

# Natural Gas Vehicles Facility Analysis

Project sponsored by DOE Clean Cities:  
Technical & Analytical Assistance

Myra Blaylock, PhD

Sandia National Laboratories

# Natural Gas Vehicles Release Characterization and Modeling



altfuels.sandia.gov

## ■ Goal:

Develop criteria for NGV and propane maintenance facilities, to inform relevant codes and standards governing these facilities.

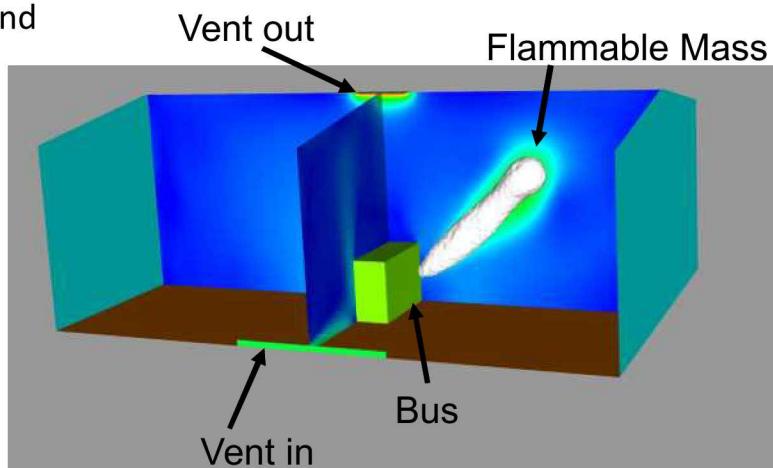
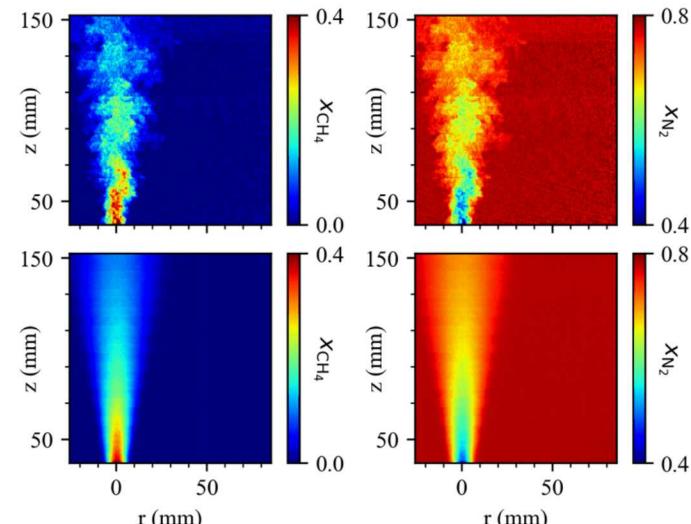
Develop relationships and educational material for outreach to standards committee members, maintenance facility owners, and vehicle operators to provide the foundation for improving requirements and standards.

## ■ Approach at Sandia National Labs:

- Develop risk analysis to determine high-risk scenarios
- Model the identified scenarios
- Develop and validate scientific models to predict hazards and harm from NG releases

## ■ Capabilities:

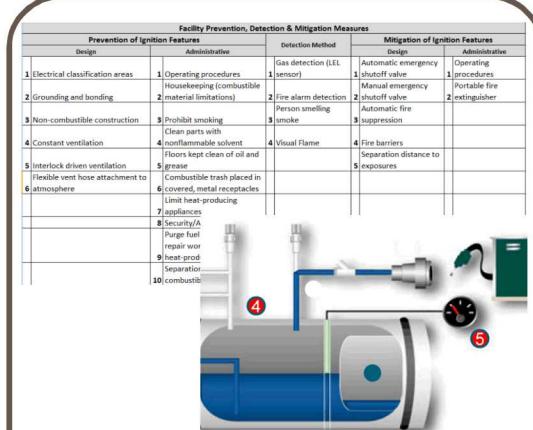
- Experimental
  - Cryogenic and other platforms with multiple fuels
  - Flexible data analysis and model validation methods
- Computer Modeling
  - Physics Models for compressed and liquid fuels
  - Computation fluid dynamics for complex leak scenarios
  - Quantitative risk assessment methods for vehicle infrastructure



Above: Experimental LNG release data

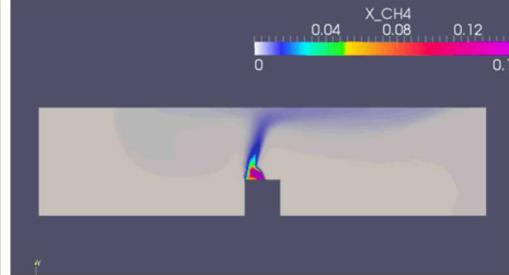
Below: CFD model results of a bus in a maintenance facility undergoing CNG high pressure release

# Project Approach:

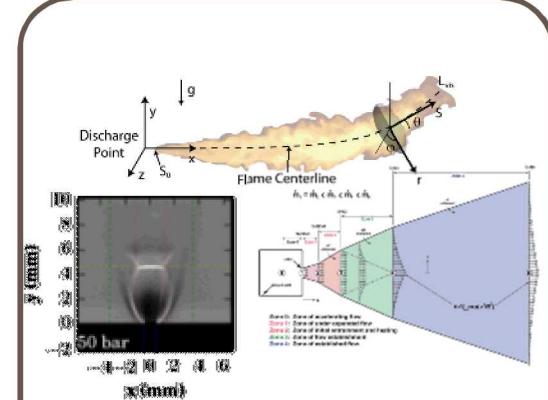


## Develop risk analysis

for determining key, high-risk scenarios to further analyze



**Apply risk analysis & behavior models to high risk scenarios**  
in alternative fuel infrastructure



## Develop and validate scientific models

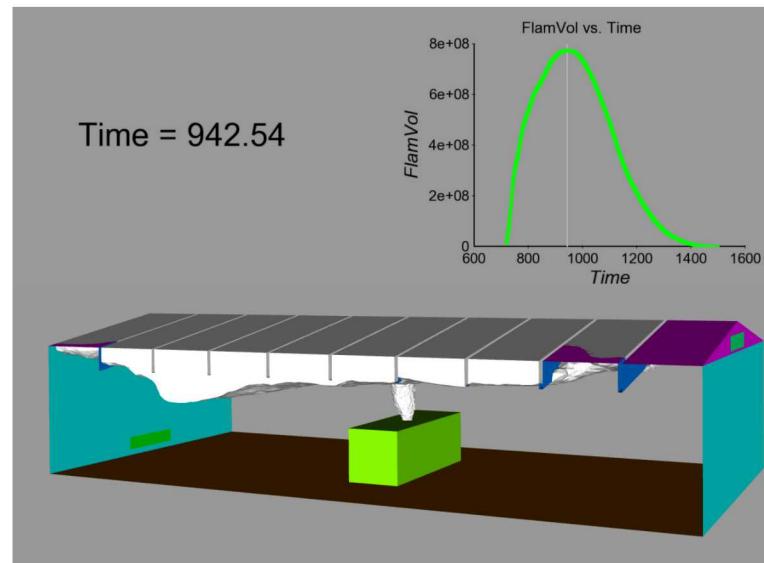
to accurately predict hazards and harm from liquid releases, flames, etc.



Scientific, risk-informed process for improving Codes & Standards to help bring advanced transportation technologies to market.

# Addressing Code Issues with Risk Assessment and Modeling

- HAZOP study identified which scenarios are most critical to alleviate and understand better through simulations
- NFPA 30A restricts sources of ignition from areas within 18" of ceiling
  - Based on legacy releases of gasoline
- IFC Relaxing Requirements for De-Fueled Vehicles
  - Exceptions for vehicles purged with N<sub>2</sub> gas
  - Vehicles contain <250 psi NG



*Modeling demonstrates that simple ceiling stand-off distance does not capture hazardous areas*

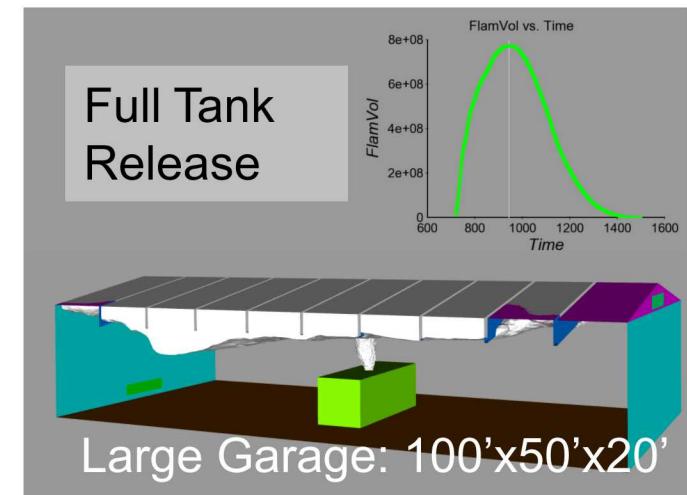
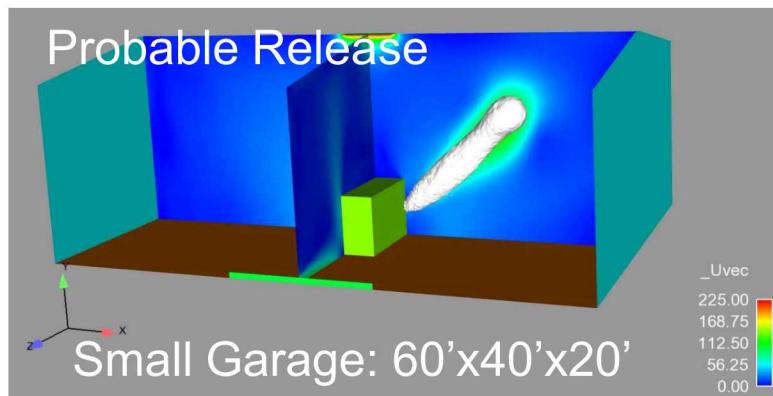
# HAZOP Identified Key Scenarios

