VENTED HYDROGEN-AIR DEFLAGRATION IN A SMALL ENCLOSED VOLUME

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Context

- Problem: Reduce green house gases, pollution and dependency on oil-based fuels
- Solution: Hydrogen, clean energy carrier (fuel cell)
- Risk: H₂ leak could fill a small confined volume in a part of a system and could ignite.
- Few studies at small scale:  - McCann (1985), CH₄/air, V=5.8 dm³ and 54.9 dm³
  - Sato (2010), C₃H₈/air, V=4 dm³

Objectives of the study

- Vented deflagration in a small confined volume (V=3.4 dm³) with a stoechiometric H₂/air mixture
- Evaluate models of literature for vented deflagrations at small scale
Contents

- Experimental setup
- Experimental results
- Molkov correlation
- Bauwens model
- Comparison between models
- Conclusions
Walls: Plexiglas

- \( \text{H}_2/\text{air}, \phi=1 \), regulated by mass flow controllers
- Ignition by spark: \( E_n=122 \text{ mJ} \)
- Pressure transducers PCB Piezotronics (±1.3%)
- High speed camera Phantom at 15000 fps
Experimental setup

- 3 ignition locations: center – back wall – front wall
- 5 centered square vent areas: 225 cm², 81 cm², 49 cm², 25 cm² and 9 cm²
- Vent cover: thin polyethylene film
Experimental results

Several pressure peaks (Cooper et al. 1986 with a 760 dm³ cubic vessel):

- $P_v$: Relief pressure
- $P_1$: Pressure generated by external explosion
- $P_2$: Pressure generated by internal combustion (flame-acoustic coupling)

$P_1$ or $P_2$ dominates the internal pressure

$\text{H}_2/\text{air}$, $\phi=1$, center ignition, raw signal (black) and filtered signal (1.5 kHz low pass filter - blue)
### Experimental results

<table>
<thead>
<tr>
<th>Vent area (cm²)</th>
<th>$K_v$</th>
<th>Center ignition</th>
<th>Back wall ignition</th>
<th>Front wall ignition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\Delta P_1$ (kPa)</td>
<td>$\Delta P_2$ (kPa)</td>
<td>$\Delta P_1$ (kPa)</td>
</tr>
<tr>
<td>225</td>
<td>1</td>
<td>3.1</td>
<td>-</td>
<td>5.0</td>
</tr>
<tr>
<td>81</td>
<td>2.8</td>
<td>11.0</td>
<td>2.5</td>
<td>25.0</td>
</tr>
<tr>
<td>49</td>
<td>4.6</td>
<td>13.0</td>
<td>10.0</td>
<td>27.8</td>
</tr>
<tr>
<td>25</td>
<td>9</td>
<td>-</td>
<td>78.9</td>
<td>-</td>
</tr>
<tr>
<td>9</td>
<td>25</td>
<td>-</td>
<td>278.4</td>
<td>-</td>
</tr>
</tbody>
</table>

- $P_1$ was included in $P_2$ which dominates for $K_v \geq 9$.
- $P_2$ was not noticed for center ignition ($K_v=1$) and back wall ignition ($K_v \leq 4.6$).
- For $K_v \geq 9$: maximal overpressures generated by internal combustion and by center ignition.
- $\Delta P_2$ was not noticed for center ignition ($K_v=1$) and back wall ignition ($K_v \leq 4.6$). 

$$K_v = \frac{V^2}{A_v}$$

- $V$ – Volume (m³)
- $A_v$ – Vent area (m²)

**For $K_v \leq 4.6$ maximal overpressures generated by external combustion (center and back wall ignition) and back wall ignition.**

**For $K_v \geq 9$: maximal overpressures generated by internal combustion and by center ignition.**

Maximal overpressure $\uparrow$ with $K_v$. 

- $\Delta P_1$ was included in $\Delta P_2$ which dominates for $K_v \geq 9$. 
- $\Delta P_2$ was not noticed for center ignition ($K_v=1$) and back wall ignition ($K_v \leq 4.6$).
Models of the literature

Actual standard to predict internal overpressure during venting explosion:


Limitations:

- $10 \text{kPa} < \Delta P_{\text{max}} < 200 \text{kPa}$
- Initial pressure $< 20 \text{kPa}$
- Static vent activation pressure $< 50 \text{kPa}$
- Deflagration index $K_G < 55 \text{MPa.m/s}$
Models of the literature

Models to answer these limitations:

**Molkov (1995)**
- Vent area
- Enclosure volume
- Sound velocity
- Burning velocity
- Specific heat
- Products expansion ratio
- Bradley number
- Empirical coefficients
- Turbulent Bradley number
- Deflagration Outflow Interaction
- $\Delta P_{\text{max}}$

**Bauwens (2010)**
- Vent area
- Enclosure lengths
- Discharge coefficient
- Sound velocity
- Burning velocity
- Lewis number
- Specific heat
- Products expansion ratio
- Universal gas constant
- Gases temperature
- Molar mass
- Flame wrinkling coefficient
- External cloud radius
- Flame area = f(ignition location)
- Flame acceleration at the exit
- External $\Delta p_{\text{max}}$
- $\Delta P_1, \Delta P_2$

- Correlations applied with our experimental setup configurations

<table>
<thead>
<tr>
<th>Ignition Location</th>
<th>Absolute average deviations for all vent areas (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Molkov 1999</td>
</tr>
<tr>
<td>Center</td>
<td>27</td>
</tr>
<tr>
<td>Back wall</td>
<td>42</td>
</tr>
<tr>
<td>Front Wall</td>
<td>133</td>
</tr>
</tbody>
</table>

- Molkov 1999 correlates better than other updated versions with small scale experimental results

