CNG, $H_2$, CNG-$H_2$ Blends – Critical Fuel Properties and Behavior

Jay Keller,
Sandia National Laboratories

Keynote Lecture presented at:
Workshop on
Compressed Natural Gas and Hydrogen Fuels:
Lessons Learned for the Safe Deployment of Vehicles

December 10-11, 2009
Hydrogen Behavior – Myth Busting

Jay Keller,
Sandia National Laboratories

Topical Lecture
Progress in Hydrogen Safety: International Short Course Series

June 15-19, 2009
Hydrogen Myths

- Hydrogen Molecular Diffusivity is 3.8 times that of CH$_4$
  - Therefore it diffuses rapidly and mitigates any hazard
- Hydrogen is 14.4 times lighter than air
  - Therefore it rapidly moves upward and out of the way
- We do not know the flammability limits for H$_2$
- We just do not understand hydrogen combustion behavior
  - Hydrogen release is different than other fuels
  - Radiation is different than other fuels
Hydrogen Myths

- Hydrogen hazards can be compared favorably to experiences with other hydrocarbon fuels
  - Less dangerous than gasoline, methane …
- Simply adding hydrogen to natural gas improves engine efficiency and lowers emissions.
- ICE’s are 33% less efficient than are Fuel Cells (@50% DOE / FreedomCar current goal)
- Hydrogen always ignites
  - Joule-Thomson heating, Static electric discharge, Shock heating …
- Hydrogen is toxic and will cause environmental harm
  - “… We need to be indemnified against a hazardous toxic hydrogen spill …” – Generic Insurance Company
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## Momentum-Dominated Jets are within the Ignition Region

### Unignited Jet Separation Distance Length Scales

<table>
<thead>
<tr>
<th>Hole Diameter</th>
<th>Flowrate</th>
<th>Xmax - Distance to 4% mole fraction</th>
<th>Start of Intermediate Region (Buoyancy)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5875 mm (1/16 inch)</td>
<td>(2,463 ft³/min)<em>&lt;br&gt;2.430x10⁻² Kg/sec&lt;br&gt;(615.9 ft³/min)</em>&lt;br&gt;6.075x10⁻³ Kg/sec&lt;br&gt;(154.1 ft³/min)*</td>
<td>7.40 m (24.28 ft)</td>
<td>14.6 m (48.0 ft)</td>
</tr>
<tr>
<td>0.794 mm (1/32 inch)</td>
<td></td>
<td>3.70 m (12.14 ft)</td>
<td>10.3 m (33.9 ft)</td>
</tr>
</tbody>
</table>

* @NTP = 21°C (70°F), 101 kPa (14.7 psia)

### Flow between exit and 4% mole fraction is in the momentum dominated regime

- Start Intermediate Region<br>
  \[ x/D = 0.5 F^{1/2}(ρ_{exit}/ρ_{amb})^{1/4} \]

- Exit Froude No.<br>
  \[ F = \frac{U_{exit}^2}{ρ_{exit}gD(ρ_{amb}−ρ_{exit})} \]
In momentum-dominated regime, the centerline decay rate follows a $1/\chi_{CL}$ dependence for all gases.

The mole fraction centerline decay rate increases with increasing molecular weight.

The decay rate for H$_2$ is significantly slower than for methane and propane.
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Buoyancy effects are characterized by Froude number

Time-averaged H₂ mole fraction distributions.

Froude number is a measure of strength of momentum force relative to the buoyant force.

Increased upward jet curvature is due to increased importance of buoyancy at lower Froude numbers.
Influence of buoyancy is quantified by the Froude number

- Jets from choked flows (Mach 1.0) are typically momentum-dominated ($P_{\text{upstream}}/P_{\text{downstream}} \sim 2$).
- Lower source pressures or very large pressure losses through cracks lead to subsonic, buoyancy-dominated plumes.

\[ Fr_{\text{den}} = \frac{U_{\text{exit}}}{(gD(\rho_{\text{amb}} - \rho_{\text{exit}})/\rho_{\text{exit}})^{1/2}} \]

Ricou and Spalding entrainment law (J. Fluid Mechanics, 11, 1961)
Small Unignited Releases: Buoyancy Effects

Data for round H₂ Jets (d₀ = 1.91 mm)