| HAZOP Number | Component                       | Hazard Scenario  | Causes  | Consequences                          | Consequence Class | Probability Class | Risk Metric | Escalation |
|--------------|---------------------------------|--|---|---------------------------------------|-------------------|-------------------|-------------|------------|
| 1            | LNG-1 (Over pressure regulator) | External leakage from regulator body                       | Seal failure, mechanical defect, damage, etc.                             | Minor leakage of GNG                  | 1                 | 4                 | 4           | L          |
| 7            | LNG-4 (LNG tank)                | Over pressure of tank and proper operation of relief valve | Excessive hold time, insulation failure                                   | Minor release of GNG                  | 1                 | 5                 | 5           | L          |
| 12           | LNG-5 (Pressure relief valve)   | Failure of PRV to reclose after proper venting, fails open | Mechanical Failure  | Total volume of tank released         | 3                 | 4                 | 12          | H          |
| 14           | CNG-1 (Cylinders)               | Overpressure of Cylinder due to an External Fire           | External fire AND successful operation of PRD                             | Potential catastrophic release of CNG | 3                 | 2                 | 6           | H          |
| 15           | CNG-1 (Cylinders)               | Outlet or fitting on tank fails                            | Manufacturing defect or installation or maintenance error                 | Potential catastrophic release of CNG | 2                 | 3                 | 6           | H          |
| 19           | CNG-3 (Pressure Relief Device)  | PRD fails open below activation pressure                   | Mechanical defect, material defect, installation error, maintenance error | Potential catastrophic release of CNG | 2                 | 4                 | 8           | H          |
| 35B          | CNG-20 (Tubing)                 | Leakage from tubing  | Mechanical damage, material failure, installation error                   | Potential release of CNG              | 3                 | 4                 | 12          | L          |
| 37           | Multiple                        | Human error or disregard for maintenance procedures        | Procedures violated (Gas train not emptied, tank not isolated)            | Total volume of system released       | 3                 | 3                 | 9           | H          |

# 3D Computational Fluid Dynamics Modeling

Risk Assessment identified several scenarios to model:

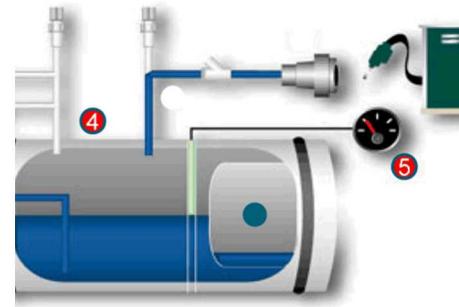
- Two sizes of garages
- Leak location and amount
- Presence of ceiling beams: **no significant difference found**
- Ventilation: **reduces but doesn't eliminate flammable concentrations**



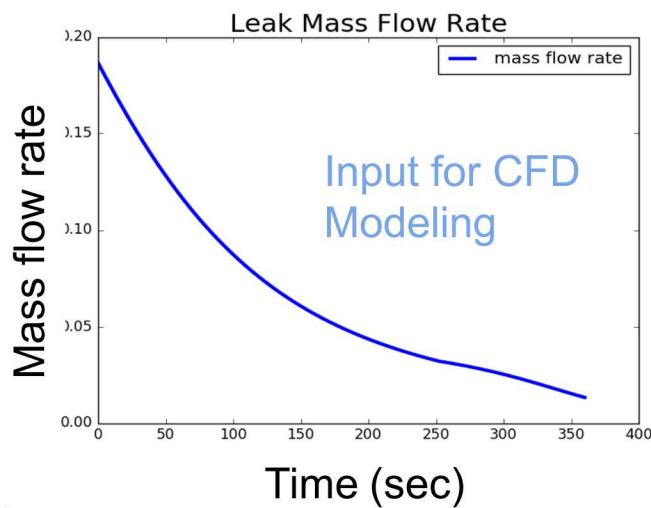
# Network Flow Modeling: Upstream of Leak

## Fast transient system analysis

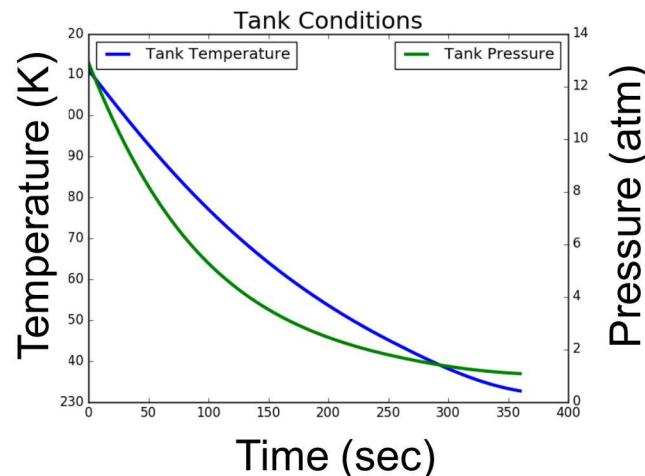
- Models venting/leaks of complex CNG/LNG tank and tubing systems
- **LNG** can leak from either saturated liquid or vapor location of tank.



Generates leak input boundary conditions for CFD modeling



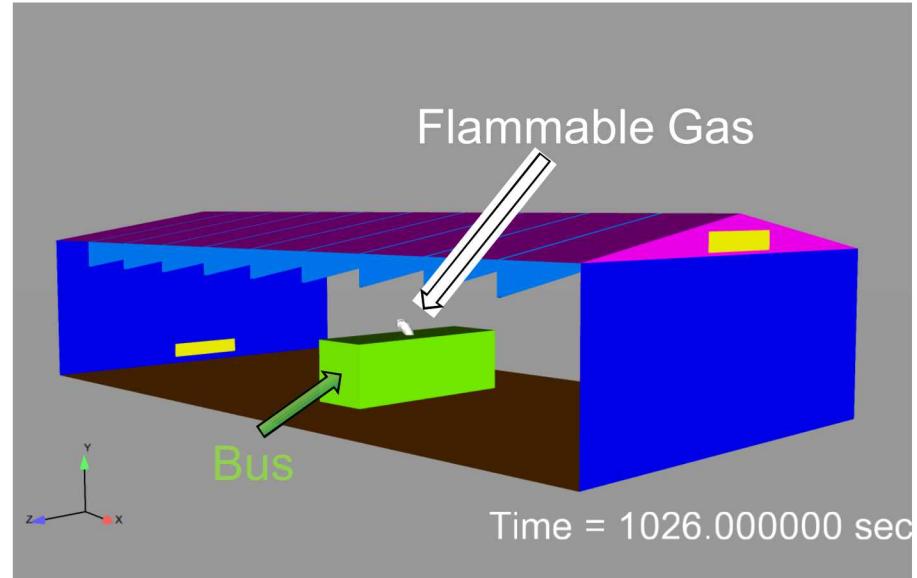
Calculates time required for tank to empty



*Fast and accurate modeling of leaking tanks and piping provides high quality CFD boundary conditions*

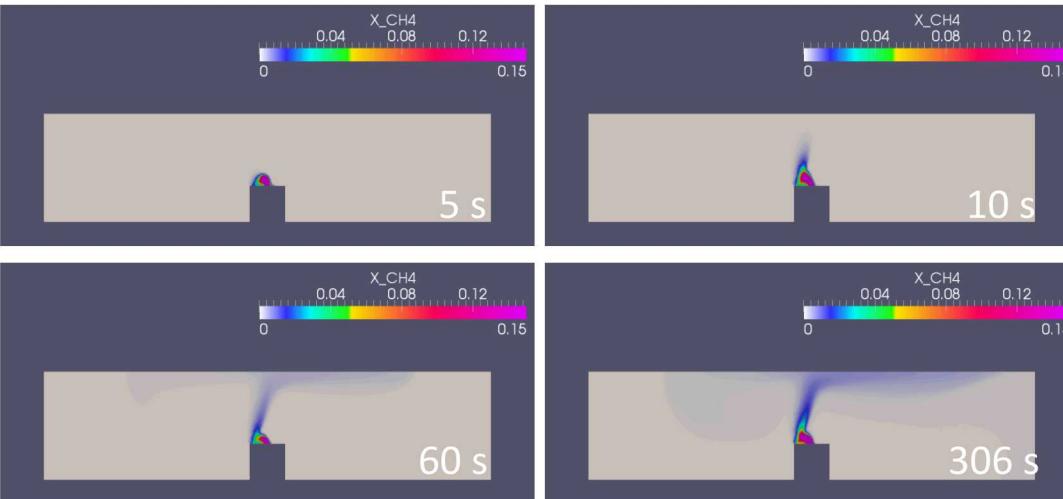
# Modeling Case A: LNG “Burping”

- After sitting for too long, an LNG tank will vent small amounts of gas (i.e. “burp”) to avoid over-pressurization of the tank. While this is a desired safety feature, it is preferable that it does not occur inside.



