# Emergency Hydrogen Refueler for Individual Consumer Fuel Cell Vehicles


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Project ID: ST140


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# Overview

***Timeline***

- Project Start Date: August 27, 2018
- Project End Date: August 26, 2020
- Percent Complete: 87.5%

***Budget***

- Total Project Budget: $999,934
  - Contractor Share: $0
  - Federal Share: $999,934
- Funds Spent: $874,942

***Barriers Addressed***

- 100% Reaction Conversion of LiH to $H_2$
- Passively Controlled $H_2$ Gas Evolution over 15 Minutes
- Technical target of 750 g $H_2$ delivered at 2000 psi

***Partners***

- US DOE: Project Sponsor and Funding
- Skyhaven: Technical R&D
- Sandia National Laboratories: Modeling

# Relevance

- A common concern for fuel cell vehicle operators is running out of hydrogen fuel
  - Sparse hydrogen filling stations
  - Operators can experience range anxiety
  - This lessens the appeal of these vehicles hindering their commercialization
- To overcome this shortfall, the DOE is interested in developing emergency hydrogen refuelers
  - Similar in concept to keeping a can of gas in the trunk
  - Compact and lightweight $H_2$ storage unit that can be stored in the vehicle trunk
  - Can be safely and reliably operated by the driver

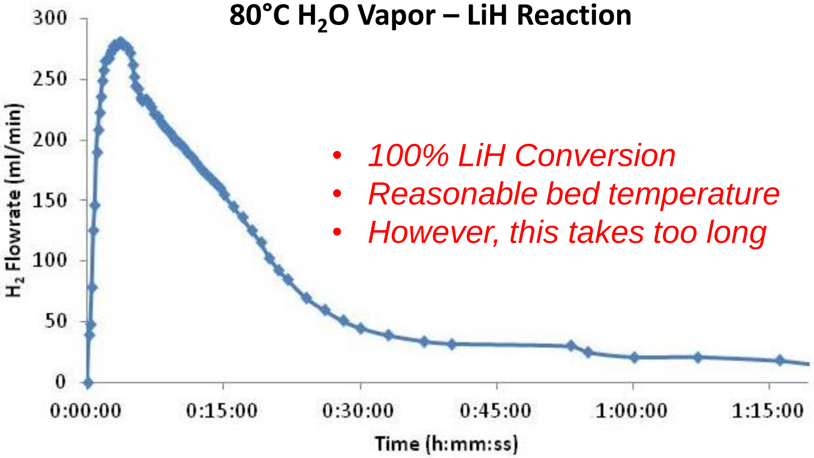
# Value Proposition

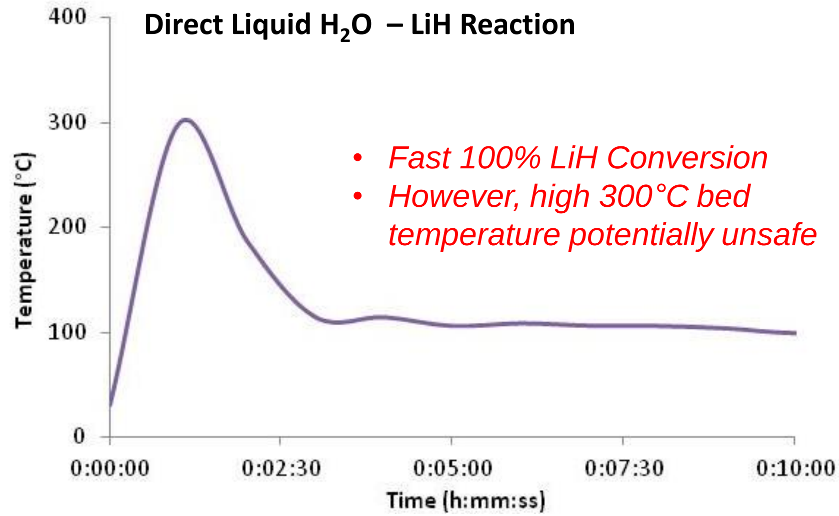
- To meet this market need, a $H_2$ gas refueler is being developed
- Skyhaven's refueler product goals
  - Provide 0.75 kg (1.7 lb) of hydrogen fuel
  - Refill the vehicle within 15 minutes
  - Activate with water giving it a long storage lifetime
  - Mass of 10 kg (22.8 lb) that includes the activating water
  - Compact space of 11 liters (0.4 $ft^3$)
  - No moving parts helping to increase reliability
- With this product, the average fuel cell vehicle will have a 50-mile range enabling the operator to reach a hydrogen refueling station

