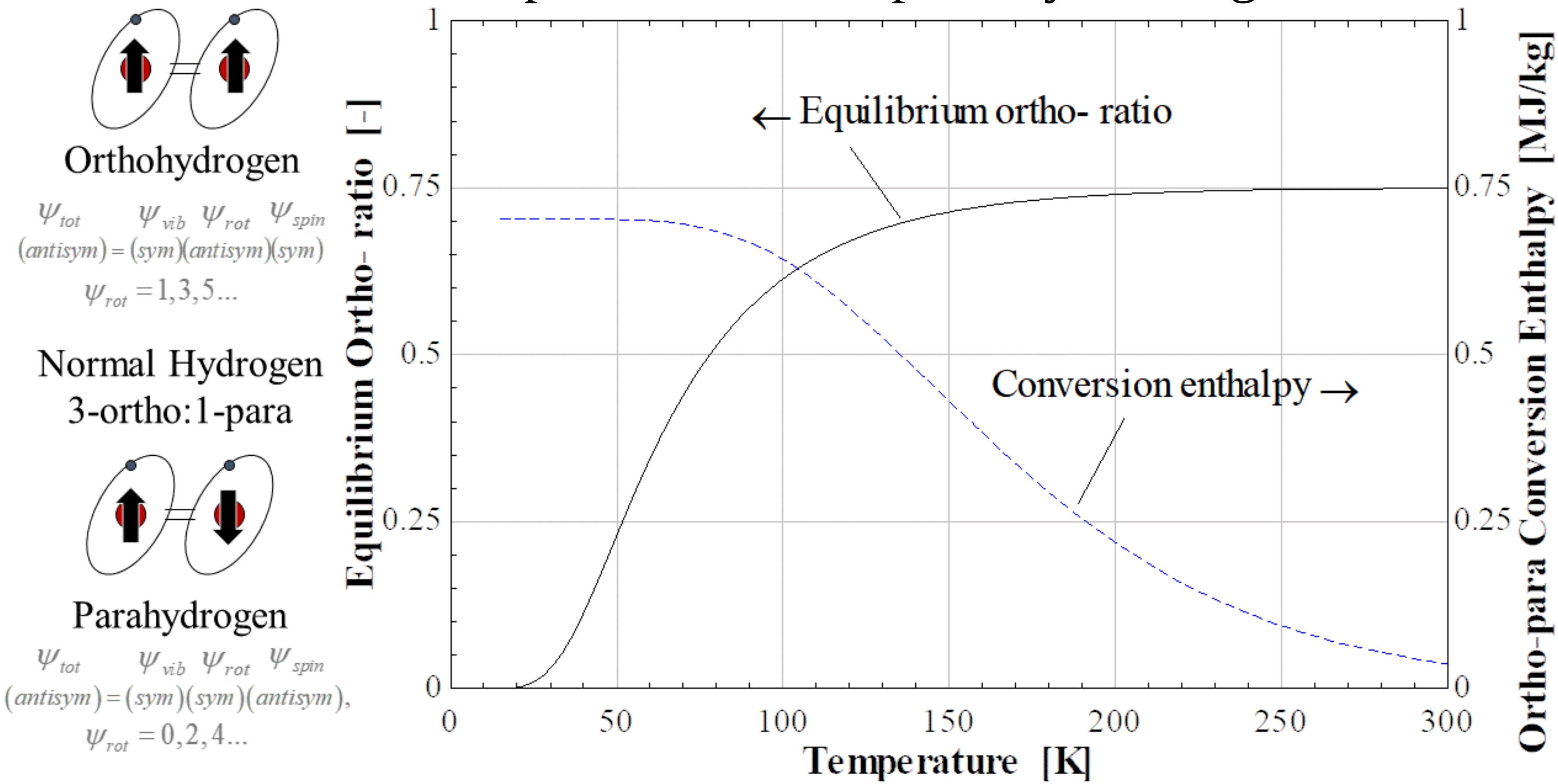
Background: Heisenberg Vortex Tube (HVT)

- Vortex tubes utilized pressurized fluid power to separate the fluid into hot and cold streams with no moving parts.
- The Heisenberg Vortex Tube (HVT) is a patented modification of conventional vortex tubes that utilizes a catalyst on the periphery to drive para-orthohydrogen conversion.

