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# Accelerating the Deployment of Hydrogen Fuel Cell Electric Vehicle (FCEV) Technologies

PRESENTED BY

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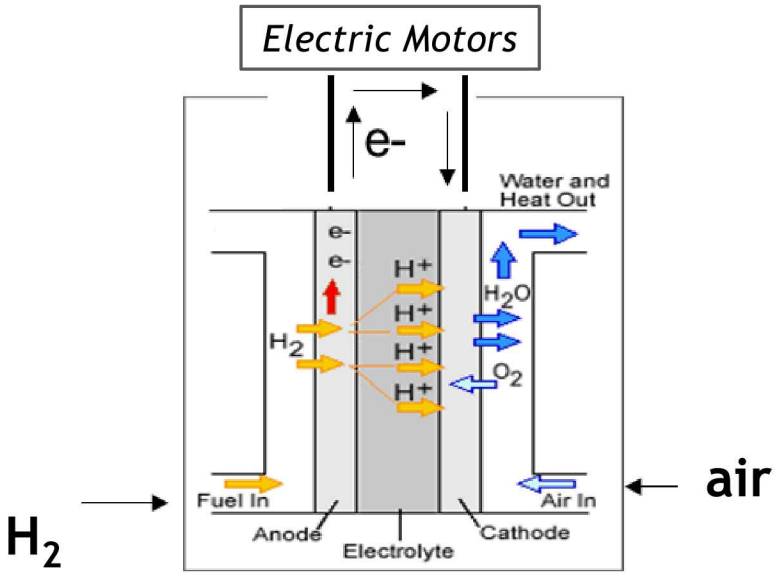
# FCEV's Research at Sandia

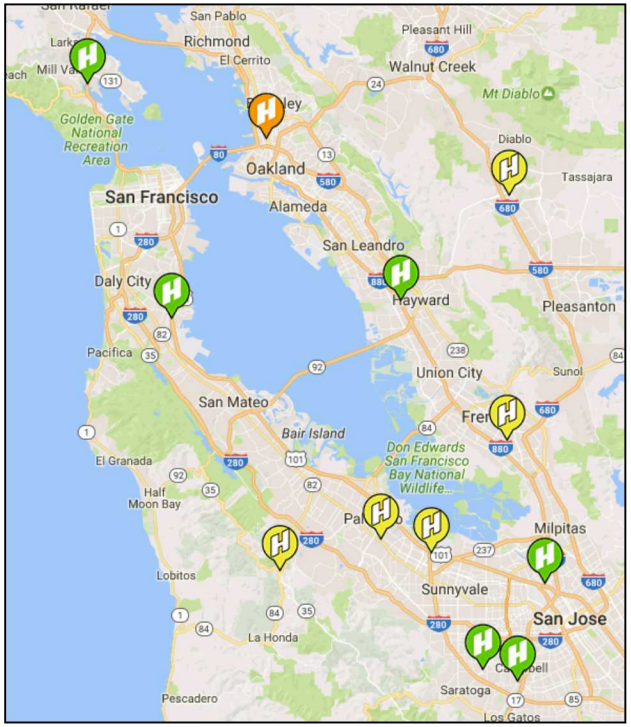
- **Motivation:** when hydrogen is used in a *Fuel Cell,* it produces ZERO pollution or greenhouse gas

- **Challenges:** safety concerns due to high flammability range and elevated cost of infrastructure.