# Approach: Refueler Innovation

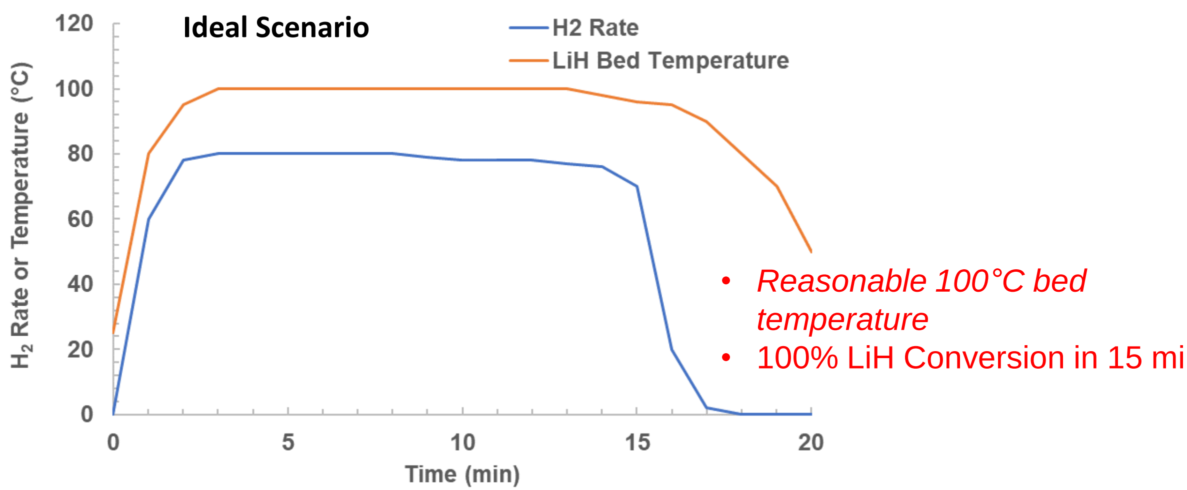
- Store lithium hydride powder in a hermetically sealed vessel
- When this chemical hydride is exposed to water vapor, it releases hydrogen gas instantaneously
  - $LiH + H_2O \rightarrow H_2 + LiOH$
- Use a network of water conduits placed throughout a packed bed of lithium hydride to shuttle liquid water
  - Liquid water pervaporates through the conduits introducing water vapor to the LiH particles
- Potential to use hydrophilic micro-wick additives within the LiH to further disperse water to all LiH particles giving 100% reaction yield