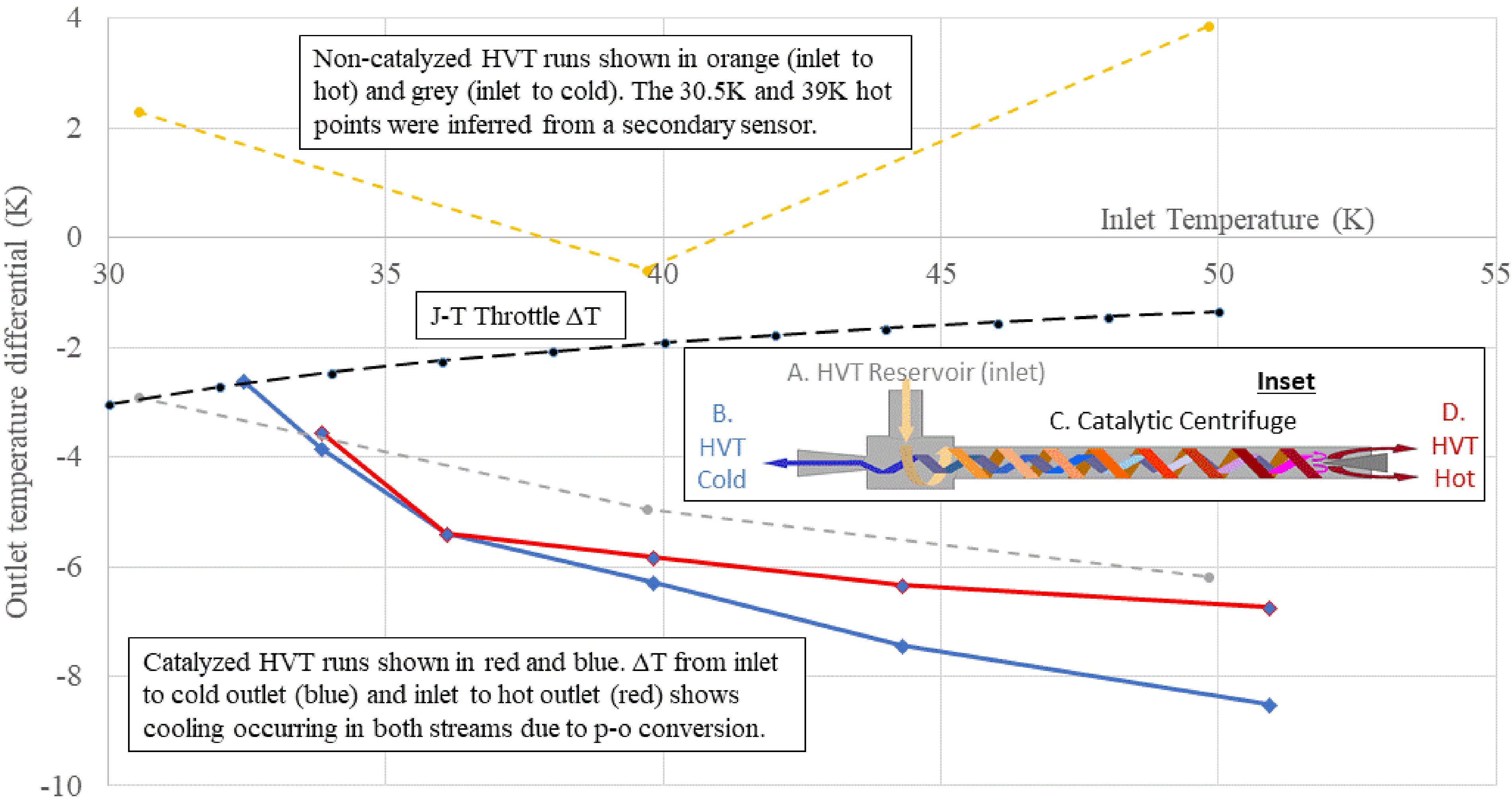


Background: Ortho-Para H_2

- Parahydrogen-orthohydrogen conversion is the largest phase change of any material at cryogenic temperatures and the vortex tube is the first concept to unlock for primary cooling.



Background: Initial Results at Onset



Project Objectives & Budget Periods

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

1. Replacing mechanical fittings and joints in condenser tank with welded parts, to minimize leaks and increase pressure capacity up to 70 bar.
2. Reducing the experimental cycle time from 5 to less than 2 days.

(Bonus) Improve ortho-parahydrogen measurements via Raman spectroscopy.

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
3. Supercritical hydrogen expander for reliquefaction of process gas.

Budget Period Year 1—Detailed Calculations of Design and Performance

Budget Period Year 2—Validating HVT Optimizations and Constructing Field Test Articles

Budget Period Year 3—Validating Field Test Article Performance

Objective 1: HVT Testing in CHEF

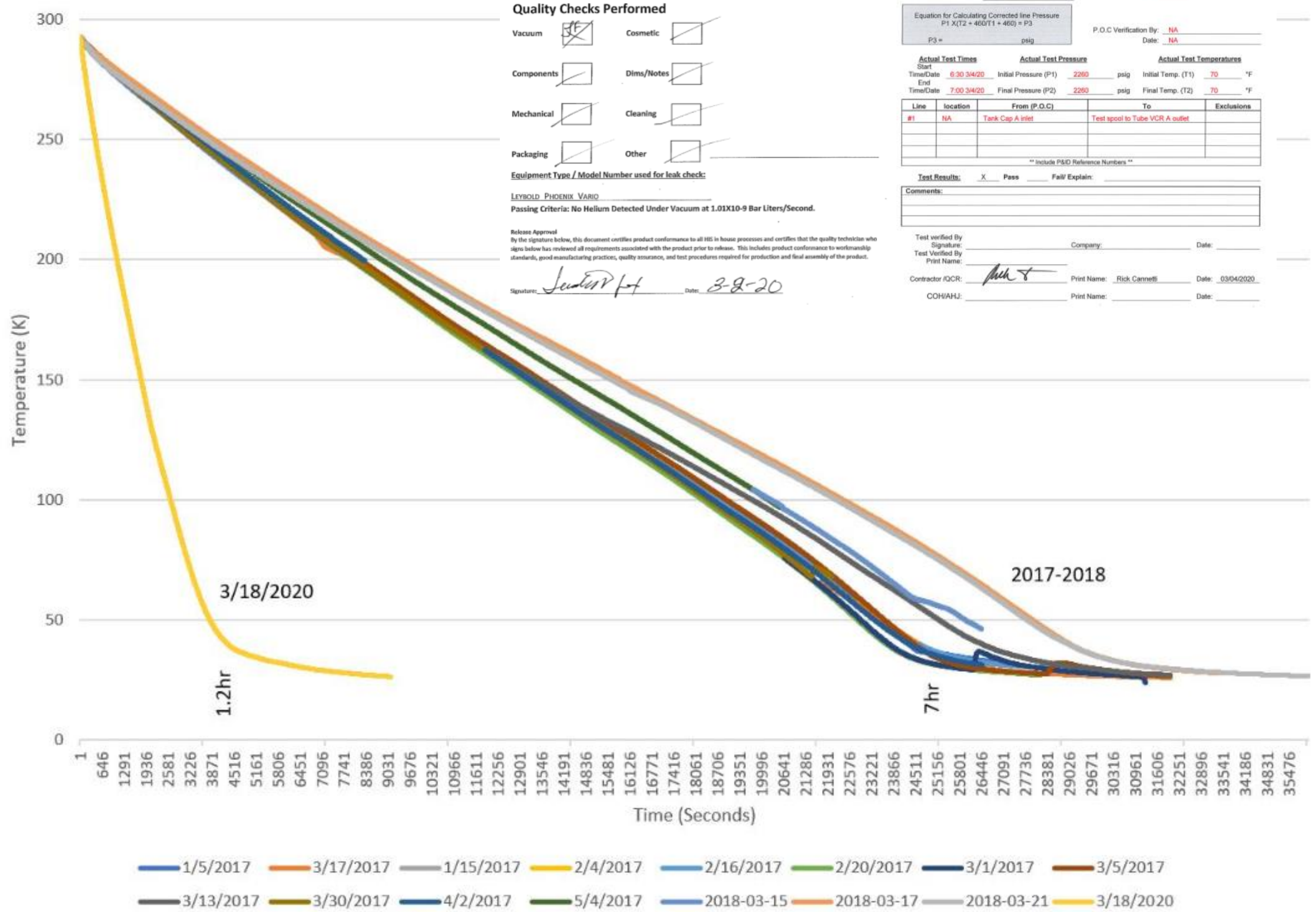
Task 1.1.1: Complete design calculations to allow CHEF operation up to 70 bar, with a factor of safety greater than three, reducing the number of possible leak points in the system, and reducing the cycle time from five to less than two days. *Output*: Submission of Safety Plan for project to DOE's Hydrogen Safety Panel, and procurement of the necessary components and materials to refurbish CHEF subsequent to approval of Safety Plan. (3 months)

Task 1.1.2: Assemble the components and materials in CHEF. *Output*: Retrofitted facility capable of 70 bar testing with a factor of safety greater than three, fewer chances for test abort, and cycle time reduced to less than two days between data points. (6 months)

Task 1.1.3: Complete safety testing and revisions to CHEF Safety Plan and Standard Operating Procedures Manual. *Output*: A functioning system and operation plan that is ready for cryogenic hydrogen testing. (3 months)

Task 1.1.1: Design Retrofit CHEF

- 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



HIS INNOVATIONS GROUP

HIS-QC 6.1-1 CERTIFICATE OF CONFORMANCE

Product Information

Part Number: Tank VCR A Rev:

Work Order: 608119 003

Quantity: 3 Built By: HIS

Quality Checks Performed

Vacuum / Cosmetic / Components / Dims/Notes / Mechanical / Cleaning / Packaging / Other

Equipment Type / Model Number used for leak check:

LEYBOLD PHOENIX VARIO

Passing Criteria: No Helium Detected Under Vacuum at 1.01X10-9 Bar Liters/Second.