# Modeling Case A: LNG Release: “Burping”

Constant release (7.6 g/s) of cool gas-phase NG (160 K) for 306 s

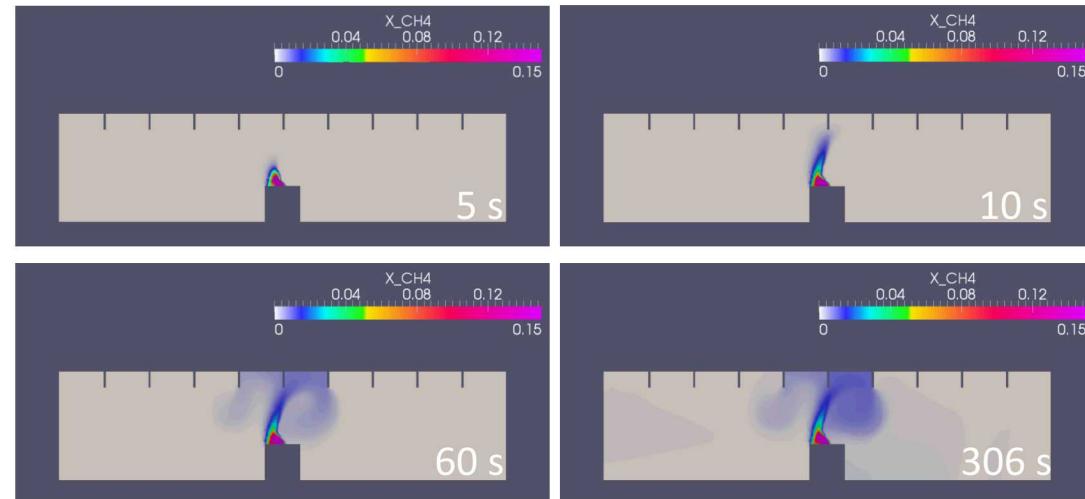


NGV facility w/o horizontal beams

- Distorted plume from vent currents
- Large cloud of overly-lean mixture spreads across the ceiling
- Only areas near NGV are flammable

NGV facility w/ horizontal beams

- Plume structure near NGV is similar to case w/o beams
- NG clouds are trapped in beam pockets but are not flammable



# Flammable volume of NG can be used to determine potential facility overpressure hazard

Flammable mass : Cumulative fuel mass mixed into flammable concentrations (mixtures between 5% and 15% by volume for NG-air)

$$\Delta p = p_0 \left\{ \left[ \frac{V_T + V_{NG}}{V_T} \frac{V_T + V_{stoich}(\sigma - 1)}{V_T} \right]^\gamma - 1 \right\}$$

C. R. Bauwens, S. Dorofeev, Proc. ICHS, 2013.

$p_0$ : Ambient pressure

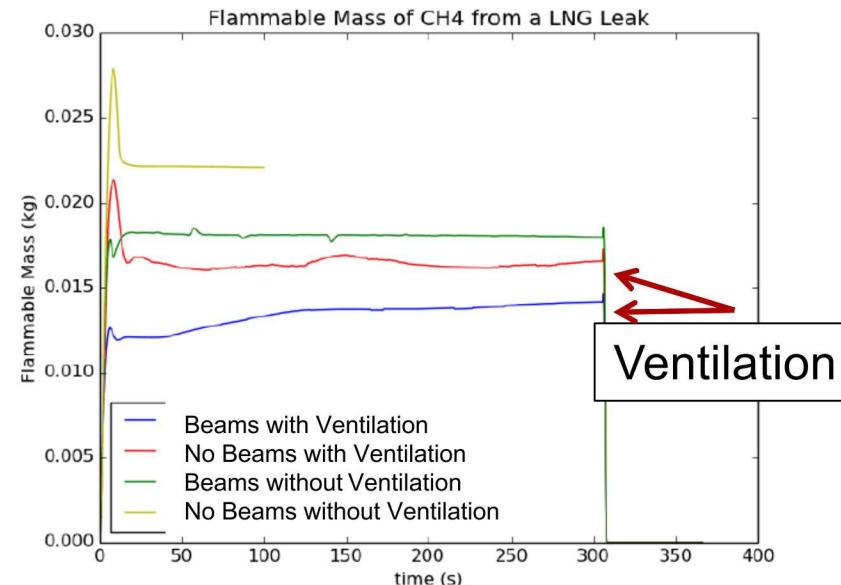
$V_T$ : Facility volume

$V_{NG}$ : Expanded volume of pure NG

$V_{stoich}$ : Stoichiometric consumed NG volume

$\sigma$ : Stoichiometric NG expansion ratio

$\gamma$ : Air specific heat ratio (1.4)



$$\Rightarrow \Delta p_{max} = 0.13 \text{ kPa} - 0.3 \text{ kPa}$$

American Institute of Chemical Engineers, 1998.

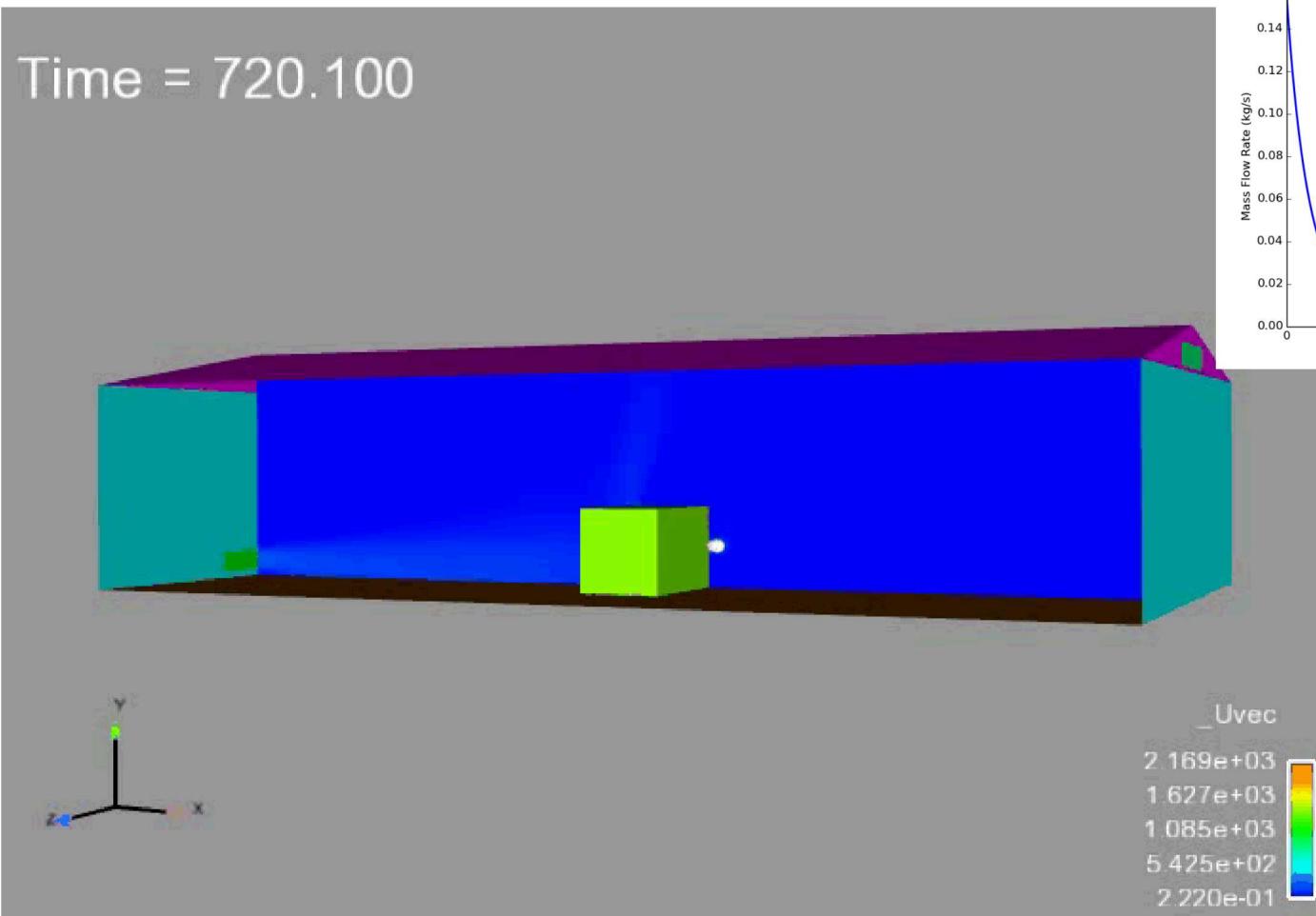
**No significant overpressure hazard for this hazard**  
**— Local blast waves not considered**

Potential Consequences:

- 1 kPa: Breaks glass
- 6.9 kPa: Injuries due to projected missiles
- 13.8 kPa: Fatality from projection against obstacles
- 13.8 kPa: Eardrum rupture
- 15-20 kPa: Unreinforced concrete wall collapse

# Modeling Case B: CNG Vehicle Fuel System Line Cracking

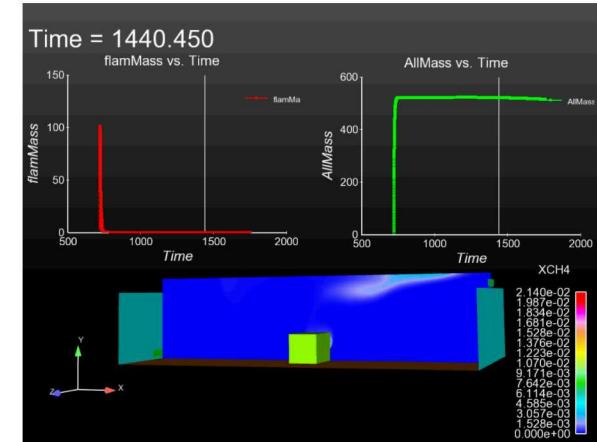
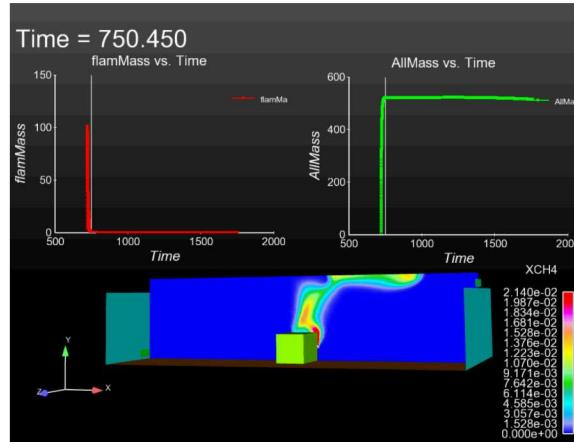
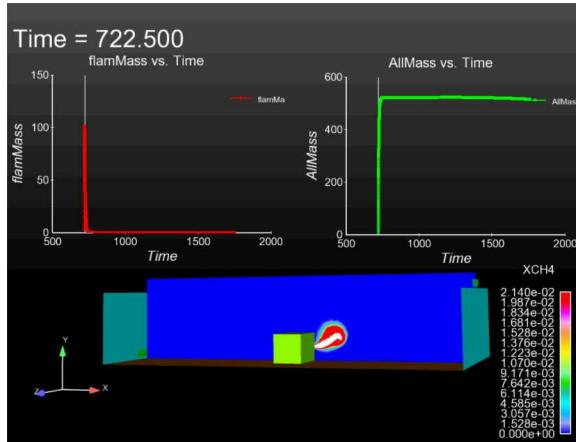
3.3 liters @ 248 bar; 3% area leak 1.27 cm ID tubing