- At the highest Fr, 1/χ_{CL} increases linearly with axial distance, indicating momentum dominates.
- As Fr increases buoyancy forces become less important and the centerline decay rate decreases.
- The transition to buoyancy-dominated regime moves downstream with increasing Fr.
**Choked & Unchoked Flows at 20 SCFM**

Tank Pressure = 3000 psig, Hole Dia. = 0.297 mm
Exit Mach Number = 1.0 (Choked Flow)
Fr ~ O(10^4)

Flowrate = 20 scfm, Hole Dia. = 9.44 mm
Exit Mach Number = 0.1 (Unchoked Flow)
Fr ~ O(100)

- Correlations based on experimental data
- Start Intermediate Region
  - \(x/D = 0.5 \ F^{1/2}(\rho_{exit}/\rho_{amb})^{1/4}\)
- End Intermediate Region
  - \(x/D = 5.0 \ F^{1/2}(\rho_{exit}/\rho_{amb})^{1/4}\)
- \(F = \text{Exit Froude No.}\)
  - \(\frac{U_{exit}^2 \rho_{exit}}{(gD(\rho_{amb} - \rho_{exit}))}\)

Start Transition Region -> \(x = 6.3\) m

Assuming gases at 1 Atm, 294K (NTP)
- Red – 10.4%
- Orange – 8.5%
- Green – 5.1%
- Blue – 2.6%

*(Chen and Rodi, 1980)*

H2 Concentration Data from:
Dr. Michael Swain
Fuel Cell Summit Meeting
June 17, 2004
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<thead>
<tr>
<th>Tube Dimensions, cm</th>
<th>Firing end</th>
<th>Limits, percent</th>
<th>Water Vapor Content</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Lower</td>
<td>Higher</td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>Length</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.5</td>
<td>150</td>
<td>Closed</td>
<td>4.15</td>
<td>75.0</td>
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<tr>
<td>5.3</td>
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<td>Open</td>
<td>4.19</td>
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<tr>
<td>5.0</td>
<td>150</td>
<td>Open</td>
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<td>5.0</td>
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<td>Close</td>
<td>4.12</td>
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<td>4.5</td>
<td>80</td>
<td>Open</td>
<td>4.00</td>
<td>72.0</td>
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### Horizontal Flame Propagation

<table>
<thead>
<tr>
<th>Tube Dimensions, cm</th>
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<tbody>
<tr>
<td></td>
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</tr>
<tr>
<td>Diameter</td>
<td>Length</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.5</td>
<td>150</td>
<td>Closed</td>
<td>6.5</td>
<td>-----</td>
</tr>
<tr>
<td>5.0</td>
<td>150</td>
<td>-----</td>
<td>6.7</td>
<td>-----</td>
</tr>
<tr>
<td>2.5</td>
<td>150</td>
<td>Open</td>
<td>7.15</td>
<td>-----</td>
</tr>
<tr>
<td>2.5</td>
<td>150</td>
<td>Open</td>
<td>6.2</td>
<td>-----</td>
</tr>
<tr>
<td>0.9</td>
<td>150</td>
<td>-----</td>
<td>6.7</td>
<td>-----</td>
</tr>
<tr>
<td>8.0</td>
<td>120</td>
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<td>9.4</td>
<td>64.8</td>
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<tr>
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<td>33</td>
<td>-----</td>
<td>8.5</td>
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</tr>
<tr>
<td>6.0</td>
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<td>N</td>
<td>9.45</td>
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### Downward Flame Propagation

<table>
<thead>
<tr>
<th>Tube Dimensions, cm</th>
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<th>Water Vapor Content</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Lower</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>Length</td>
<td></td>
<td></td>
<td></td>
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<td>31</td>
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<tr>
<td>8.0</td>
<td>37</td>
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<td>8.5</td>
<td>67.5</td>
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<td>150</td>
<td>N</td>
<td>8.8</td>
<td>-----</td>
</tr>
<tr>
<td>7.0</td>
<td>150</td>
<td>N</td>
<td>8.8</td>
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<td>120</td>
<td>N</td>
<td>9.45</td>
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</tr>
</tbody>
</table>