Release Approval

By the signature below, this document certifies product conformance to all HIS in house processes and certifies that the quality technician who signs below has reviewed all requirements associated with the product prior to release. This includes product conformance to workmanship standards, good manufacturing practices, quality assurance, and test procedures required for production and final assembly of the product.

Signature: Date: 3-8-20

Apollo

Pressure Test Report

Project: HIS Tank Cap A Location: Tigard, OR Fab shop,

Tool ID: Tank Cap A and Tube VCR A Job #: HIS 001

Service: NA Tester: Rick Cannetti

Date: 03/04/2020 Contractor: Apollo Mechanical

Specified REQ: X Current Client Specs; Other:

Test Type: Hydro Test; X Pneumatic; Service; Other:

Test Requirements: Min Duration: 30 minutes; Min. Pressure: 2250 psig; Max pressure: 2400 psig

Test Medium: Water; air; X High Purity Argon; Nitrogen; Other:

Test Instruments: Gauge S/N: 06100J01; Gauge Due: 05/08/2020

Equation for Calculating Corrected line Pressure P1 X(T2 + 460/T1 + 460) = P3

P3 = psig

P.O.C Verification By: NA Date: NA

Actual Test Times: Start Time/Date 6:30 3/4/20; End Time/Date 7:00 3/4/20

Actual Test Pressure: Initial Pressure (P1) 2260 psig; Final Pressure (P2) 2260 psig

Actual Test Temperatures: Initial Temp. (T1) 70 °F; Final Temp. (T2) 70 °F

Line	location	From (P.O.C)	To	Exclusions
#1	NA	Tank Cap A inlet	Test spool to Tube VCR A outlet	

** Include P&ID Reference Numbers **

Test Results: X Pass Fail/ Explain:

Comments:

Test verified By Signature: Company: Date:

Test Verified By Print Name:

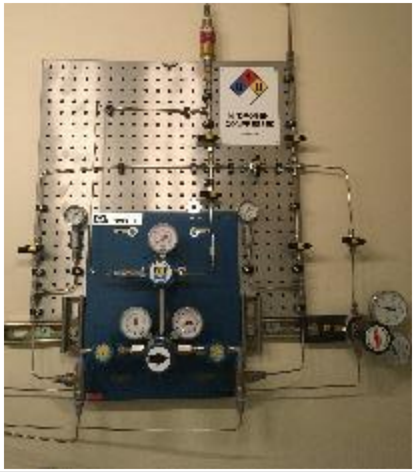
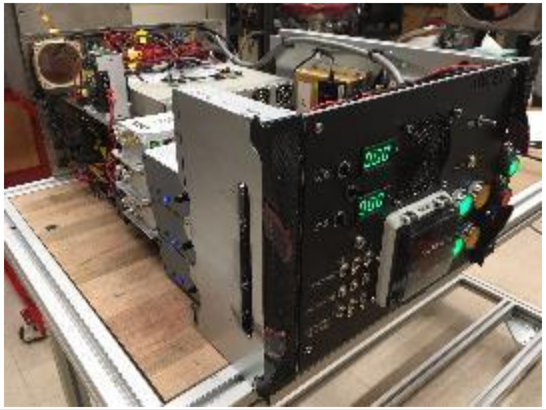
Contractor /QCR: Print Name: Rick Cannetti Date: 03/04/2020

COH/AHJ: Print Name: Date:

Task 1.1.2: Complete CHEF Retrofit

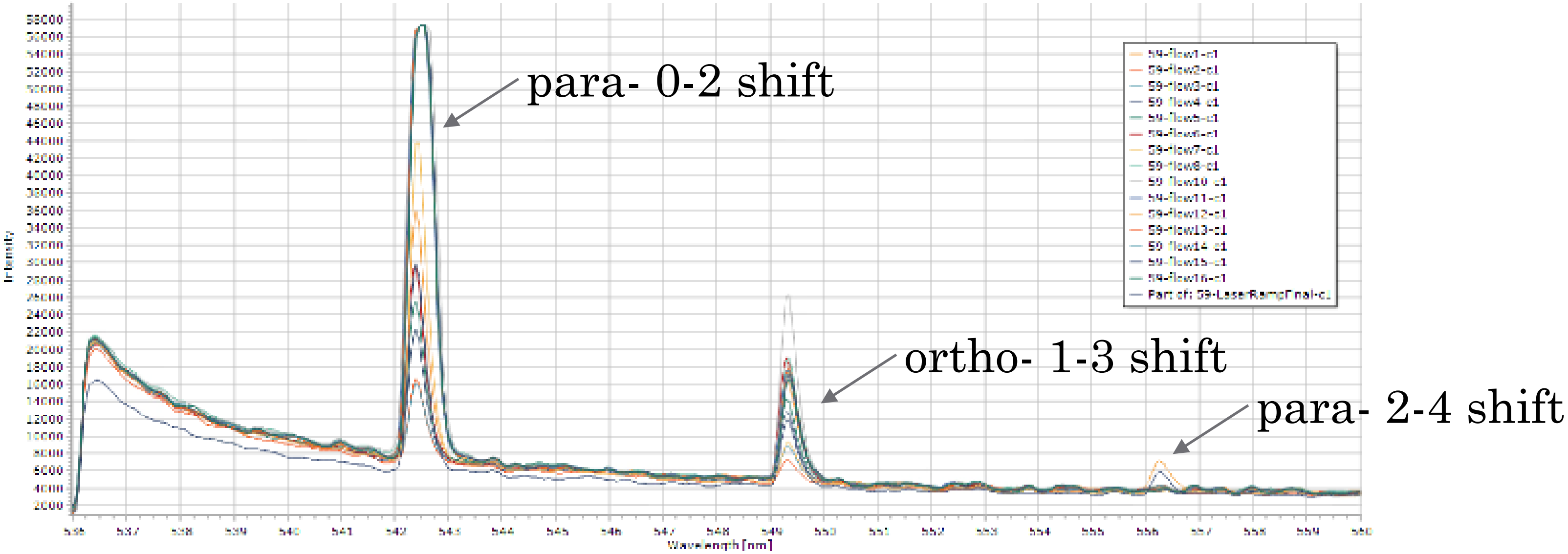
- Experiment upgrade is complete
  - Number of connections in vacuum chamber reduced from 103 to 63
    - All weld or VCR type
    - Indium-Cu seal on optic lenses
  - All components are helium leak tight
    - Internals are leak-tight to 17.3K
    - 4.2e-7 torr vacuum level
  - Control box complete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



Task 1.1.3: Validate Operation

- 1st cryogenic Raman spectroscopy system successfully implemented to measure ortho-parahydrogen ratios of flowing hydrogen:
  - Utilizing fiber optics to sample ratios before and at both outlets of HVT with accuracy within ± 2%
  - High resolution even shows parahydrogen 2-4 rotational energy mode shift near 556 nm at 40 K.