**Hydrogen Fuel Cell**

$2\ H_2 + O_2 \rightarrow 2\ H_2O$

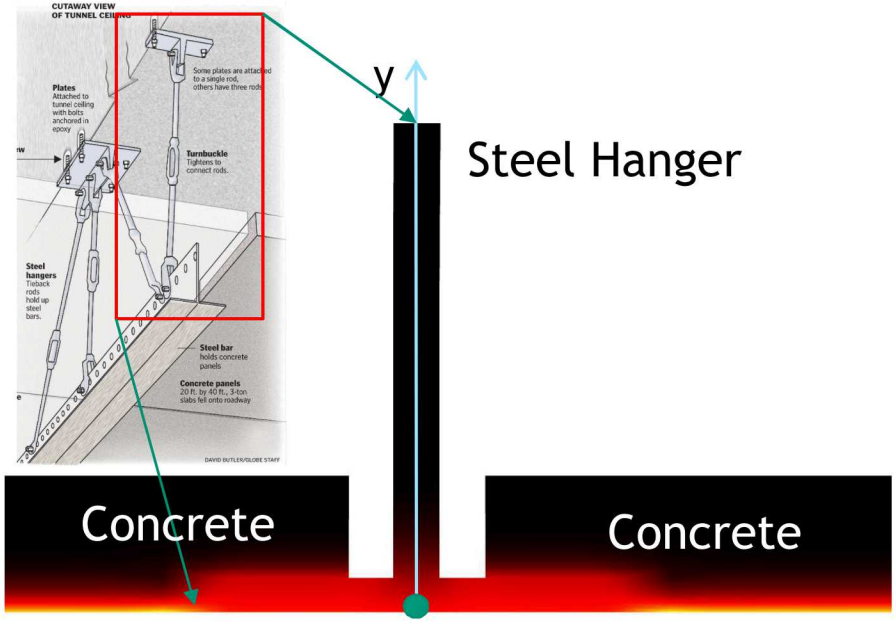


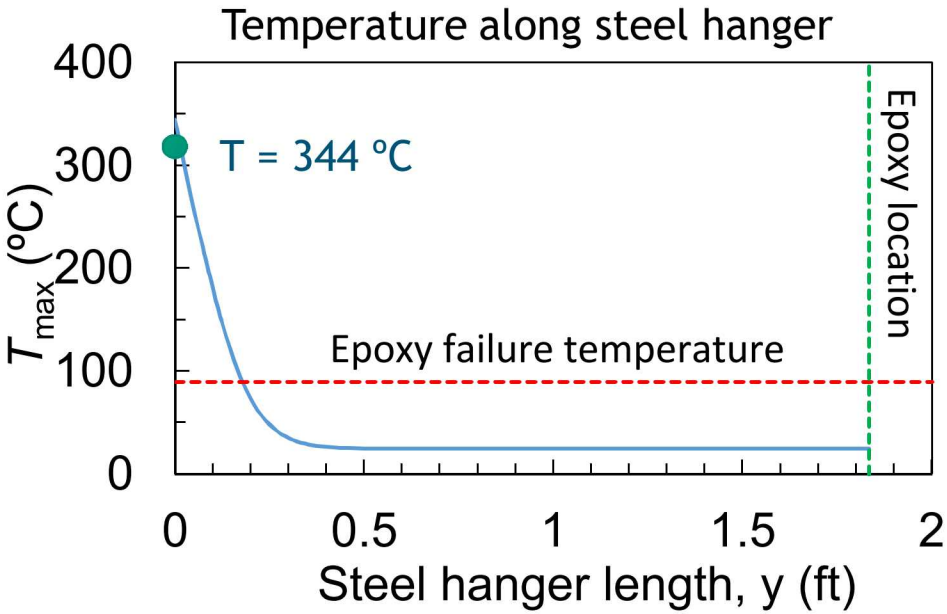



# Simulation of a H2 Jet Fire in a Tunnel

**GOAL:** Determine the tunnel structural damage due to a hydrogen TPRD release jet flame

1. Network Flow Model
   - $H_2$ tank blowdown
   - Boundary conditions for CFD Model
2. CFD Model (Sierra -Fuego)
   - H2 jet flame
   - Boundary conditions for Heat Transfer Model
3. Heat transfer model (Sierra – Aria)
   - Ceiling Structure
   - Temperature profiles
4. Solid mechanics Model (Sierra – Adagio)
   - Displacements on ceiling structures due to thermal expansion



# Numerical Modeling of Emergency Hydrogen Refueler for Fuel Cell Electric Vehicles

- **GOAL:** Develop a numerical model of the emergency hydrogen refueler to improve performance
- Multiphysics numerical simulation of a reacting two-phase flow in a porous media

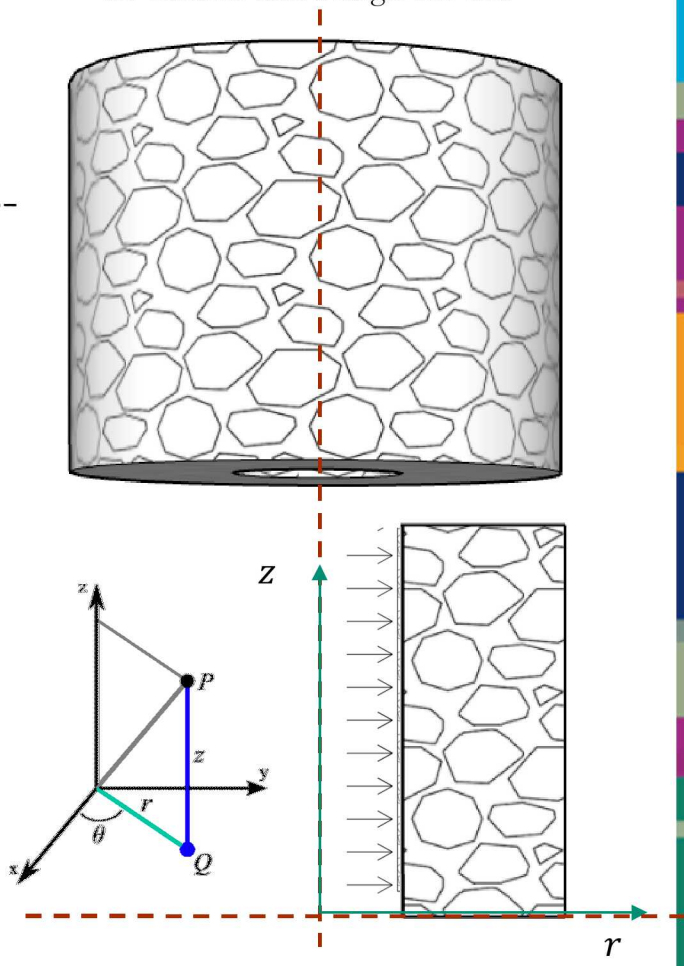
$$LiH(s) + H_2O(l) \rightarrow LiOH(s) + H_2(g) \quad (1)$$