### Propagation in a Spherical Vessel

<table>
<thead>
<tr>
<th>Capacity, cc</th>
<th>Firing end</th>
<th>Limits, percent</th>
<th>Water Vapor Content</th>
<th>Reference</th>
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<tr>
<td></td>
<td></td>
<td>Lower</td>
<td>Higher</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Closed</td>
<td>9.2</td>
<td>-----</td>
</tr>
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<td>Not stated</td>
<td>N</td>
<td>8.5</td>
<td>67.5</td>
<td></td>
</tr>
<tr>
<td>Not stated</td>
<td>N</td>
<td>8.7</td>
<td>75.5</td>
<td></td>
</tr>
<tr>
<td>1,000</td>
<td>N</td>
<td>5.0</td>
<td>73.5</td>
<td></td>
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<tr>
<td>810</td>
<td>N</td>
<td>4.6</td>
<td>70.3</td>
<td></td>
</tr>
<tr>
<td>350</td>
<td>N</td>
<td>9.4</td>
<td>64.8</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>N</td>
<td>9.4</td>
<td>64.8</td>
<td></td>
</tr>
</tbody>
</table>
78 investigations of hydrogen flammability limits were identified between 1920 and 1950.

Hydrogen flammability limits are well established.

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<tbody>
<tr>
<td>7.5 150</td>
<td>Closed</td>
<td>4.15 75.0</td>
<td>Half-saturated</td>
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## Horizontal Flame Propagation

<table>
<thead>
<tr>
<th>Tube Dimensions, cm</th>
<th>Firing end</th>
<th>Limits, percent</th>
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</tr>
</thead>
<tbody>
<tr>
<td>21.0 31</td>
<td>Open</td>
<td>9.3</td>
<td>Saturated</td>
<td>63</td>
</tr>
<tr>
<td>8.0 37</td>
<td>Closed</td>
<td>8.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.5 150</td>
<td>N</td>
<td>8.8</td>
<td></td>
<td></td>
</tr>
<tr>
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<td></td>
</tr>
<tr>
<td>6.2 33</td>
<td>Open</td>
<td>8.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.0 120</td>
<td>N</td>
<td>9.45</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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<table>
<thead>
<tr>
<th>Tube Dimensions, cm</th>
<th>Firing end</th>
<th>Limits, percent</th>
<th>Water Vapor Content</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Not stated</td>
<td>Not stated</td>
<td>9.2</td>
<td>Saturated</td>
<td>271</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Diameter</th>
<th>Length</th>
<th>Not stated</th>
<th>Lower</th>
<th>Higher</th>
<th>Content</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,000</td>
<td></td>
<td>N</td>
<td>8.7</td>
<td>75.5</td>
<td>N</td>
<td>95</td>
</tr>
<tr>
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<td></td>
<td>N</td>
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<td>73.5</td>
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<td>N</td>
<td>4.6</td>
<td>70.3</td>
<td>N</td>
<td>368</td>
</tr>
<tr>
<td>35</td>
<td></td>
<td>N</td>
<td>9.4</td>
<td>64.8</td>
<td>N</td>
<td>297</td>
</tr>
</tbody>
</table>
What is a Reasonable Flame Stabilization Limit?

Which volume fraction contour is relevant:
- lean flammability limit? … 4% or 8%
- detonation limit? … 18%
- a fraction of the lowest lean flammability limit? … 1%

Ignition of hydrogen in turbulent jets occurs around 8% as measured by Swain.
- This is consistent with the downward propagating limit of 8%
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  - Hydrogen release is different than other fuels
  - Radiation is different than other fuels
Hydrogen jets and flames are similar to other flammable gases

- Fraction of chemical energy converted to thermal radiation
- Radiation heat flux distribution
- Jet length
**H₂ Flame Radiation**

Orange emission due to excited H₂O vapor

Blue continuum due to emission from OH + H → H₂O + hν

UV emission due to OH*

IR emission due to H₂O vibration-rotation bands

H₂O emission in IR accounts for 99.6% of flame radiation
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- Jet length
Thermal Radiation from Hydrogen Flames

- Previous radiation data for nonsooting CO/H₂ and CH₄ flames correlate well with flame residence time.
- Sandia’s H₂ flame data is a factor of two lower than the hydrocarbon flame data.

- Radiation heat flux data collapses on single line when plotted against product \( \tau \times a_p \times T_f^4 \).
- \( a_p \) (absorption coefficient) is factor with most significant impact on data normalization.