Objective 2: CFD & Atomistic Optimization of HVT

Task 1.2.1: Select host platforms for Computational Fluid Dynamics (CFD) and atomistic software to begin parametric analysis of HVT. *Output:* Computational facilities ready to begin parametric analysis. (2 months)

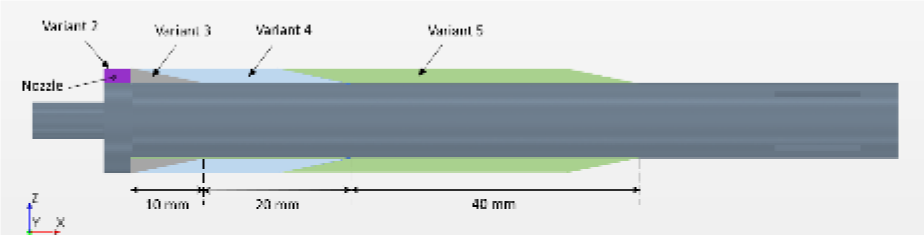
Task 1.2.2: Import and mesh existing computer aided drafting model of HVT and complete initial CFD verification and validation study. *Output:* CFD performance prediction of HVT comparable to existing experimental measurements. (5-6 months)

Task 1.2.3: Conduct parametric study of validated CFD code near anticipated HVT design points for optimization based on prior EERE/NREL HOQ analysis. *Output:* Optimal HVT design for specific state points relevant to Plug Power. (6 months)

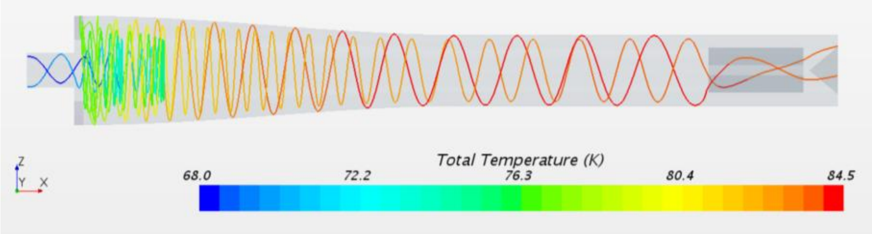
Task 1.2.4: Perform simulations to determine important physical quantities associated with para-orthohydrogen conversion on interior HVT wall. *Output:* Sensitivity study of HVT catalysis. (6 months)

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



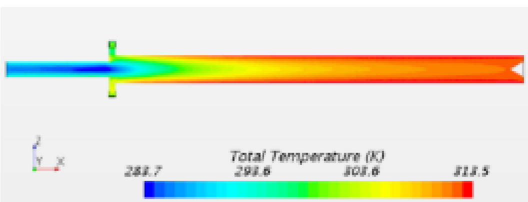
VT with conical sections for room air



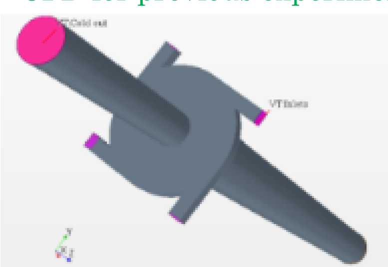
Cyclonic VT for cryogenic H2

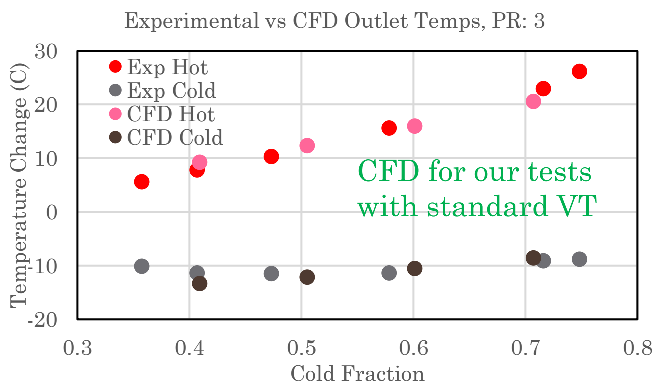
Task 1.2.2: Verification of CFD

- Verification and validation (V&V) CFD studies were carried out in a broad range of conditions using (1) data available in the literature, (2) data from our own newly built setup for air-based VT, and (3) results from initial cryo-HVT tests in CHEF (w/t & w/o catalyst)