# Modeling Case B: CNG Fuel System Line Cracking

3.3 liters @ 248 bar; 3% area leak 1.27 cm ID tubing

**No significant overpressure hazard**

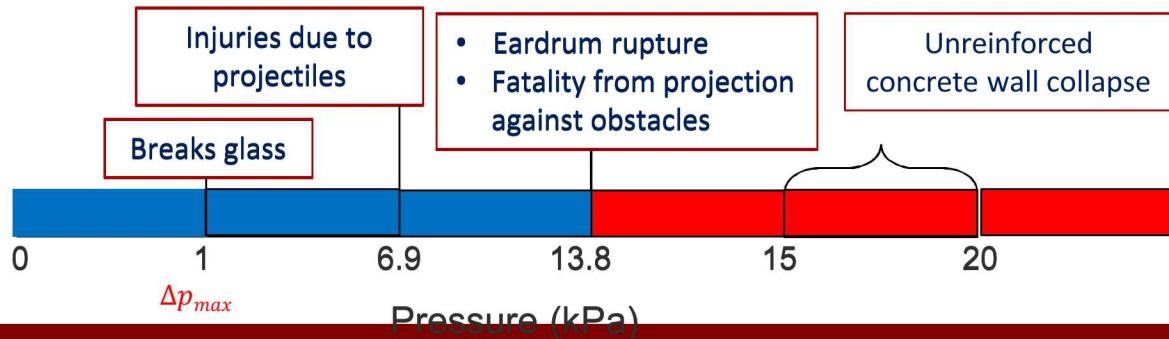
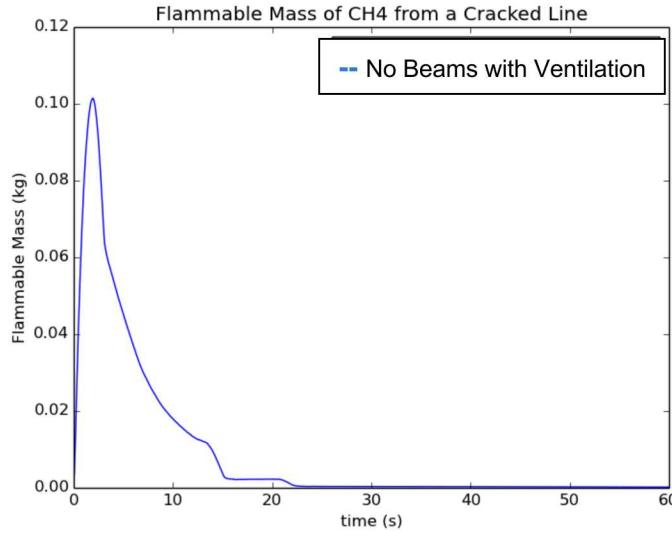


$$\Delta p_{max, expansion} = 0.43 \text{ kPa to } 1.3 \text{ kPa}$$

## Potential Consequences:

- 1 kPa: Threshold for glass breakage

American Institute of Chemical Engineers, 1998.



# Modeling Case D: CNG Fuel System

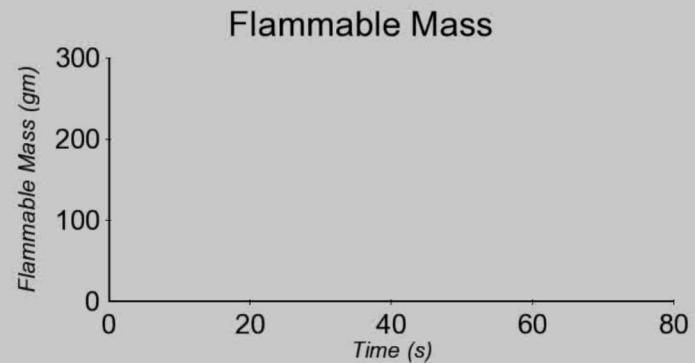
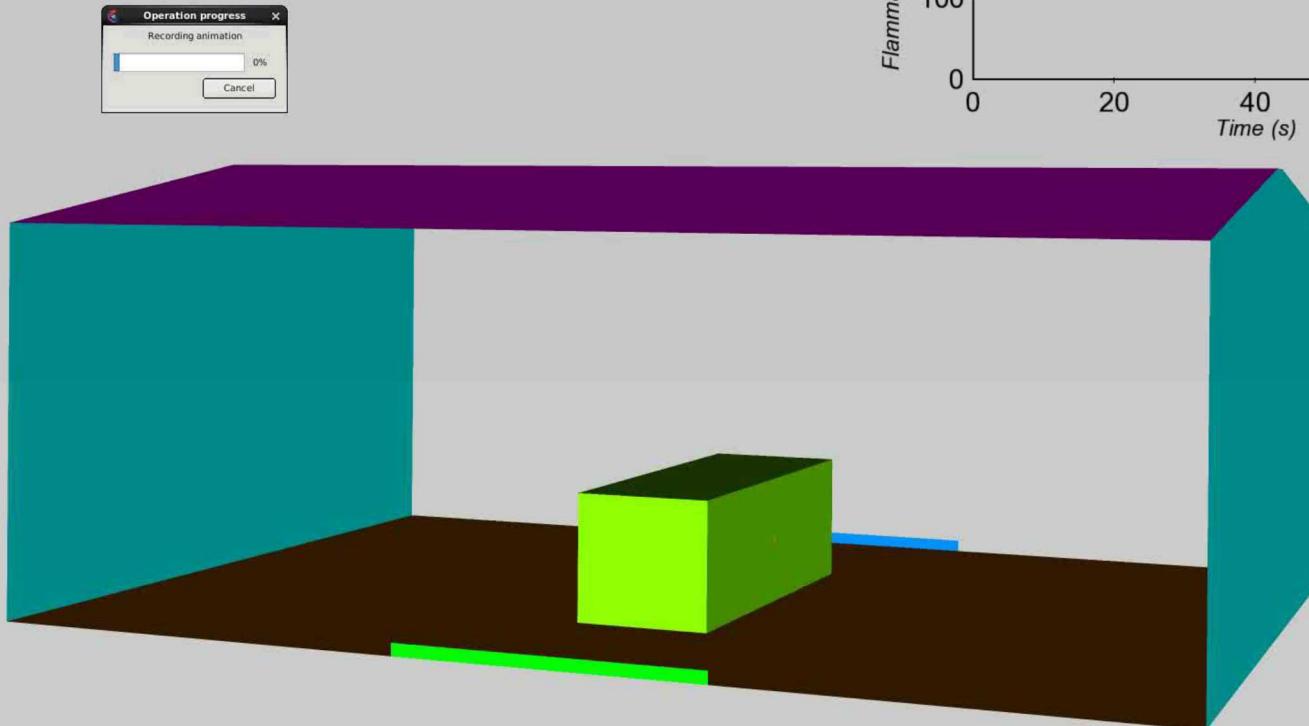
## Line Cracking – smaller garage