- Plank mean absorption coefficient for different gases must be considered.
Hydrogen Myths

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  - Less dangerous than gasoline, methane …
- Simply adding hydrogen to natural gas improves engine efficiency and lowers emissions.
- ICE’s are 33% less efficient than are Fuel Cells (@50% DOE / FreedomCar current goal)
- Hydrogen always ignites
  - Joule-Thomson heating, Static electric discharge, Shock heating …
- Hydrogen is toxic and will cause environmental harm
  - “… We need to be indemnified against a hazardous toxic hydrogen spill …” – Generic Insurance Company
Comparisons of NG and H$_2$ Behaviors

- Assume 3.175 mm (1/8 inch) dia. hole
- Unignited jet lower flammability limits
  - LFL H$_2$ - 4% mole fraction
  - LFL NG - 5% mole fraction
- Flame blow-off velocities for H$_2$ are much greater than NG
- Flow through 1/8” diameter hole is choked
  - $V_{\text{sonic}} = 450$ m/sec for NG (300K)
  - $V_{\text{sonic}} = 1320$ m/sec for H$_2$ (300K)
- Hole exit (sonic) velocity for NG is greater than NG blow-off velocity
  - No NG jet flame for 1/8” hole
- Hole exit (sonic) velocity for H$_2$ is much less than blow-off velocity for H$_2$
  - H$_2$ jet flame present for 1/8” hole
Small Unignited Releases: 
Momentum-Dominated Regime

Data for round turbulent jets

In momentum-dominated regime, the centerline decay rate follows a $1/\chi_{CL}$ dependence for all gases.

The mole fraction centerline decay rate increases with increasing molecular weight.

The decay rate for H$_2$ is significantly slower than for methane and propane.
Distance on Jet Centerline to Lower Flammability Limit
for Natural Gas and Hydrogen

<table>
<thead>
<tr>
<th>Tank Pressure</th>
<th>Hole Diameter</th>
<th>Distance to 5% Mole Fraction Natural Gas</th>
<th>Distance to 4% Mole Fraction Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>18.25 bar (250 psig)</td>
<td>3.175 mm (1/8 inch)</td>
<td>1.19 m (3.90 ft)</td>
<td>4.24 m (13.91 ft)</td>
</tr>
<tr>
<td></td>
<td>1.587 mm (1/16 inch)</td>
<td>0.59 m (1.93 ft)</td>
<td>2.12 m (6.95 ft)</td>
</tr>
<tr>
<td>207.8 bar (3000 psig)</td>
<td>3.175 mm (1/8 inch)</td>
<td>3.92 m (12.86 ft)</td>
<td>13.54 m (44.42 ft)</td>
</tr>
<tr>
<td></td>
<td>1.587 mm (1/16 inch)</td>
<td>1.96 m (6.43 ft)</td>
<td>6.77 m (22.21 ft)</td>
</tr>
</tbody>
</table>

Distance to the lower flammability limit for hydrogen is about 3 times longer than for natural gas.
Maximum LFL Extents vs Time – Horizontal H2 and CH₄ Jets along Horizontal Surface

Features: strong transient overextent of the hydrogen cloud (larger than at steady state), not observed in case of methane

Much stronger effect of surface on methane jets vs hydrogen jets:

- While methane free jet max LFL extent is almost 3 times shorter than that of hydrogen, at 0.5 m above ground the max LFL extents for both gases become almost equal
Small Unignited Releases: Ignitable Gas Envelope

H₂ Jet at Re=2,384; Fr = 268

CH₄ Jet at Re=6,813; Fr = 478

- H₂ flammability limits: LFL 4.0%; RFR 75%
- CH₄ flammability limits: LFL 5.2%; RFR 15%

Radial profiles in H₂ jet, d = 1.91 mm, Re = 2384
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Lean Premixed Combustion for NOx Control

At ultra lean conditions a tradeoff exists between NOx and CO emissions. Ultimately, lean operation is limited by the onset of flame instability and blowout.

$H_2$ addition extends lean flammability limit and reduces CO emissions.
Effect of Hydrogen -Enrichment on Flame Stability

- Data points indicate minimum equivalence ratio at which a stable flame can be maintained.
- Hydrogen addition significantly extends lean flame stability.
- Expected NO$_x$ levels less than 3 ppm can be achieved with 20% hydrogen addition.