# Approach: Water Activation of LiH to Release $H_2$ Gas: Vapor Versus Liquid Feed

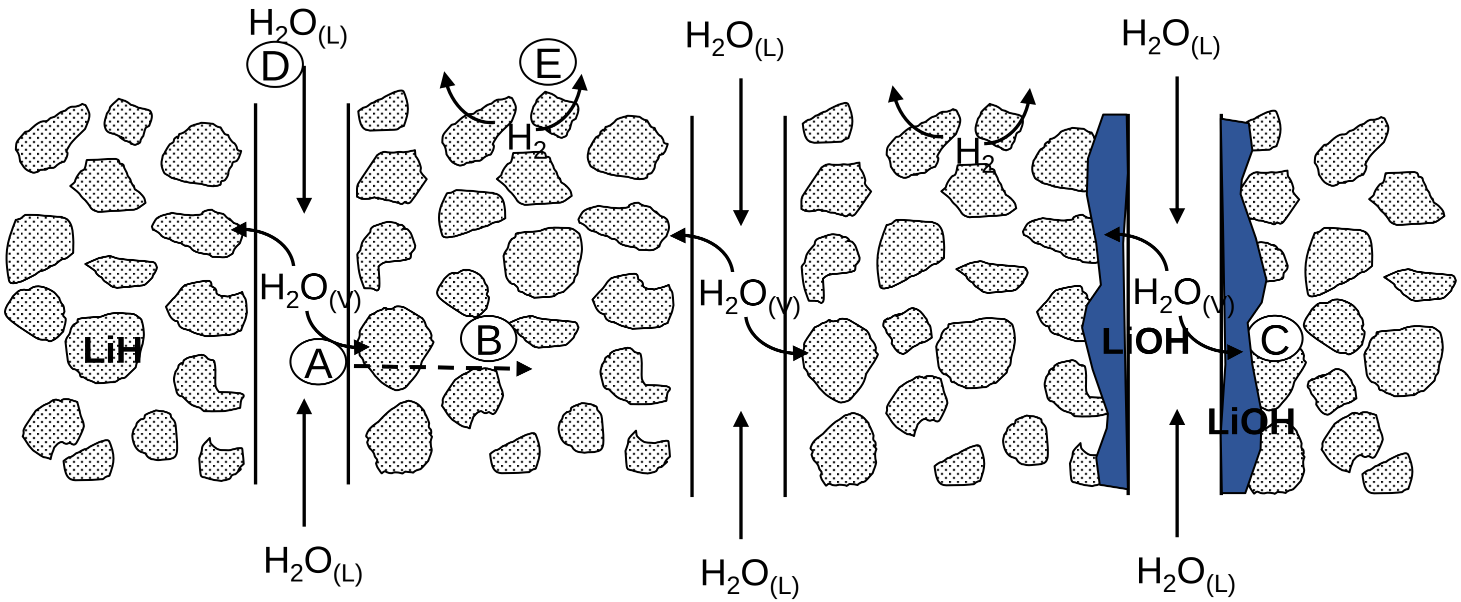



- Ideal scenario
  - React all LiH within 10-15 minutes
  - Maintain bed temperature less than 100°C using water vapor feed
  - Liquid water for bootstrapping



# Refueler Technical Challenges




A : Maximizing the water vapor transport rate through conduit

B: Maximizing the distance that water vapor can transport into the LiH bed

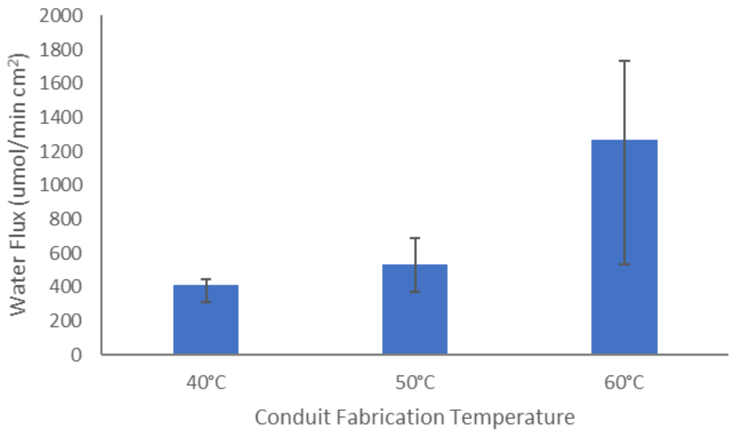
C: Overcoming LiOH films that hinder water transport to LiH particles

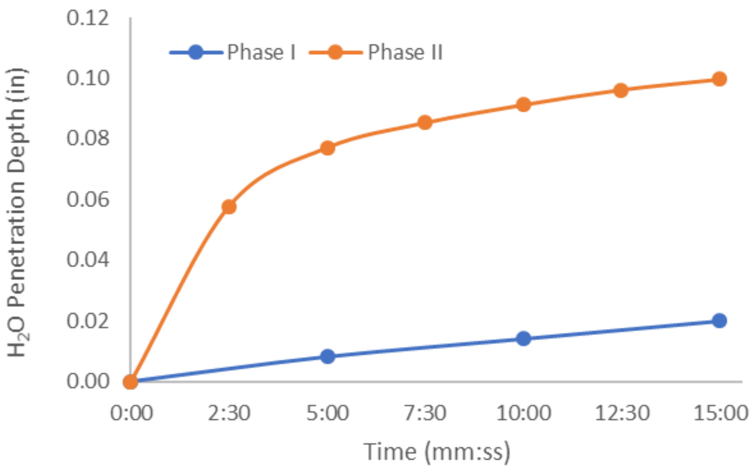
D: Introducing liquid water into the conduits without pumps

E: System engineering – start up, heat removal, $H_2$ purity, reliability, refueler design, cost