### CNG Fuel System Line Cracking

No ventilation

Flammable Mass region shown in white

Time = 0.00 sec



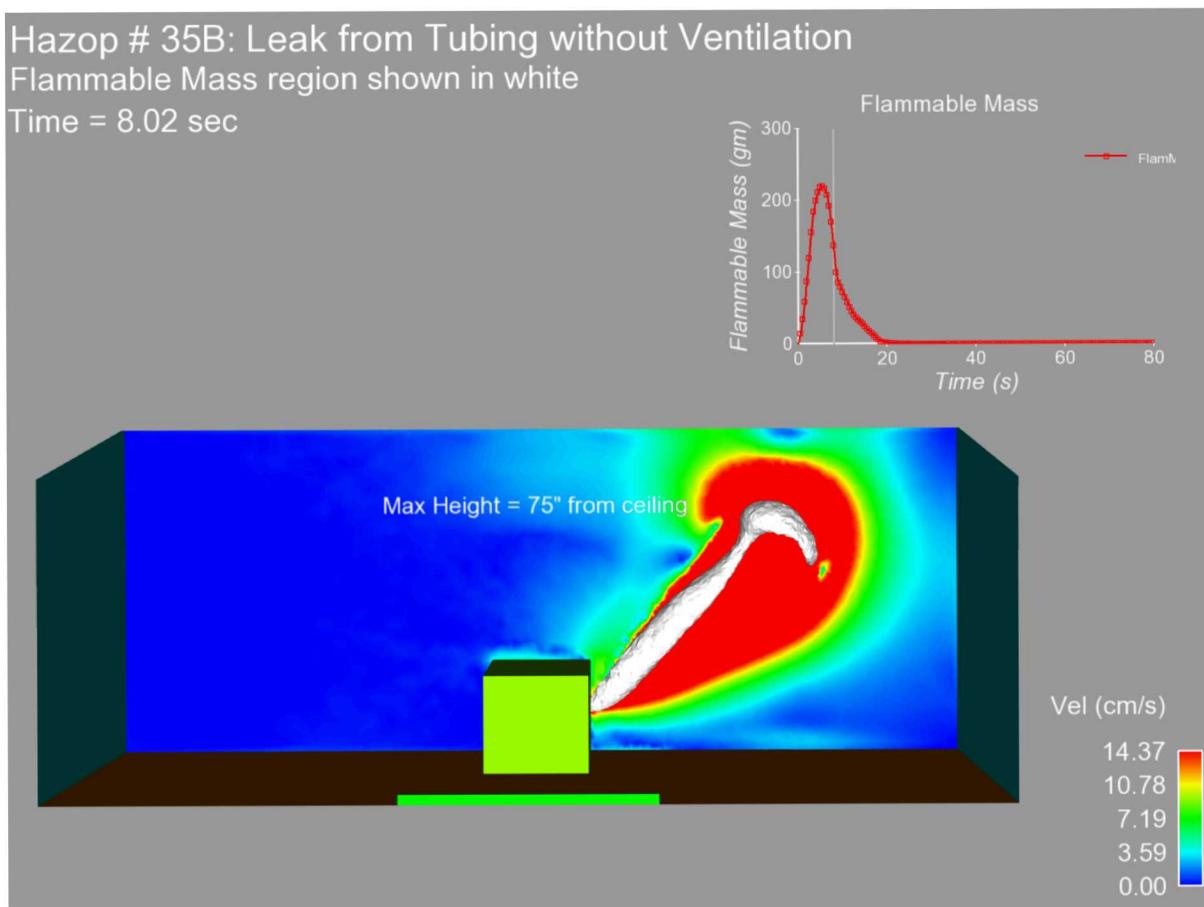
# Modeling Case D: CNG Fuel System Line

## Cracking – smaller garage

Hazop # 35B: Leak from Tubing without Ventilation

Flammable Mass region shown in white

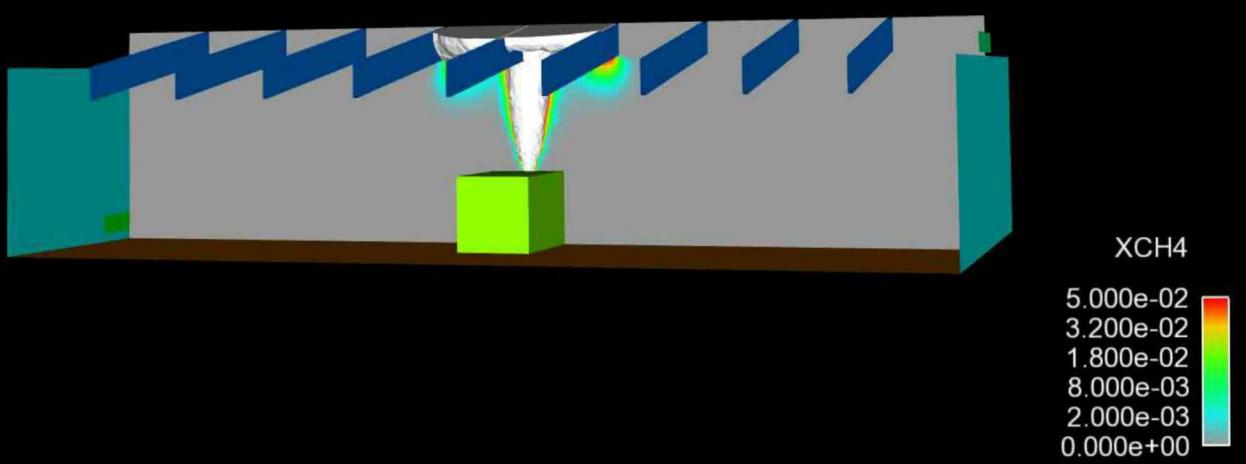
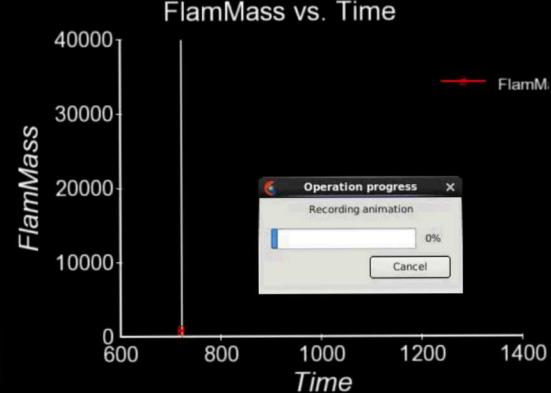
Time = 8.02 sec



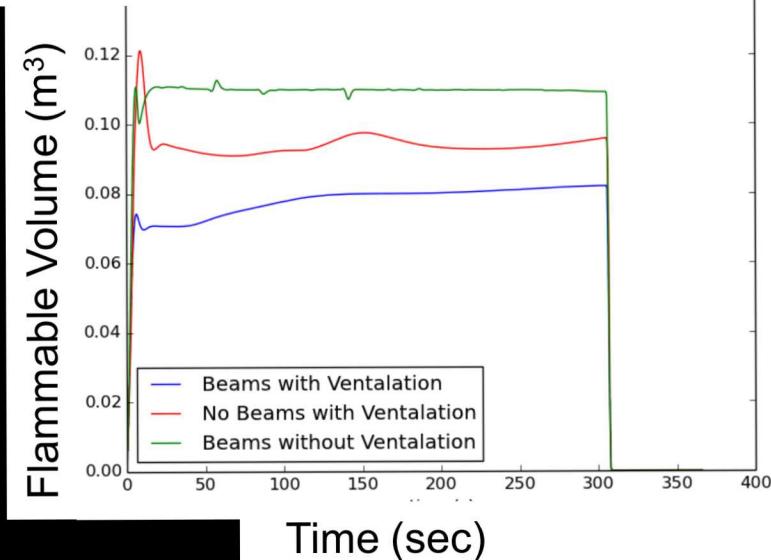
|                  | Maximum Height | Distance to Ceiling | Flammable Mass | Over-pressure |
|------------------|----------------|---------------------|----------------|---------------|
| No Ventilation   | 215" (5.46 m)  | 75" (1.91 m)        | 0.22 kg        | 2 kPa         |
| With Ventilation | 222" (5.64 m)  | 68" (1.73 m)        | 0.17 kg        | 1.5 kPa       |

# Modeling Case C: CNG Blowdown

## Full CNG Tank Blowdown in Large Garage



## Effects of Beams and Ventilation



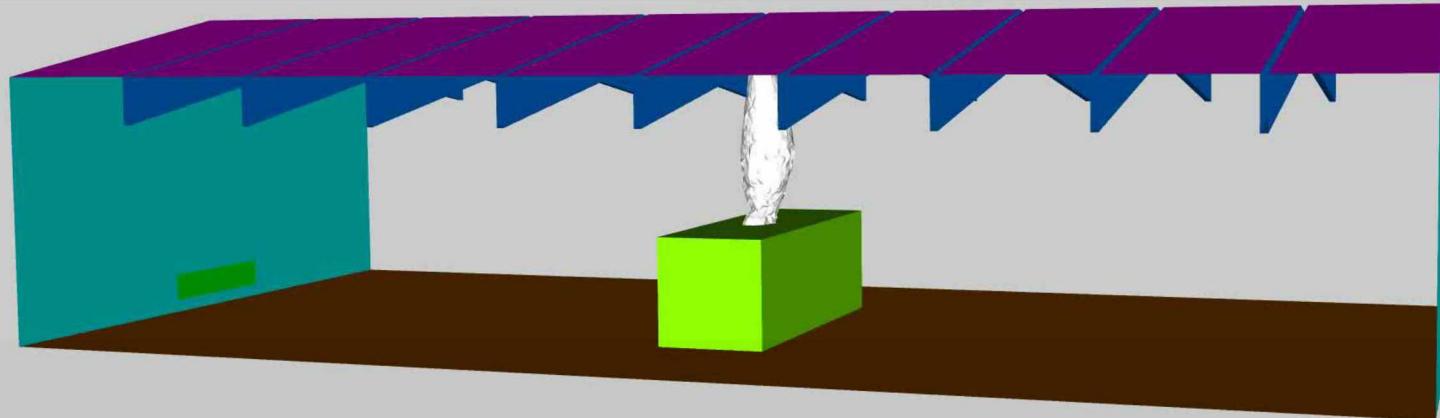
$$\Delta p_{max, expansion} = 220 \text{ kPa}$$

Wall collapse

# Modeling Case F: LNG Blowdown

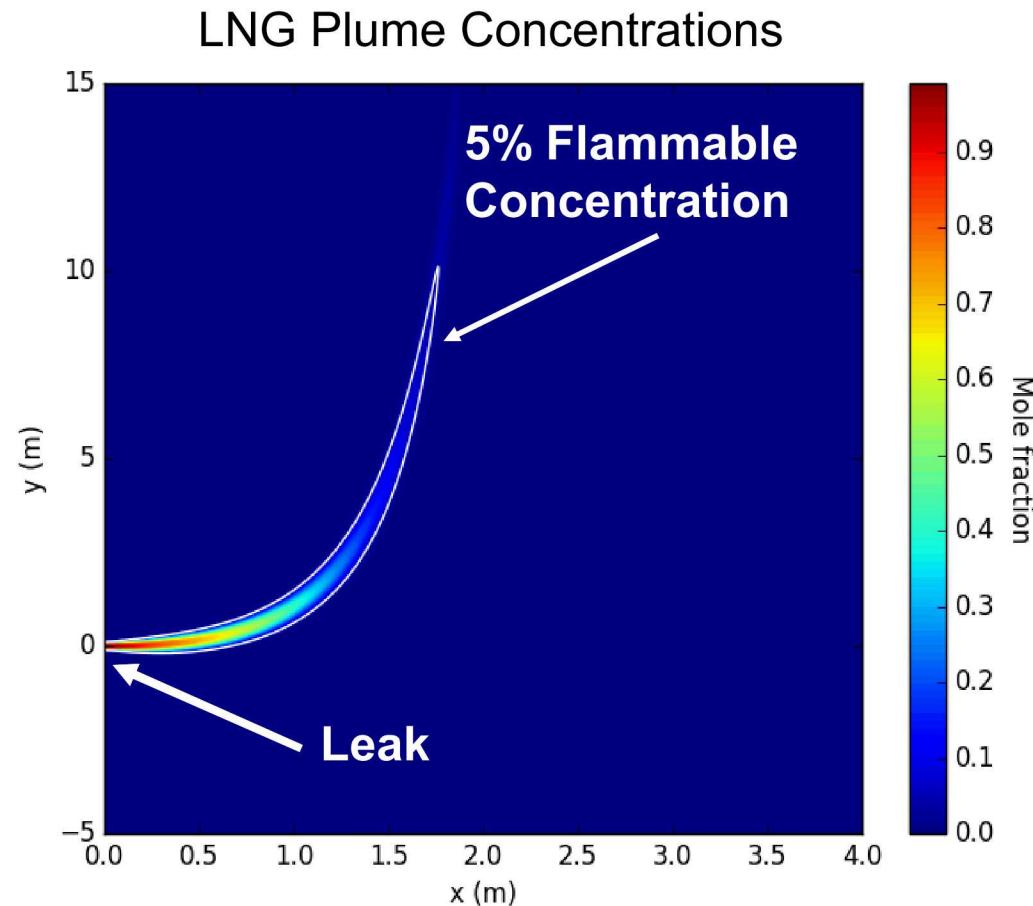
Full LNG Tank Blowdown

Time = 0.54



# 2D Plume Modeling

- Fast 2D models of leaks
  - buoyancy effects and
  - plume concentrations
- LNG cryogenic releases
  - Leaks can be from either saturated liquid or vapor location of tank.
- Outflow leak conditions taken from network flow modeling