$$LiH(s) + H_2O(g) \rightarrow LiOH(s) + H_2(g) \quad (2)$$

$$H_2O(l) \rightarrow H_2O(g) \quad (3)$$

- General assumptions
  - 2D axis-symmetric domain
    - System is dependent on z and r only
    - Cylindrical coordinate system
  - Solid is stationary

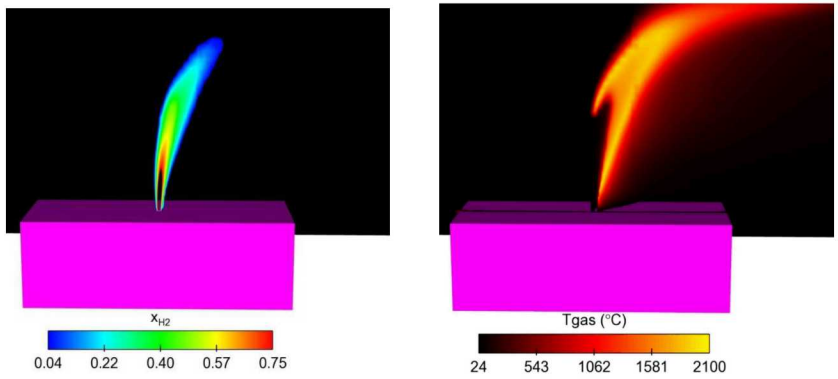
3D refueler with a single cell unit



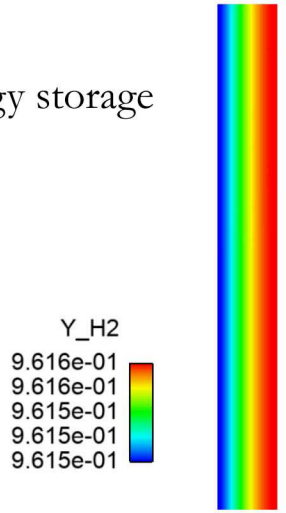

2D axis-symmetric domain for numerical simulation

# Research Focus

- Investigate safety of hydrogen releases
  - Gaseous and liquid hydrogen
  - Unattended releases
  - Controlled releases
  - Models can be applied to other fuels




- Developing numerical models to predict system performance of two phase flow in porous reacting media
  - Hydrogen production
  - Isotope exchange
  - Thermochemical energy storage
  - Thermal batteries




## Research Needs

- Models to predict material specific characteristics
  - Evaporation, solubility, permeability, diffusion coefficient, thermal conductivity
- Experimental results to validate our numerical models

# Questions

# Backup Slides

# Sandia Computational Resources

- SIERRA Multi-mechanics Module: Aria
  - General three-dimensional, transient capability to solve a non-isothermal multi-component, two-phase transport of a reacting flow in a porous medium.
  - Generalized volumetric sources that can be a function of space, time, chemistry, temperature, or any field variable.
  - Aria's codes own an in-memory parallel distributed mesh and field database, which can be fully distributed among parallel processors via domain decomposition.
  - **Sandia developers maintain the Sierra Platform**
- SNL's High Performance Computing (HPC)
  - Skybridge, Chama, Ghost, Uno
  - Skybridge contains 1,848 nodes, each equipped with one 16-core processor.

# Benefits to Sandia National Labs

- Challenges of this work
  - Couple a porous reactant media to a phase changing flow domain
  - Allow mass exchange between phases
  - Inlet boundary to permeate liquid water
- SNL developers have implemented new models into the Sierra-Aria platform
  - Modified Van Genuchten model for capillary pressure
  - Added advection contributions to one temperature porous enthalpy models for multiphase flow
  - Added open boundary option for one temperature porous enthalpy for multiphase flow
  - The new capabilities will be validated against experimental data produced by Skyhaven.

SNL will be able to use these new models for projects that deal with similar physics, such as thermal battery models.

# Sandia National Laboratories
## "Exceptional service in the national interest"

- Largest National Lab in U.S.
  - U.S. Department of Energy (DOE)
  - ~12,000 employees
  - ~US$2.3B/yr from DOE, other federal agencies, and private industry
  - $H_2$ Program in Livermore, CA (HQ in Albuquerque, NM)
- Hydrogen program: 60+ years technical depth in a wide range of areas, which we apply to enable impactful clean energy solutions