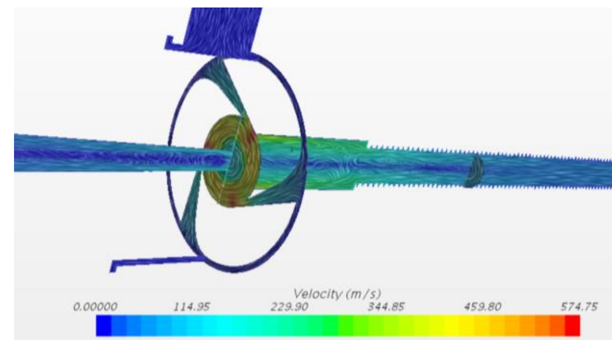


CFD for previous experiments





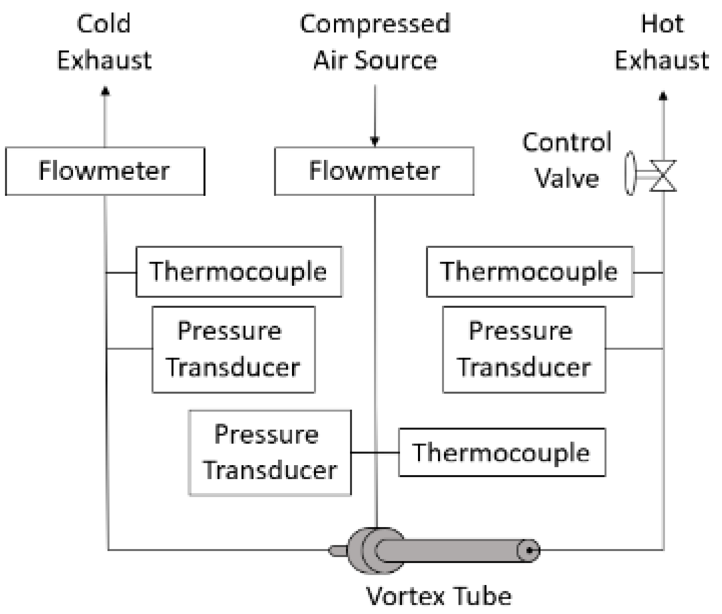
CFD for our tests with standard VT

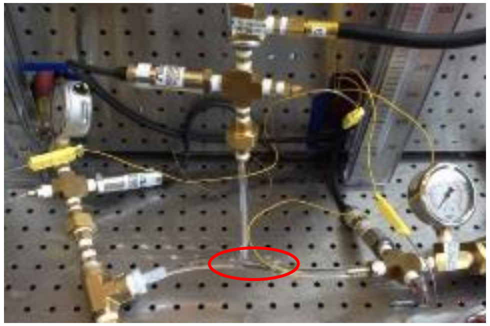


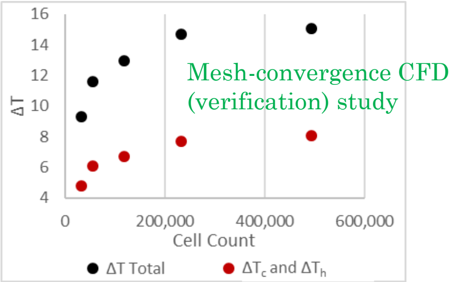
CFD for initial experiments in CHEF

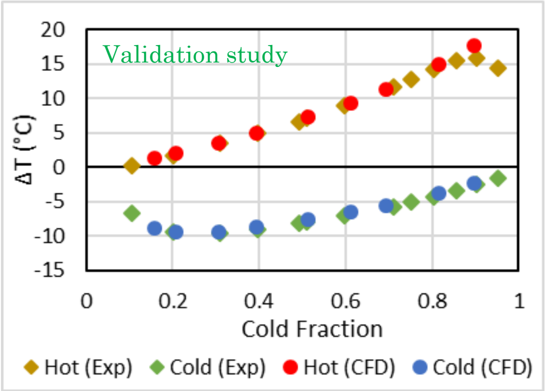
Task 1.2.2: 1st 3D printed Vortex Tube

- 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



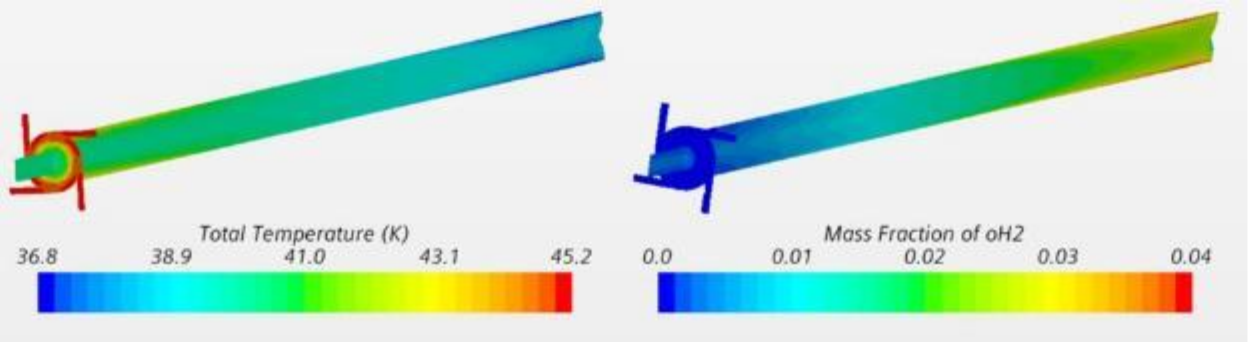






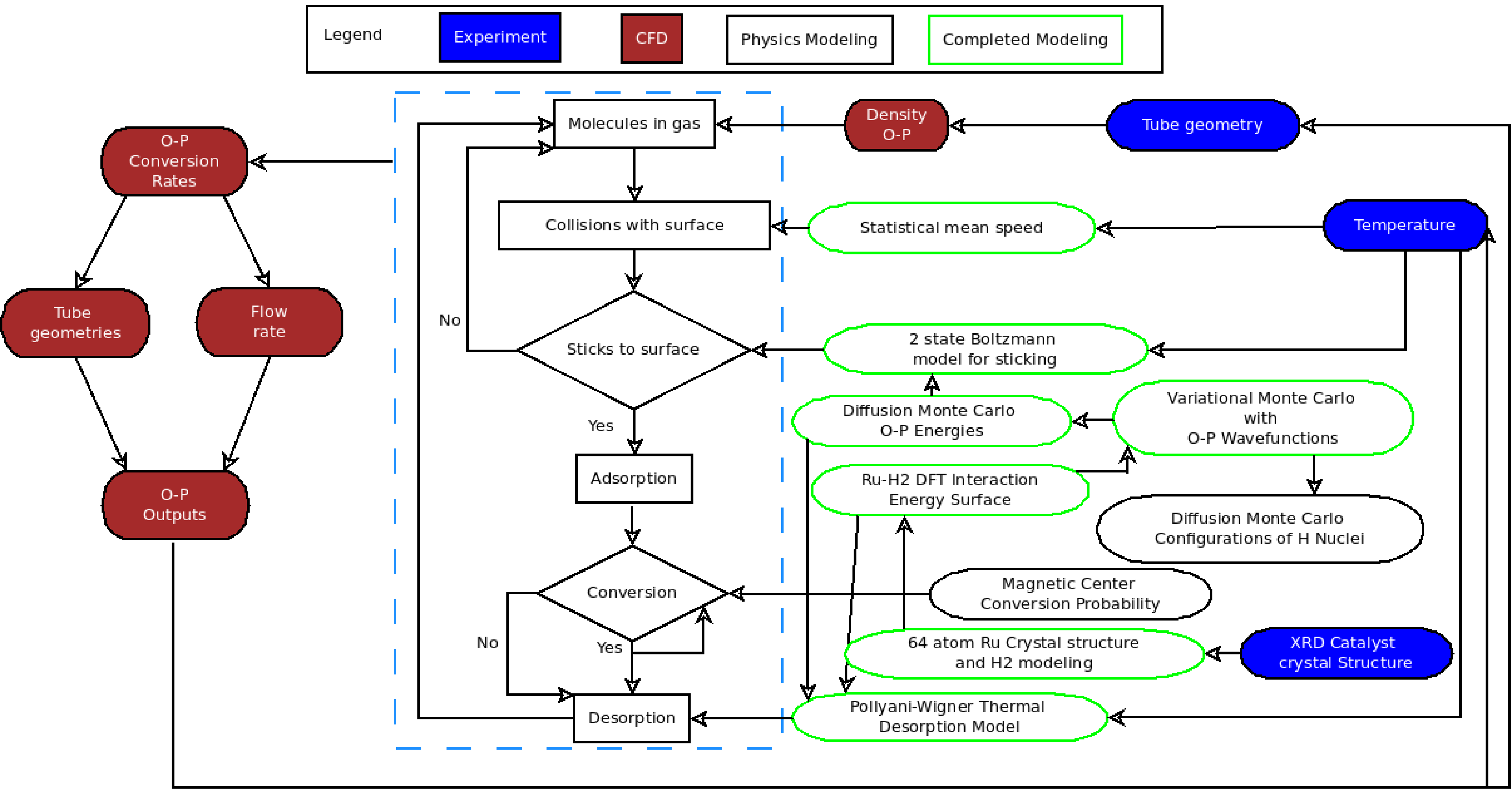
Task 1.2.3: Parametric Study of HVT

- 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



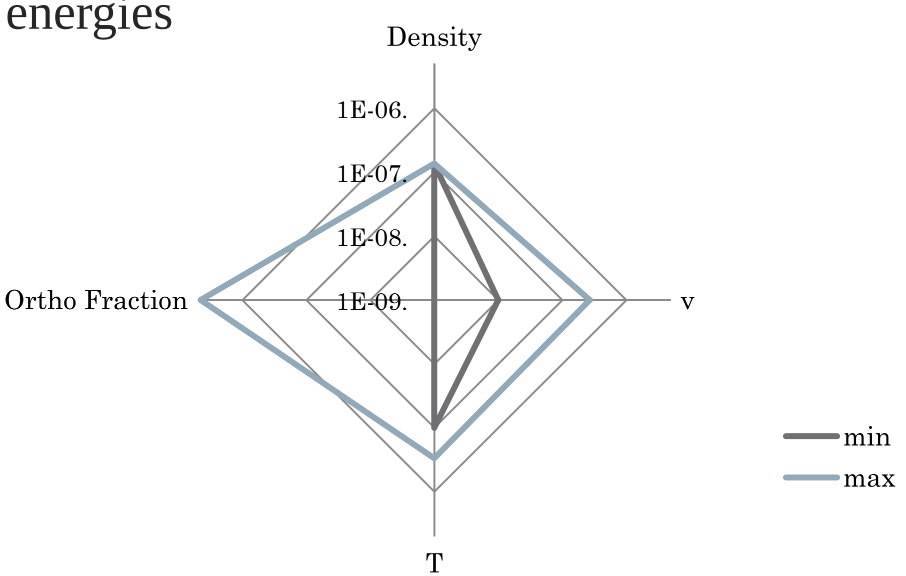
Example of temperature field and ortho-H2 distribution from CFD simulations