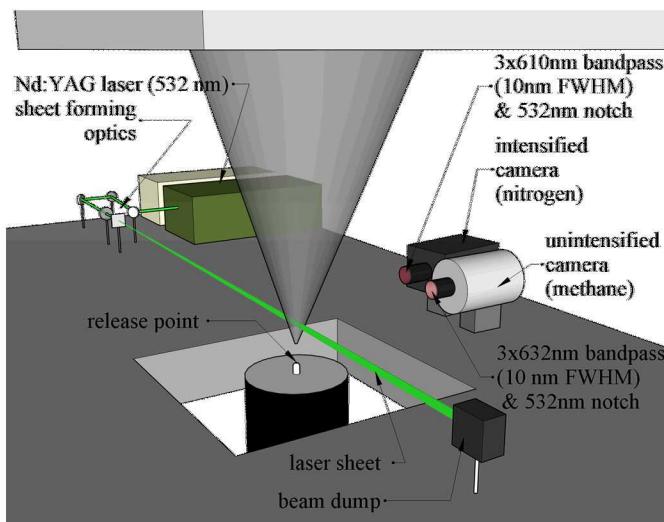


*Fast modeling of CNG and LNG leak plumes provides 1<sup>st</sup> order estimate of leak shape*

# LNG Experiments for Model Validation

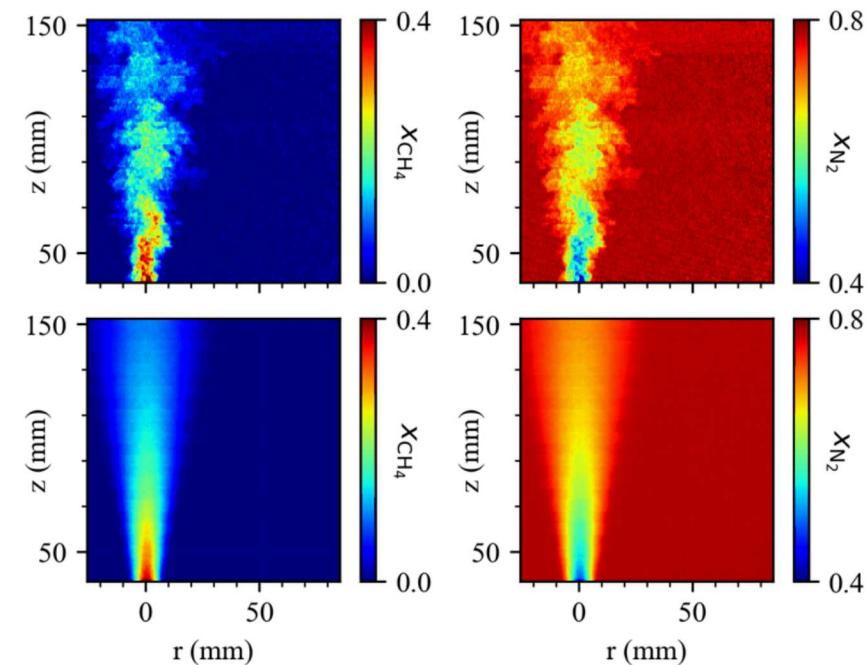
LNG experiments for understanding leak behaviors and model validation

## Experimental setup for liquid CH<sub>4</sub> (Planar laser Raman imaging)



Instantaneous  
Time Averaged

Example cryogenic CH<sub>4</sub> data



# Publications and Presentations

- <http://altfuels.sandia.gov>
- “Analyses in Support of Risk-Informed Natural Gas Vehicle Maintenance Facility Codes and Standards: Phase I”, by Isaac W. Ekoto, Myra L. Blaylock, Christine A. LaFleur, Jeffery L. LaChance, Douglas B. Horne, Sandia National Laboratories, March 2014. SAND2014-2342.
- Presentation slides
- “Analyses in Support of Risk-Informed Natural Gas Vehicle Maintenance Facility Codes and Standards: Phase II”

# Observations

- Little sensitivity was observed for ventilation or roof supports due to the short durations of the releases relative to the ventilation rates and the propensity of the support structures to enhance mixing .
  - Ventilation reduced but didn't completely eliminate flammable concentrations
  - Beams did not increase risk of concentration build-up
- For the low-flow release scenarios the flammable masses, volumes, and extents were low, and the flammable regions disappeared quickly after the conclusion of the leaks. Moreover, predicted peak overpressures indicated there was no significant hazard expected.
- For the larger release, the release plume quickly achieved a nearly steady flammable volume that extended from the release point at the vehicle up to the ceiling, before spreading across the ceiling.
- LNG release has the potential to result in flammable concentrations throughout the height of the facility.

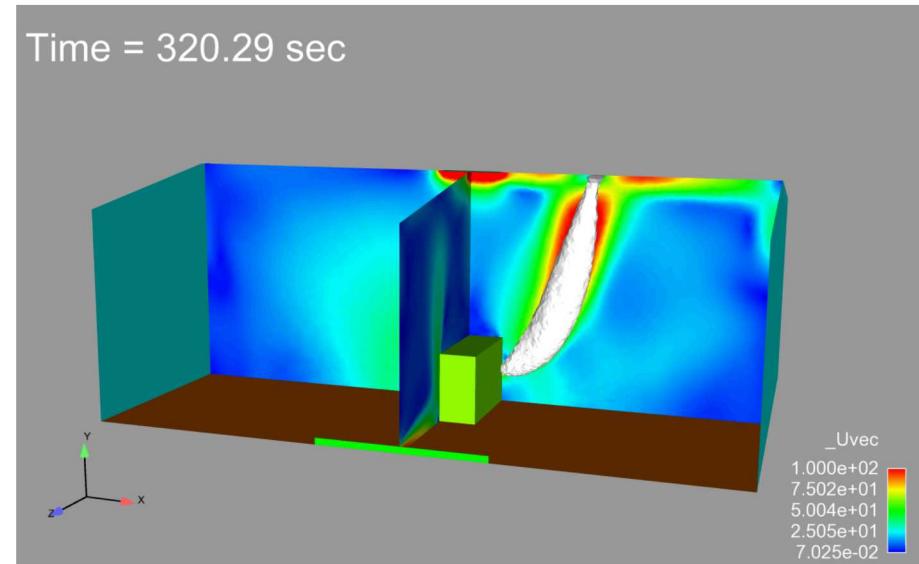
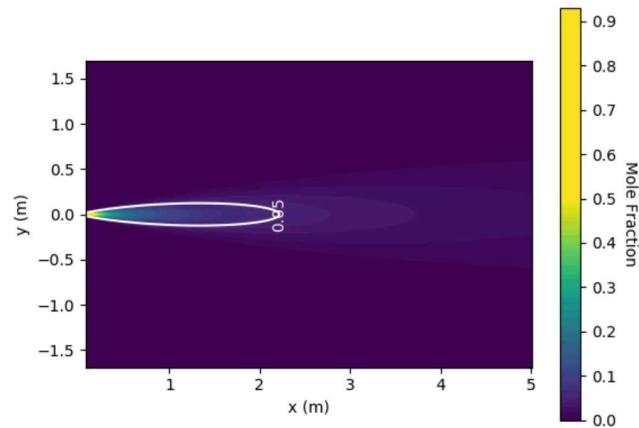
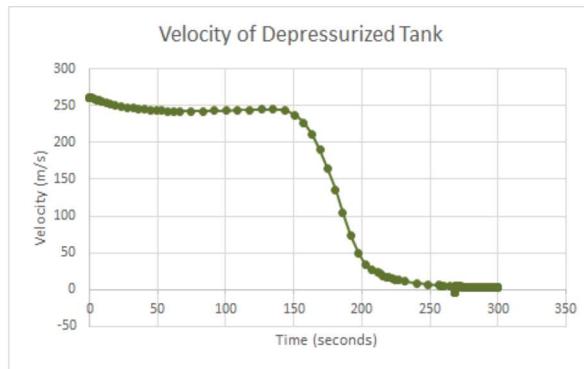
Thank you!

Questions?