# Accomplishments: Improved $H_2O$ Transport Through Conduit and LiH Bed

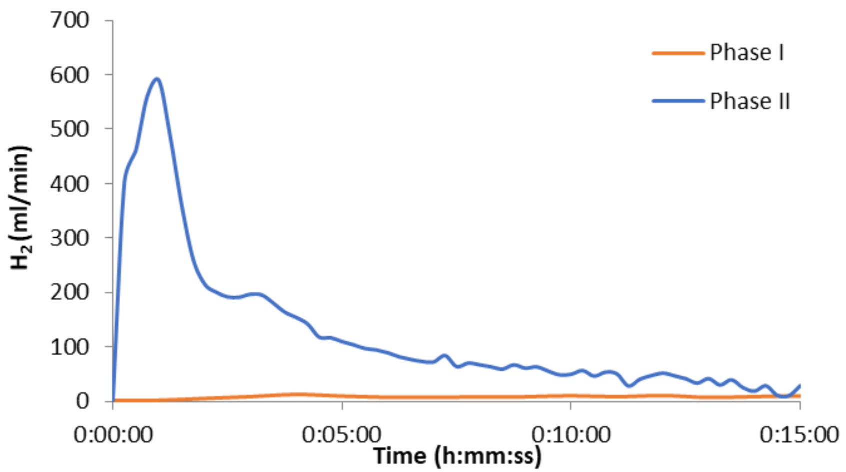
- Goals:
  - Rapidly transport water through conduit wall to produce $H_2$ gas immediately
  - Want water to diffuse through long distances of LiH particles (and through LiOH films)
- Accomplishments:
  - Change in conduit material and refueler operation design increased water transport through conduit wall and LiH bed
  - Results in minimizing number of water conduits minimizing cost, weight, volume of refueler

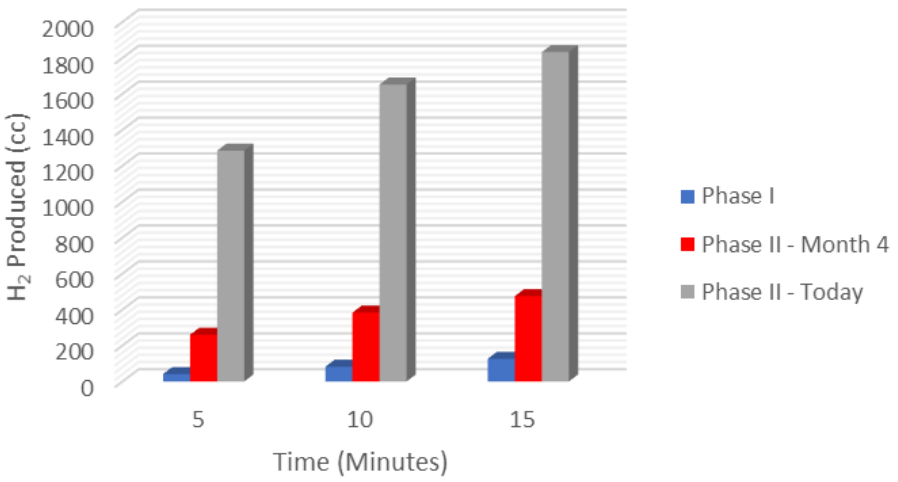


# Accomplishments: Increased Single Conduit $H_2$ Production

- Goals:
  - Immediate hydrogen production
  - Increase hydrogen production rate during duration of operation
- Accomplishments:
  - Improvements in material and design resulted in single conduit performance showing instantaneous hydrogen production at significantly higher production rates than those measured in earlier work