Task 1.2.4: Catalysis Modeling Process



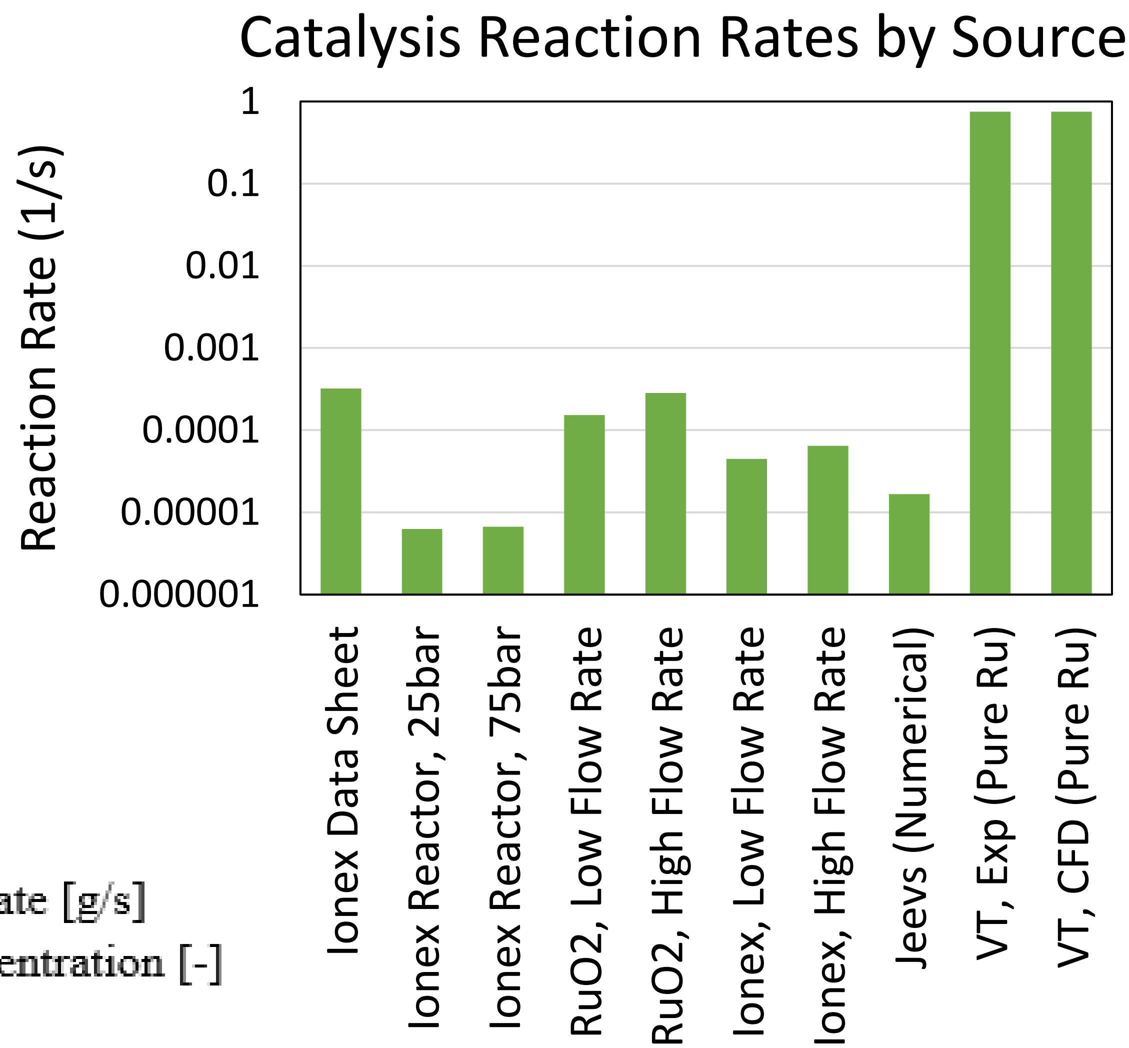
Task 1.2.4: Catalysis Sensitivity Results

- Molecular Density Functional Theory simulations
  - Energy of interaction between H_2 and Ru surface
- Monte Carlo Rotational wavefunction simulations
  - Rotational state dependent adsorption energies
- Process models
  - Adsorption model and rate
    - Sticking model
  - Desorption model and rate
  - Conversion rate code
    - Gives rate of conversion in kg/m^2s
- Uncertainties
  - Sticking probability is less than model
  - Temperature and density inside tube dependent on CFD



Task 1.2.4: Catalysis Activity Results

- Closest experimental conditions to model are with RuO2, which are 3 orders of magnitude lower in performance than preliminary HVT results.



$$\dot{r} = \frac{\dot{m}_{H2} * \Delta Ortho}{m_{cat}}$$

$\dot{r}$:	Reaction Rate [1/s]
$\dot{m}_{H2}$:	Hydrogen Mass Flowrate [g/s]
$\Delta Ortho$:	Change in Ortho Concentration [-]
m_{cat}:	Mass of Catalyst [g]

Objective 3: Design HVT Field Trials

Task 1.3.1: Develop design specifications and a House of Quality (HOQ) for the three test applications comparing the HVT to J-T and other competing technologies. *Output:* Quantifiable design specification document allowing objective comparisons between design alternatives. (3 months)

Task 1.3.2: 0-1st order design calculations of HVT performance for three identified applications. *Output:* Functioning parametric models to aid in system designs. (12 months)

Task 1.3.3: Design field test articles and select field test locations to allow both J-T and HVT testing. *Output:* Dimensioned drawings ready for procurement or production. (9 months)

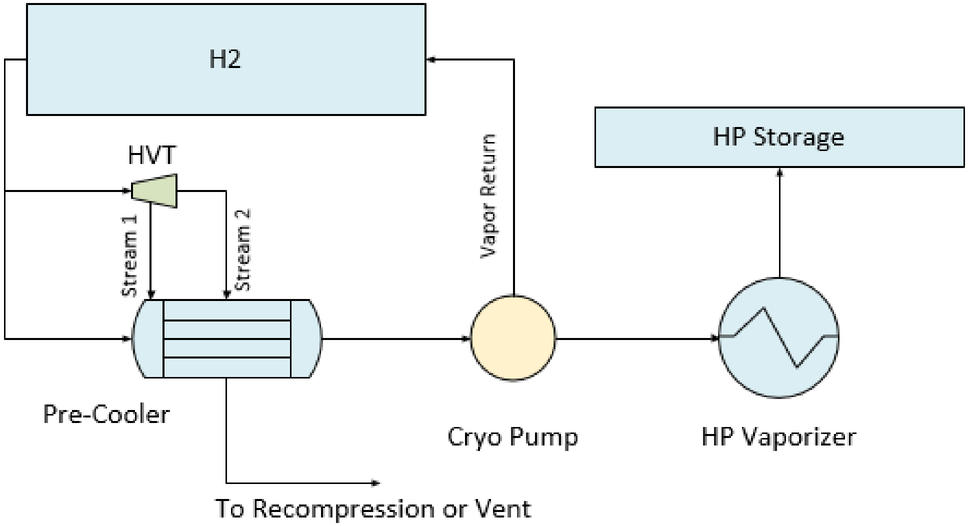
Task 1.3.1: Application 1: Pump Pre-Cool HOQ & Needs

Objective: Increase liquid hydrogen pump volumetric efficiency by 20% through vapor separation and subcooling of the liquid.