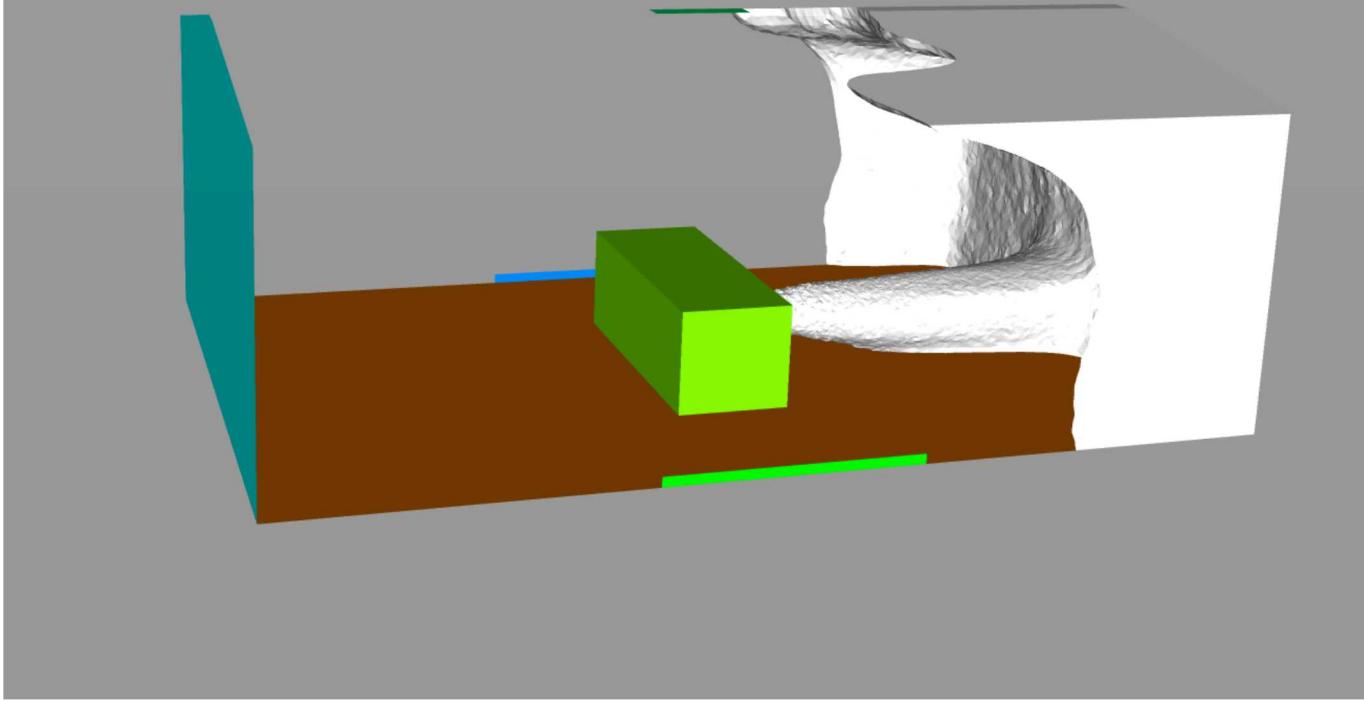
# Defueling to 250 psi

- Recently adopted IFC wording addressing reducing CNG cylinder pressure down to 250 psi that would allow CNG vehicles into the unmodified building.
  - 123 Gal tank