# Accomplishments: Reaction Completion Percentage Improves to Near 100%

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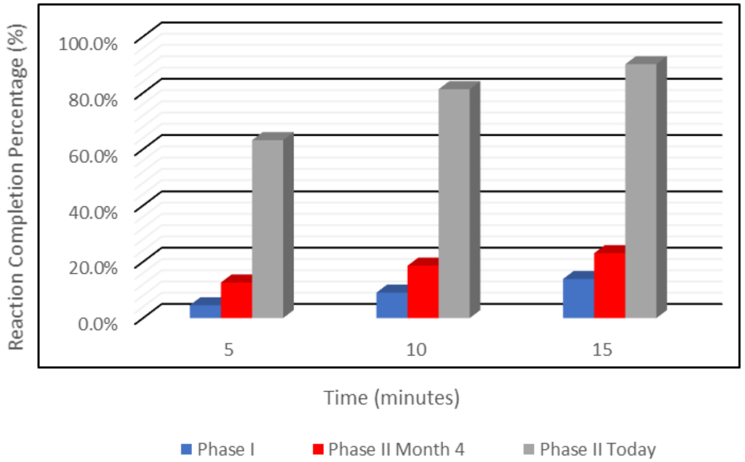
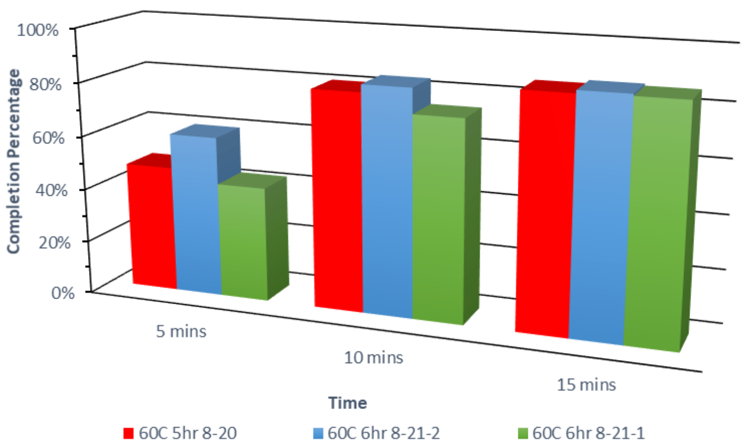
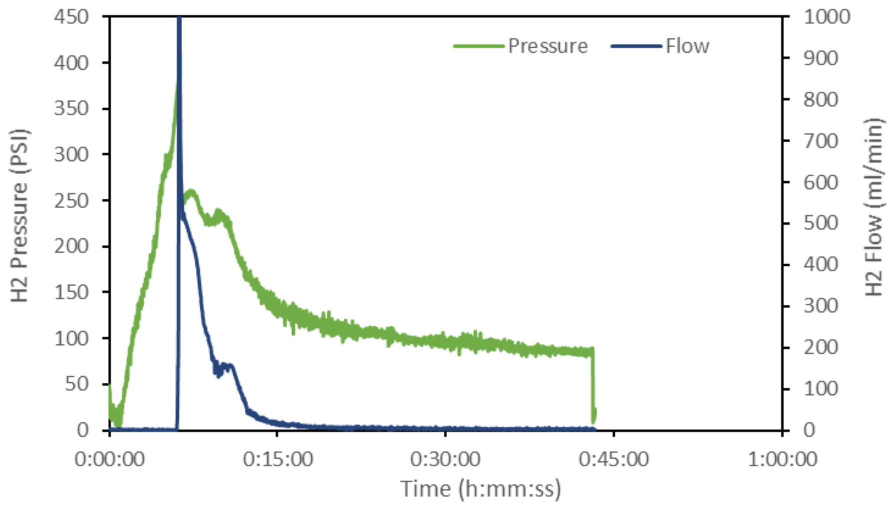
- Goals:
  - Achieve 100% reaction completion within 15 minutes in single conduit refueler
- Accomplishments:
  - Near 100% reaction completion within 15 minutes shown with improved Phase II conduit/design
  - Variations in conduit properties (i.e. wall thickness, water flux) due to processing affect refueler performance initially, however, over 15 minutes, similar reaction completion percentages are achieved, simplifying conduit manufacturing quality control



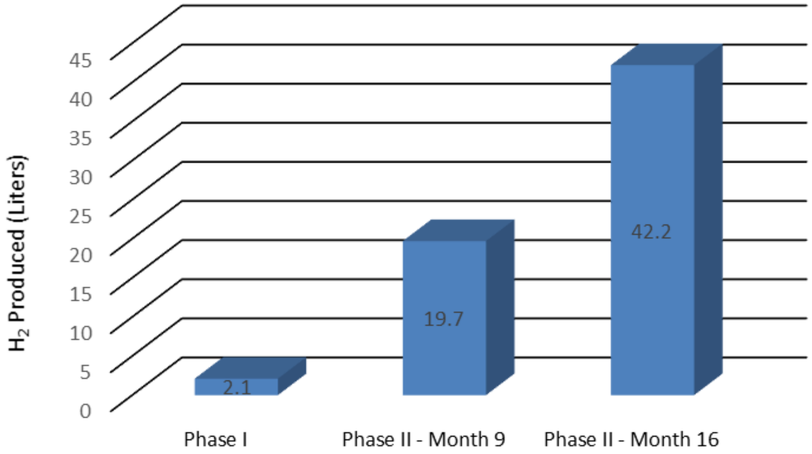
# Accomplishments: Generated Pressurized $H_2$ In Hydrogen Refueler