Key HVT Metrics:

- Provide Reduced Temperature LH2 for use as HX cold stream
- Minimize Expansion PR to enable recompression of cold stream
- Robust to variation in tank H2 conditions
- Exceed Performance of Throttle Valve

Conclusion: CFD indicates little cooling of liquid and pump cavitation not as severe as expected.

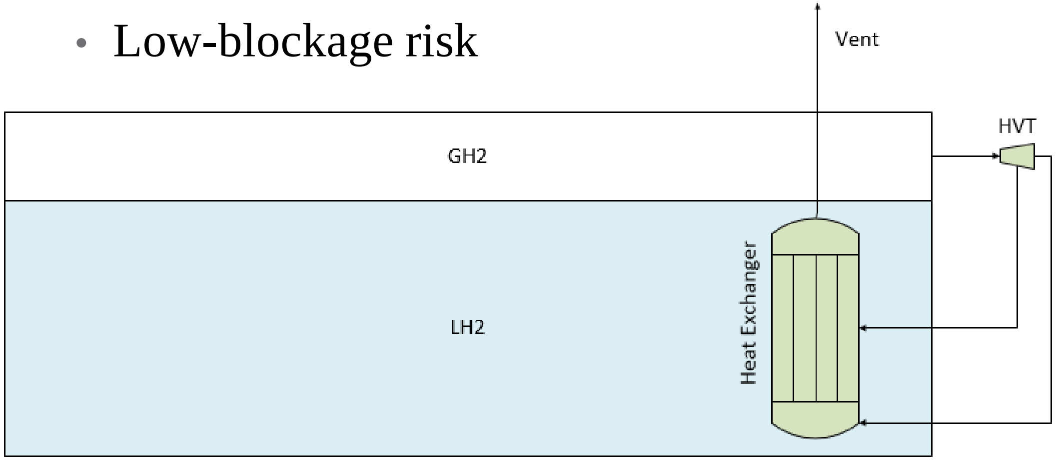


Task 1.3.1: Application 2: Liquid Tank Thermal Vapor Shielding

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.

Key HVT Metrics:

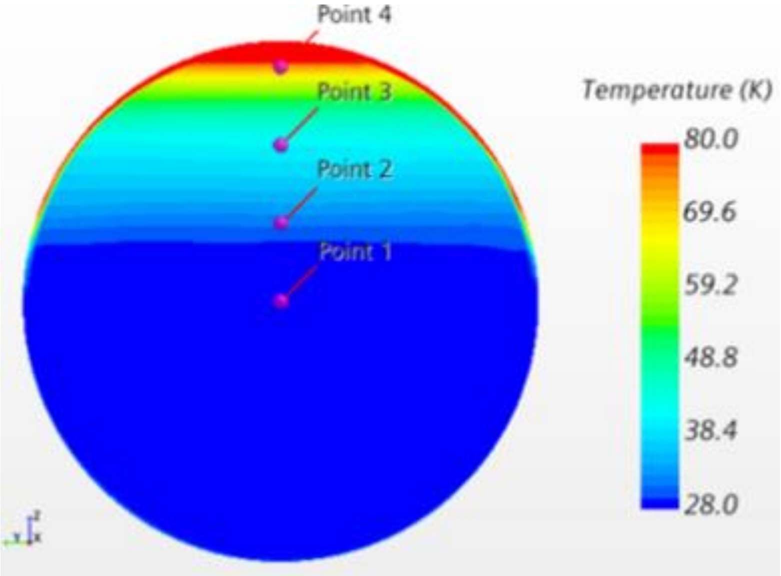
- Maximize entropy of vent stream
- Minimize thermal mass
- Fast response time
- Low-blockage risk

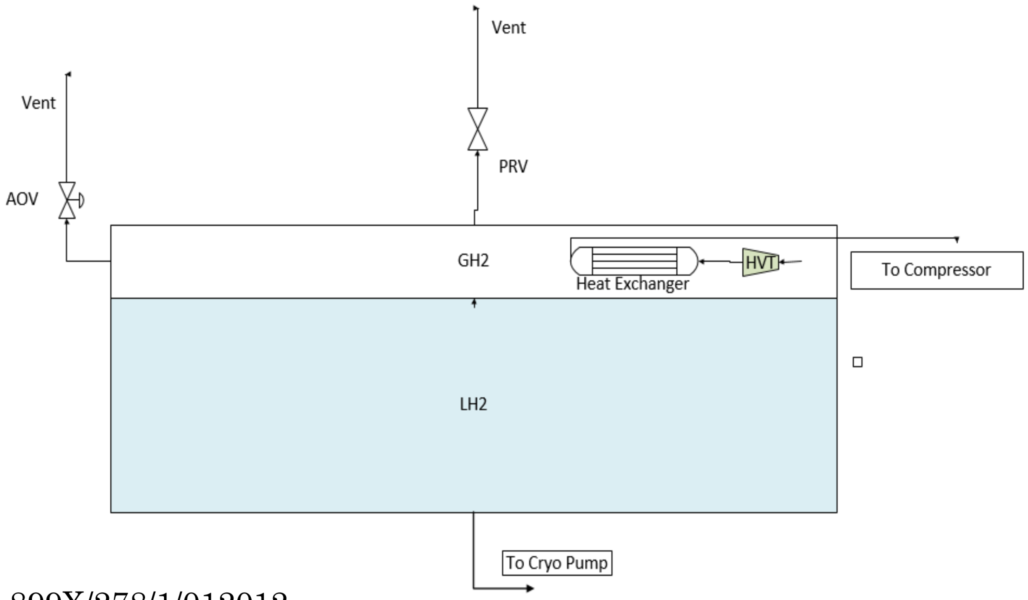


Conclusion: Para-orthohydrogen conversion to equilibrium within the vapor ullage (<77 K) increases the energy removed from the tank by the Boil-off-Gas (BOG) compressor by up to 35%, thereby increasing utilization by reducing hydrogen vents, warranting additional consideration.

Task 1.3.2: Design Calcs for App. #2; TVS

- Maximum temperature in tank vapor ullage is currently unknown. Conducted CFD analysis of simplified tank stratification for estimate.
- Extrapolation from NASA studies[1] indicates max temperature could approach 77 K; tank ullage temperature is highly variable based on tank utilization, warranting further studies outside original scope.