# Modeling Case E: CNG Blowdown in smaller garage

HAZOP #15: Full CNG Cylinder Blowdown

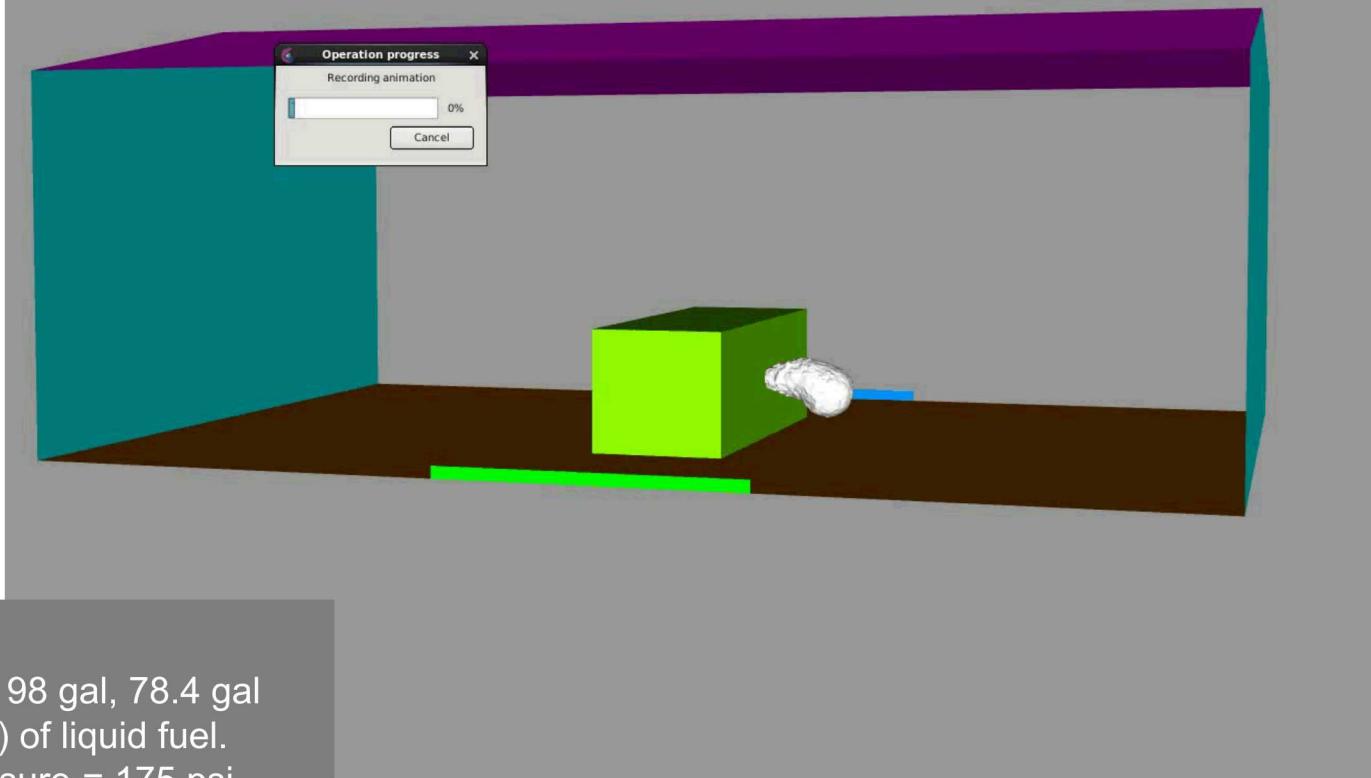


# Propane

## Propane Leak with Top Down Ventilation

Flammable Volume in white

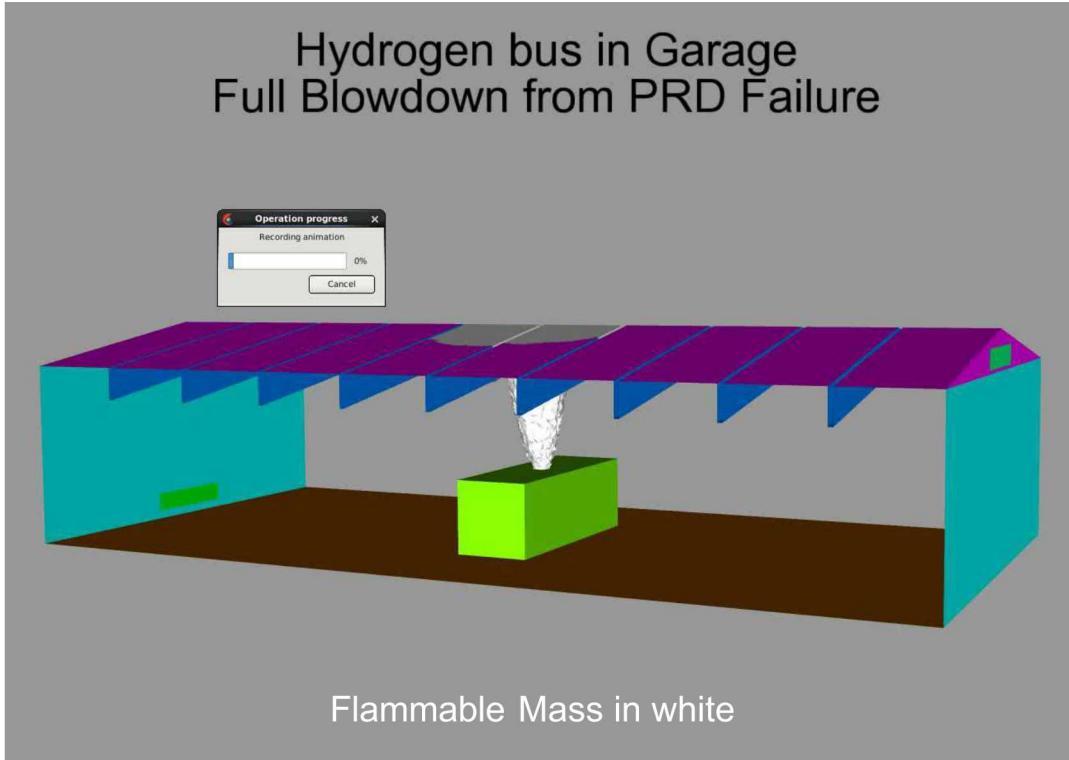
Time = 643.0629



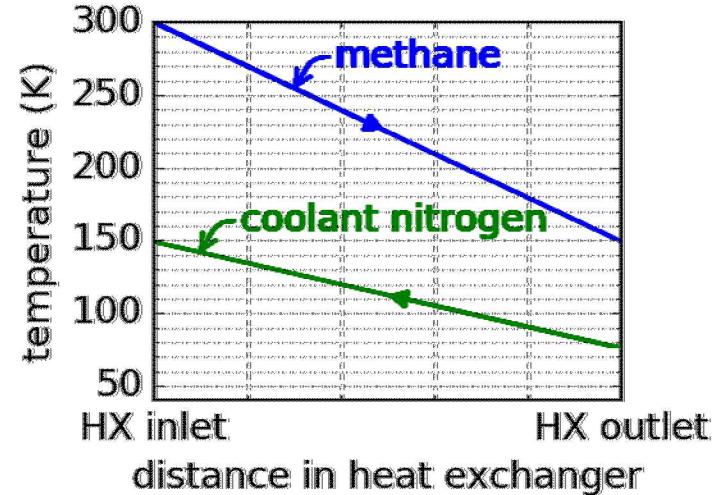
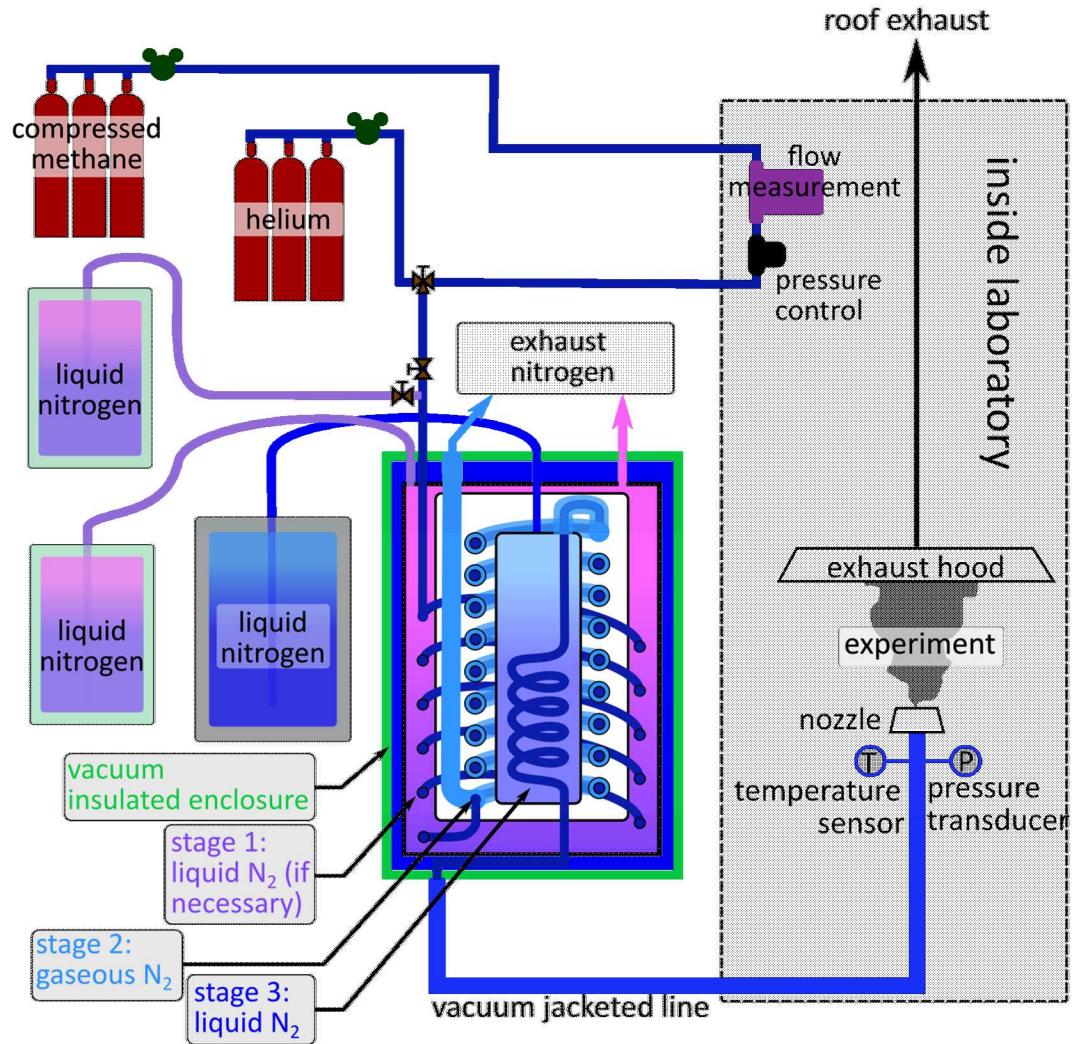
- **Tank:**

- Vol= 98 gal, 78.4 gal (80%) of liquid fuel.
- Pressure = 175 psi.
- Leak orifice = 6.2mm.
- Temp = 70° F

# Hydrogen Fuel Cell Bus Full Tank Blowdown

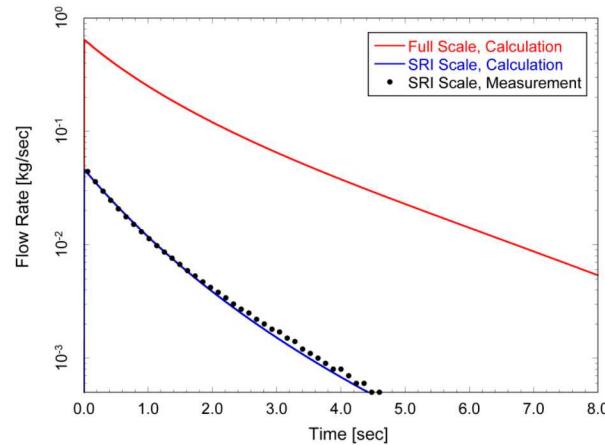


# LNG Experimental Setup



- Accurate control/measurement of boundary conditions

# Simulation Methodology

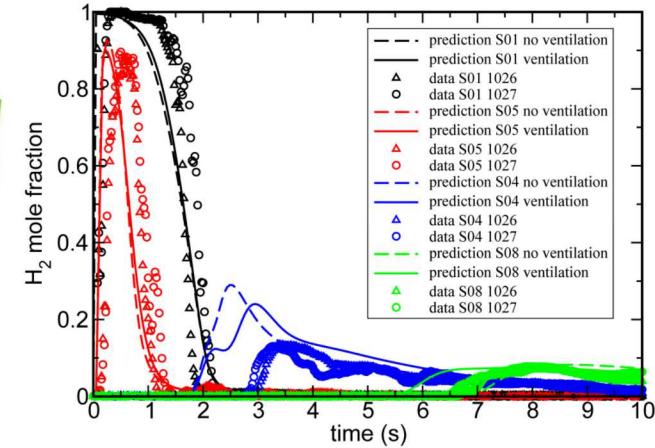
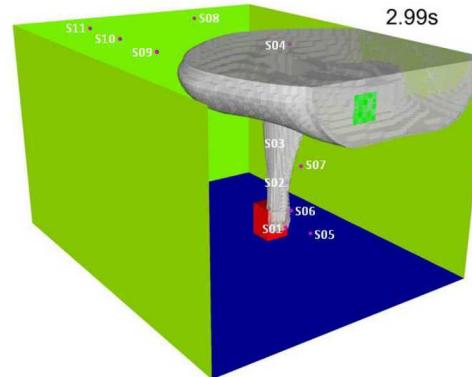


Blowdown release rates calculated via Sandia network flow solver (NETFLOW)

Winters, SAND Report 2009-6838.

## Sandia FUEGO flow solver

- Finite volume
- Compressible Navier-Stokes
- $k-\epsilon$  turbulence model
- Slip isothermal walls (294 K)
- $\sim 10$  cm mesh spacing



Houf et al., Int J H2Energy, 2013.

Methodology previously validated against large-scale hydrogen blowdown release experiments

# Modeling Scenarios

| Modeling Scenario | Scenario Description                              | Garage Details  | Tank/Leak Volume | Tank Pressure | Orifice Diameter |
|-------------------|---|---|------------------|---------------|------------------|
| A                 | LNG Blow-Off “weeping”                            | Heavy Duty: 100' x 50' x 20'  | 1.7% of 700 L    | 248 bar       | 6.2 mm           |
| B                 | CNG Fuel System Line Cracking                     | Heavy Duty: 100' x 50' x 20'  | 3.3 liters       | 8.62 bar      | 1.65 mm          |
| C                 | Full blowdown of an CNG cylinder                  | Heavy Duty: 100' x 50' x 20'  | 700 liters       | 248 bar       | 6.2 mm           |
| D                 | CNG Fuel System Line Cracking                     | Light Duty: 60' x 40' x 20'   | 3.3 liters       | 248 bar       | 1.65 mm          |
| E                 | PRD failure for a CNG cylinder                    | Light Duty: 60' x 40' x 20'   | 370 liter        | 248 bar       | 6.2 mm           |
| F                 | Full blowdown of an LNG cylinder                  | Heavy Duty: 100' x 50' x 20'  | 405.5 liter      | 24 bar        | 1.1 cm           |
| G                 | Overpressure of CNG cylinder due to external fire | Model under development. External fire would cause release and ignition, leading to jet fire. |                  |               |                  |

# Modeling/HAZOP Cross Reference

| HAZOP Scenario Number |   | Heavy-Duty Facility Modeling Scenario<br>(100' x 50' x 20') |                                      | Light-Duty Facility Modeling Scenario<br>(60' x 40' x 20') |                                      |
|-----------------------|---|---|--------------------------------------|--|--------------------------------------|
| 1                     | External leakage from LNG regulator body                      | A/B   | LNG blow-off                         | N/A  |                                      |
| 7                     | Overpressure of LNG tank and proper operation of relief valve | A   | LNG "Burping"/ "Weeping"             | N/A  |                                      |
| 12                    | Failure of LNG PRV to reclose after proper venting            | F   | Full blowdown of an LNG cylinder     | N/A  |                                      |
| 14                    | Overpressure of cylinder due to external fire                 | G   | Analytical Jet Fire (In development) | G  | Analytical Jet Fire (In development) |
| 15                    | PRD Outlet or fitting on CNG cylinder fails                   | C   | Full blowdown of a CNG cylinder      | E  | PRD failure for a CNG cylinder       |
| 19                    | CNG PRD fails open below activation pressure                  | C   | Full blowdown of a CNG cylinder      | E  | PRD failure for a CNG cylinder       |
| 35B                   | Leakage from CNG tubing                                       | B   | CNG fuel system line cracking        | D  | CNG fuel system line cracking        |
| 37                    | Human error or disregard for maintenance procedures           | All   | Covered by other scenarios           | All  | Covered by other scenarios           |

A: weeping  
 B & D: small leak (more probable)  
 C & E: CNG blowdown (worst case)  
 F: LNG blowdown

# SNL Project Motivation

- Improve **codes and standards** for gaseous fuel vehicle **maintenance facility** design and operation to reflect technology advancements
- Develop **Risk-Informed** guidelines for modification and construction of maintenance facilities using **Quantitative Risk Assessment**
- **CFD**