- Goals:
  - Pressurize hydrogen gas inside refueler
  - Release pressurized hydrogen gas stream to fuel cell
- Accomplishments:
  - Test system designed to generate then release $H_2$ at 350 psi in sub scale refueler
  - Demonstrated hydrogen pressure generation of 350 psi inside refueler
  - Released pressurized hydrogen stream from refueler at 350 psi



# Accomplishments: Scaleup Demonstrates Refueler Delivering 42 L $H_2$

- Goals:
  - Increase hydrogen production by packing numerous conduits in parallel increasing LiH content in refueler
- Accomplishments:
  - Scale up of hydrogen refuelers has increased the number of conduits in a refueler from 1 to 13 increasing LiH content in refueler
  - Hydrogen production increased from 2.1 L to 42 L during the Phase II program



# Response to Previous Years Reviewers Comments

- This project was not reviewed last year

# Collaborations: HPC4Materials Program

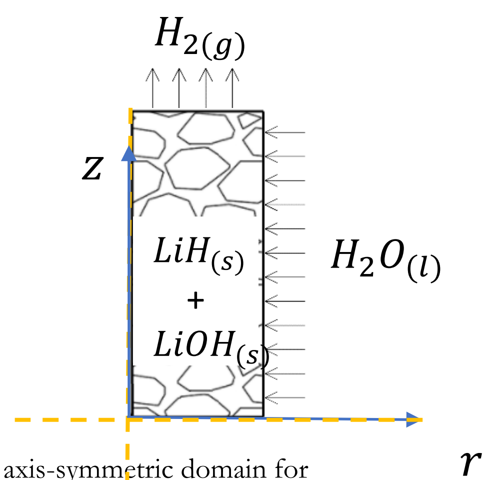
- HPC4Materials program seeks qualified industry partners to participate in short-term, collaborative projects with the DOE's national laboratories
- Industry partners granted access to High Performance Computing (HPC) facilities and experienced staff at DOE National Laboratories
- Collaborative effort addresses key challenges in developing, modifying, and/or qualifying new or modified materials through the application of high performance computing, modeling, simulation, and data analysis
- The technical goal is to developed a robust multiphysics model of the refueler reactor that will be used to improve the design and performance of the current refueler prototype.
- Specifically, the following performance goal need to be achieved:
  - 100% LiH reaction conversion within 15 minutes
  - Maximum pressure inside the reactor bed below 2,000 psia
  - Temperature inside the reactor bed below 100 degrees Celsius
  - Reduce the reactor's mass and volume

# Collaborations: CRADA Partnership

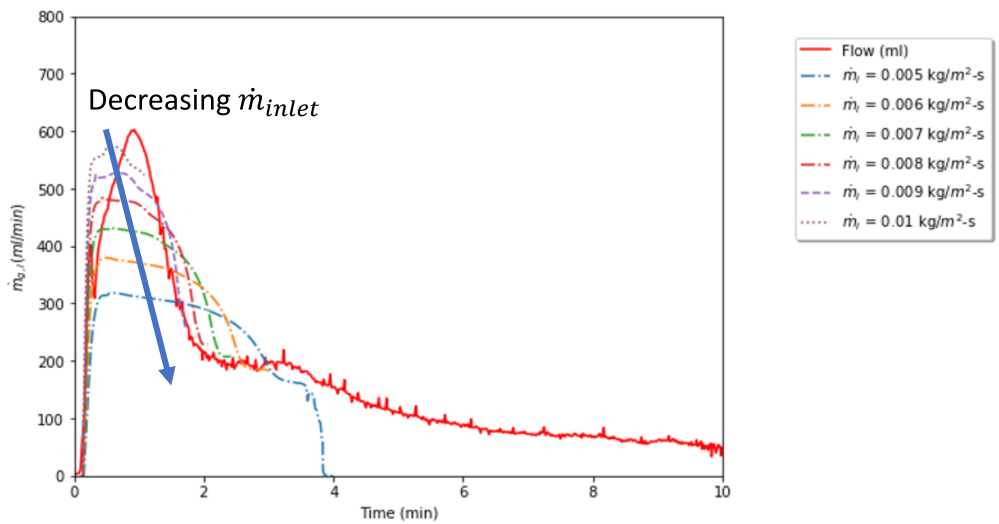
- Skyhaven will develop and conduct experimental measurements to ascertain physical and transport properties in LiH and LiH/LiOH mixtures including:
  - Thermal conductivities, water and hydrogen diffusivities, reaction rate expressions and reaction rate constants
- Sandia National Laboratories will develop and incorporate the physical and transport properties into a multiphysics model that solves the highly-coupled equations that describe the hydrogen generation process accounting for mass, energy, flow, and reaction rates
- Model will be developed in Aria, which is a Sandia National Laboratories in-house Galerkin finite element based program for solving coupled-PDE physics problems
- Aria is capable of solving nonlinear, implicit, transient state problems in 2D and 3D on parallel architectures