**Present Day H₂ICEs: Emissions**

- **NOₓ** is the only non-trivial engine-out emission pollutant
  - Engine out Dial-a-NOₓ value ~ 5-6 ppm
  - With after-treatment NOₓ values can be near zero ***
    - Measured tailpipe NOₓ emissions equal to ambient levels of about 50 ppb
- **HC, CO** all near zero engine-out emissions **
  - Trace amounts from lubricating oil
    - CO – O(1) ppm, HC – O(5) ppm for a reduction of a factor of 1000, 250 respectively compared to gasoline

- **BMW presentation @ 2006 National Hydrogen Association Meeting March, 2006**
- **SAE Papers #’s 2002-01-0240 thru 0243 and 2003-01-0631; Ford Research**
- **James Heffel, University of California, Riverside, College of Engineering – Center for Environmental Research and Technology (CE-CERT); Personal Communication; Under the technical guidance and contract to Sandia National Laboratories, funding from the Hydrogen Program Office; OPT**

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*Closed symbols* engine out
*Open symbols* after treatment with TWC
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- Hydrogen hazards can be compared favorably to experiences with other hydrocarbon fuels
  - Less dangerous than gasoline, methane …
- Simply adding hydrogen to natural gas improves engine efficiency and lowers emissions.
- ICE’s are 33% less efficient than are Fuel Cells (50% @ rate power DOE / FreedomCar 2010 & 2015 goal)
- Hydrogen always ignites
  - Joule-Thomson heating, Static electric discharge, Shock heating …
- Hydrogen is toxic and will cause environmental harm
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Brake Thermal Efficiency Trend – Projected to Multi-cylinder Engine

- 3+ years of data
- Different injection rates
- Mostly 1500-4500 RPM
- Naturally aspirated & boosted.
- Discrete clouds - different boost condition.
Hydrogen Myths

- Hydrogen hazards can be compared favorably to experiences with other hydrocarbon fuels
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81 ignitions of H₂ releases have been reported (MHIDAS database). In 11 cases the ignition source was identified (flame, electric, hot surface). *In the remaining 70 no ignition source could be identified.*

Proposed causes include the following:

- Joule-Thomson
- **Static charge buildup in the flow**
- Shock heating that leads to ignition of H₂/air mixtures
- Catalytic reaction with materials present in the flow (iron oxide)
- Friction heating of particulates / hot surface ignition

**Area of current research**
81 ignitions of H₂ releases have been reported (MHIDAS database). In 11 cases the ignition source was identified (flame, electric, hot surface). In the remaining 70 no ignition source could be identified.

Proposed causes include the following:

- Joule-Thomson
- Static charge buildup in the flow
- Shock heating that leads to ignition of H₂/air mixtures
- Catalytic reaction with materials present in the flow (iron oxide)
- Friction heating of particulates / hot surface ignition
The direction and magnitude of temperature change is determined by the Joule-Thomson coefficient which is a function of upstream pressure \( P_1 \).

\[
\mu_{JT} = \left( \frac{\delta T}{\delta P} \right)_H = \left( \frac{\Delta T}{\Delta P} \right)_H
\]

Above the inversion temperature, the expanding gas temperature increases.

The inversion temperature of \( H_2 \) is between 28 and 200 K (depending on pressure); at ambient temperature the expanding \( H_2 \) increases in temperature.

For initial compressed gas pressure of 14 MPa, the estimated temperature rise is approximately \( \sim 6 \) K.

At pressures up to 250 MPa, the maximum estimated coefficient is 0.53 K/MPa. Thus, at future \( H_2 \) storage pressures of 100 MPa, the maximum temperature rise would be 53 K.\(^1\) If the initial temperature was 300K (room temperature) the exit gas temp would be 353K.


Given the \( H_2 \) auto-ignition temperature of 858 K, Joule-Thomson heating is insufficient to cause ignition.
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White, Chris, Sandia National Laboratories
### Publication list

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Nighttime photograph of ∼40 MPa large-scale H2 jet-flame test (dj = 5.08mm, Lvis = 10.6 m) from Sandia/SRI tests.
Some people just do not get it!

$\Rightarrow H_2$
- is not toxic,
- it is environmentally benign
- we just borrow it -- ($2H_2O + E \rightarrow 2H_2 + O_2$; then $2H_2+O_2 \rightarrow 2H_2O + E$)

$\Rightarrow H_2$ is a fuel and as such has stored chemical energy
- It has hazards associated with it
  - It is no more dangerous than the other fuels that store chemical energy
  - IT IS JUST different; -- WE UNDERSTAND THE SCIENCE

Following NFPA 52 / 2 - Hydrogen Installations are no more dangerous than current refueling stations.
Presentation End