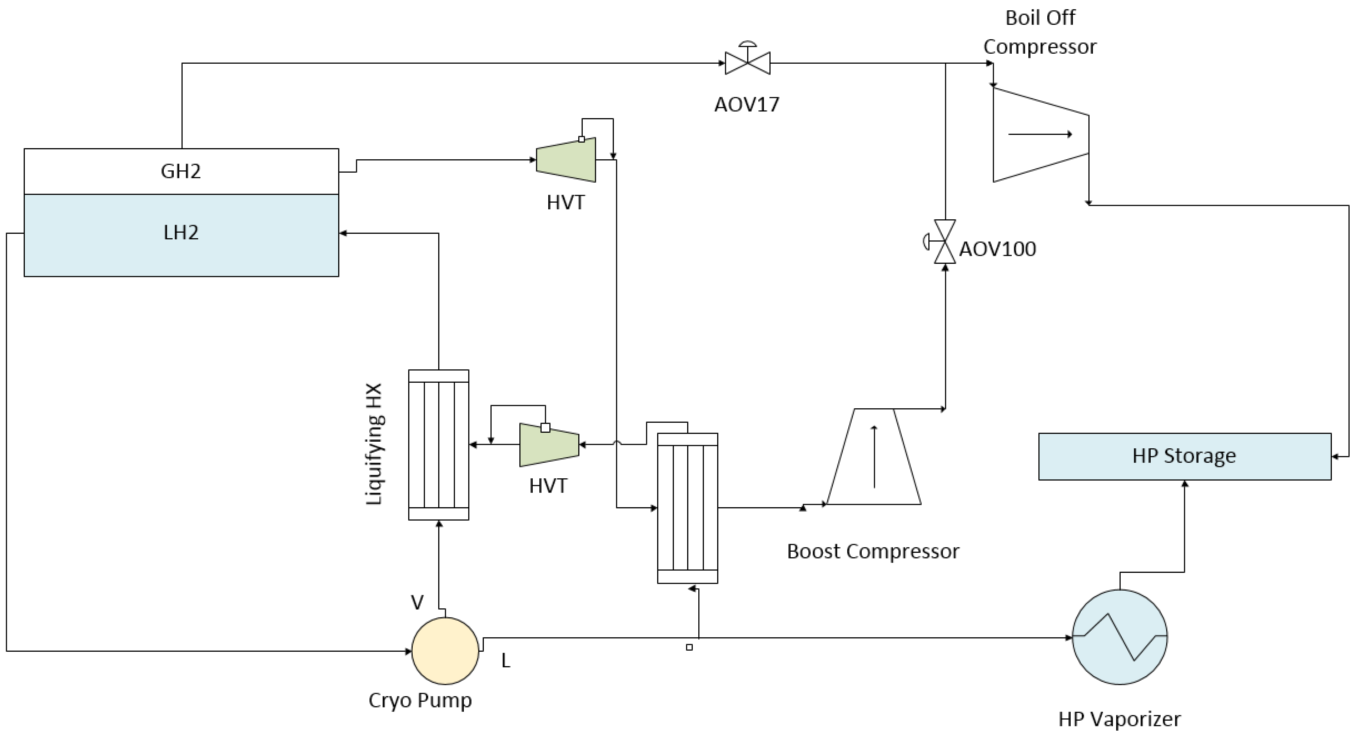


1. Notardonato et al. **278** (2017) 012012 doi:10.1088/1757-899X/278/1/012012

Task 1.3.1: Application 3: Supercritical re-liquefier

Objective: Reliquefaction of Boil-off-Gas (BOG) via supercritical expansion.

Concept: Increase compression of BOG above supercritical, cool, then expand via HVT for reliquefaction.



Key HVT Metrics: Provide Reduced Temperature LH2, Minimize Expansion PR to enable recompression of cold stream, Robust to variation in tank H2 conditions, Exceed Performance of throttle valve.

Conclusion: CFD modeling of supercritical expansion in HVT indicated insufficient cooling to warrant the concept.

Task 1.3.3: Field article design

- LH_2 tank suppliers already install hangers at the top of tanks so catalyzed heat exchanger (or HVT) can be readily incorporated into new tanks.
- 1^{st} order numerical calculations show that either a packed bed HEX (with Ionex catalyst) or HVT (with Ruthenium catalyst) can achieve the needed conversion, with acceptable weight and dimensions, within the allowable pressure drop for the BOG compressor. However, HVT pressure drop is orders of magnitude less than packed bed.

Required Slides

1. Accomplishments and Progress
2. Collaborations
3. Remaining Challenges and Barriers
4. Proposed Future Work
5. Technology Transfer Activities
6. Summary

Accomplishments and Progress

- Retrofitted the Cryocatalysis Hydrogen Experimental Facility (CHEF) for para-orthohydrogen catalysis measurements up to 70 bar, with a cycle time less than two days, and a novel Raman spectroscopy system for direct determination of the ortho-parahydrogen ratio before and after the HVT.
- Verified CFD and atomistic catalysis simulations for modeling the HVT. Showed potential to achieve the year 1 Go/No-Go performance criteria for 40% isentropic expansion efficiency.
- Successfully manufactured and tested world's first 3D printed vortex tube.
- Designed a Thermal-Vapor-Shielding (TVS) system to reduce Boil-off-Gas (BOG) compressor load up to 35%.

Collaborations

- No collaborations outside the WSU-Plug Power team occurred.

Remaining Challenges and Barriers

- COVID-19 delayed CHEF experiments to reproduce 2018 HVT measurements, those tests to be completed in June 2020.
- Although the HVT is shown to improve the TVS application, shape and catalyst optimization is required in order to show improved performance characteristics versus a packed bed HEX and the potential lifetime of the catalyst within the HEX.
- A detailed model of liquid hydrogen tank operation to show the effect of this HEX on the ullage volume temperature and pressure, considering thermal and mass transport effects, is required.
- Identifying a new tank to be produced with an HVT to enable field trials will be a logistical challenge.

Proposed Future Work

- In Budget Year 2 we propose to continue our initial plan of conducting HVT measurements in CHEF to improve model accuracy. We will continue numerical optimization of HVT for specific operational conditions and will begin manufacturing of a scaled field-test article.
- In addition to our initially proposed work scope, we propose development of a liquid hydrogen tank stratification model with adjustable parameters that can be customized to each of Plug Power's liquid hydrogen tanks. This model can incorporate the HVT in a TVS configuration to show whether performance is degrading over time.

Technology Transfer Activities

- No technology transfer activities at this time.

Summary

- Retrofitted the Cryocatalysis Hydrogen Experimental Facility (CHEF) for para-orthohydrogen catalysis measurements up to 70 bar, with a cycle time less than two days, and a novel Raman spectroscopy system for direct determination of the ortho-parahydrogen ratio before and after the HVT.
- Verified CFD and atomistic catalysis simulations for modeling the HVT. Showed potential to achieve the year 1 Go/No-Go performance criteria.
- Successfully manufactured and tested world's first 3D printed vortex tube.
- Designed a Thermal-Vapor-Shielding (TVS) system to reduce hydrogen venting by increasing energy transferred to the boil-off-gas compressor as much as 35%.