# Modeling $H_2$ Flow in Single Conduit at Varying Liquid Water Mass Flow Rates

- High performance modeling of the liquid water mass flow rate ranging from 0.005 kg/m$^2$-s to 0.01 kg/m$^2$-s demonstrates:
  - Decreasing water flux decreases maximum and overall $H_2$ production
  - Importance of water flux to overcome LiOH film to maintain a high $H_2$ flow rate/reaction completion percentage
  - Water flux modeling results combined with temperature and porosity modeling results will be used to design the hydrogen refueler to achieve 100% reaction completion while minimizing size, weight, volume

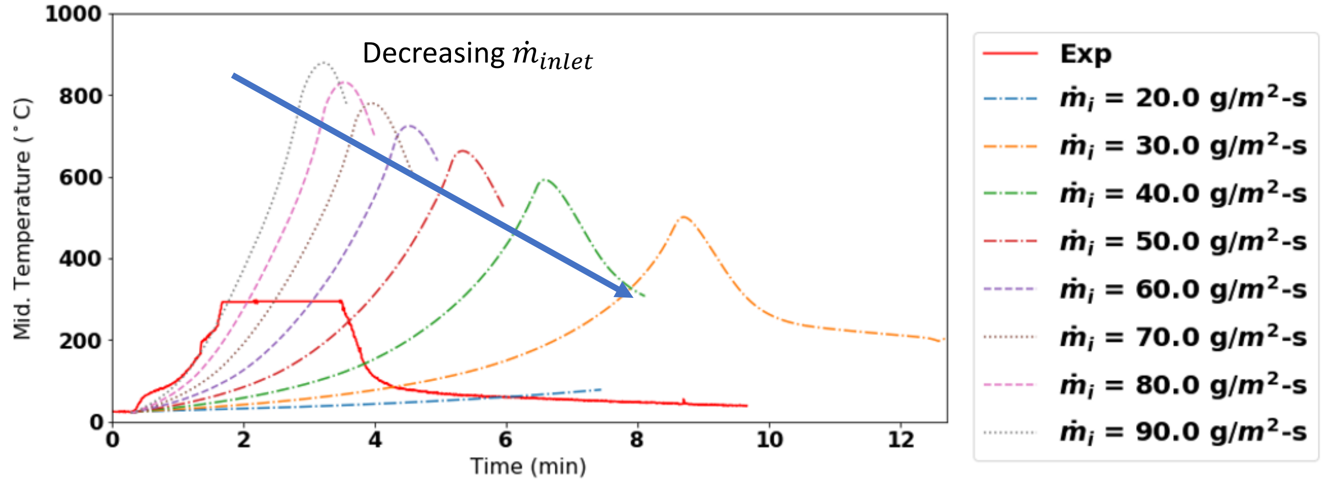



2D axis-symmetric domain for numerical simulation



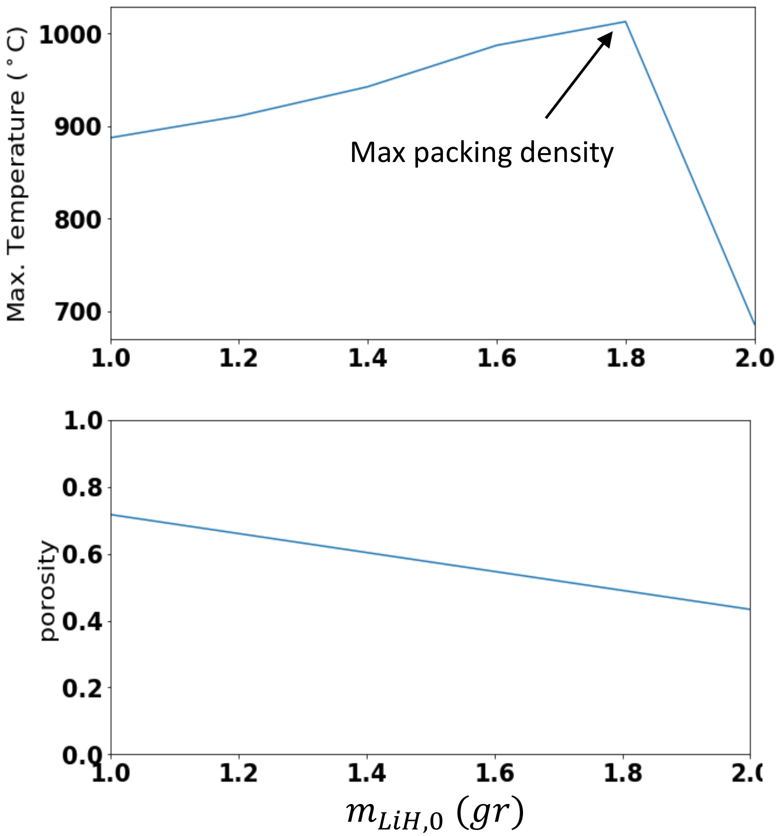
# Modeling LiH Bed Temperature as Function of Water Flux

- Significant decreases in LiH bed temperature are seen as liquid water mass flow rate decreases from 0.01 kg/m$^2$-s to 0.005 kg/m$^2$-s
- Model demonstrates importance of a controlled water feed to LiH to control LiH bed temperature
- Bed temperature modeling will assist in the thermal management of the hydrogen refueler (i.e. design of internal/external heat transfer fins)



# Modeling LiH Packaging in Single Conduit Refueler

- LiH packing in refueler predicts porosity affects on temperature
- As LiH content reaches 1.8 g in the single conduit refueler, modeled bed temperature rapidly decreases
  - Decreased porosity as LiH content increases prevents water from penetrating due to dense LiOH film produced from reaction
  - Terminating reaction and lowering temperature
- Use model to determine ideal packing density of LiH for 100% reaction completion and low bed temperature



# Remaining Challenges

- Maintaining low refueler temperature as scale up continues
  - Increased LiH = more heat generated in refueler
- Introduction of water using the new design approach
- Fabrication and manufacturing methodologies for full scale refueler
  - Producing conduits in volume
  - Packaging numerous conduits at scale
  - Filling refueler with LiH at scale
  - Pressure vessel design

# Proposed Future Work

- DOE SBIR Phase II Program will be used to focus on further development of technology including:
  - Demonstrate the refueler meeting hydrogen safety standard J2719
  - Demonstrate the refueler operating up to 2000 psia
  - Show that the refueler can operate from sub-freezing to 40 °C environmental temperatures
  - Show that the refueler will dispense 750 g of hydrogen over a 15-minute refueling operation reacting 100% of the lithium hydride
  - Develop and integrate a water conduit network into a 3000 g lithium hydride packed bed to safely operate and control the hydrogen evolution reaction
  - Develop internal and external heat transfer cooling mechanisms to maintain the refueler outer surface temperature less than 100 °C
- HPC4Materials program will be used to further develop a robust multiphysics model of the refueler reactor that will be used to improve the design and performance of the refueler

*Any Proposed Future Work is Subject to Change Based on Funding Levels*

# Technology Transfer

- Currently in discussions with the U.S Army (Ground Vehicle Power and Mobility) about a 2-year program to continue development of the hydrogen refueler
- This program would deliver an emergency hydrogen refueler to the Army with the form factor of a 20-liter fuel canister producing a pressurized hydrogen gas stream
- Responded to SBIR DE-FOA-0002156, FY 2020 SBIR/STTR Phase II Release 2 with Phase IIa proposal
  - Proposed program will further the Phase II advancements to examine thermal management within the context of the new packaging design, develop refuelers that can introduce water to the outside of a plurality of tubular conduits, and develop the manufacturing and assembly methods to produce multiple LiH packed conduits in volume

# Summary: Technology Status Today

- Phase I and II DOE programs have shown the technical feasibility of the hydrogen refueler
  - Demonstrated mechanisms to gravity feed water to the conduits
  - Showed conduit material change increases the water transport rate through the conduits
  - Showed that material and design changes have significantly increased reaction completion percentages and overall hydrogen production
  - Examined scale up packaging numerous conduits inside a larger refueler producing 42 liters of hydrogen
- HPC4Materials program has used Sandia's multiphysics model to describe the hydrogen generation process inside a single conduit refueler