- Molkov 1999 has been chosen to be compared to Bauwens model
<table>
<thead>
<tr>
<th>$A_v$ (cm²)</th>
<th>$K_v$</th>
<th>Molkov (1999) $\Delta P_{max}$ (kPa)</th>
<th>Center ignition</th>
<th>Back wall ignition</th>
<th>Front wall ignition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Measured $\Delta P_{max}$ (kPa)</td>
<td>Dev. (%)</td>
<td>Measured $\Delta P_{max}$ (kPa)</td>
<td>Dev. (%)</td>
</tr>
<tr>
<td>225</td>
<td>1</td>
<td>3.1</td>
<td>-35.5</td>
<td>5</td>
<td>-60</td>
</tr>
<tr>
<td>81</td>
<td>2.8</td>
<td>11</td>
<td>-18.2</td>
<td>25</td>
<td>-64</td>
</tr>
<tr>
<td>49</td>
<td>4.6</td>
<td>13</td>
<td>69.2</td>
<td>27.8</td>
<td>-20.1</td>
</tr>
<tr>
<td>25</td>
<td>9</td>
<td>78.9</td>
<td>-10</td>
<td>61.5</td>
<td>15.5</td>
</tr>
<tr>
<td>9</td>
<td>25</td>
<td>278.4</td>
<td>-1.6</td>
<td>180.8</td>
<td>51.6</td>
</tr>
</tbody>
</table>

- Correlation rather consistent with center ignition
- Overestimation for front wall ignition
- Not conservative for center and back wall ignition
Assumptions for Bauwens model:

- $\Delta P_2$ asymptotically approaches a constant volume explosion pressure $P_{cv} = 811.7$ kPa when $Av \to 0$ m$^2$ (Bauwens 2012)

- Initial flame velocity=laminal flame velocity $S_L = 2.14$ m.s$^{-1}$ ($Le \approx 0.9$ for stoechiometric $H_2$/air mixture – $S_{u0} = 0.9Le^{-1}S_L$)

- Bauwens model: vented gas composed of 90% of products and 10% of reactants $\to$ 100% products considered in the present study

- New fitting value of $k_T = 9.26$ m$^{-1}$ (for $\Delta P_1$) based on Bauwens (2010, 2011) and Chao (2011) experiments with a linear law.

- Flame wrinkling factor $\Xi_A = 1$ (for $\Delta P_2$) to avoid higher overpressures generated at large scale ($S_u = \Xi_A S_L$)
## Bauwens model – $\Delta P_1$

<table>
<thead>
<tr>
<th>$A_v$ (cm$^2$)</th>
<th>$K_v$</th>
<th>Center ignition $\Delta P_1$ (kPa)</th>
<th>Back wall ignition $\Delta P_1$ (kPa)</th>
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<tr>
<td></td>
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<td>Bauwens</td>
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<td>225</td>
<td>1</td>
<td>3.1</td>
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<td>81</td>
<td>2.8</td>
<td>11.0</td>
<td>7.1</td>
</tr>
<tr>
<td>49</td>
<td>4.6</td>
<td>13.0</td>
<td>8.3</td>
</tr>
<tr>
<td>25</td>
<td>9</td>
<td>-</td>
<td>10.1</td>
</tr>
<tr>
<td>9</td>
<td>25</td>
<td>-</td>
<td>13.6</td>
</tr>
</tbody>
</table>

- Deviations varying from -36% to 58% for center ignition
- Deviations varying from -20% to 72% for back wall ignition
- Not conservative for some configurations
<table>
<thead>
<tr>
<th>$A_v$ (cm$^2$)</th>
<th>$K_v$</th>
<th>Center ignition $\Delta P_2$ (kPa)</th>
<th>Back wall ignition $\Delta P_2$ (kPa)</th>
<th>Front wall ignition $\Delta P_2$ (kPa)</th>
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<tr>
<td></td>
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<td>Measured  Bauwens  Dev. (%)</td>
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</tr>
<tr>
<td>225</td>
<td>1</td>
<td>-   0.6   -</td>
<td>-   0.4   -</td>
<td>1.3   0.6   -53.9</td>
</tr>
<tr>
<td>81</td>
<td>2.8</td>
<td>2.5  5.6  124</td>
<td>-   3.8   -</td>
<td>2.5   4.4   76</td>
</tr>
<tr>
<td>49</td>
<td>4.6</td>
<td>10   15.7  57</td>
<td>-   10.8  -</td>
<td>6.6   11.8  78.8</td>
</tr>
<tr>
<td>25</td>
<td>9</td>
<td>78.9 58.8  -26</td>
<td>61.5 41.6  -32.4</td>
<td>40  43.4  8.5</td>
</tr>
<tr>
<td>9</td>
<td>25</td>
<td>278.4 295.9  6</td>
<td>180.8 235  30</td>
<td>196.4 237.5  20.9</td>
</tr>
</tbody>
</table>

- Model more accurate for small vent areas $K_v \geq 9$
- Not conservative for some configurations
Comparison between models - $\Delta P_{\text{max}}$

$\Delta P_{\text{max}}$ modeled is compared to $\Delta P_{\text{max}}$ measured ($\Delta P_1$ or $\Delta P_2$)

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</table>

- Bauwens model is globally more accurate than Molkov 1999
- Results of both models are close for center and back wall ignition
- Molkov 1999 overpredicts pressure for front wall ignition but is conservative for this location
Consideration of ignition location given $\Delta P_{\text{max}}$ for each vent area

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<td>Locations for $\Delta P_{\text{max}}$</td>
<td>Molkov 1999</td>
</tr>
<tr>
<td></td>
<td>31</td>
</tr>
</tbody>
</table>

- The critical case is only considered for each vent area
- Both models give $\approx$ similars results
- Bauwens model for $K_v \leq 4.6$
- Molkov model for $K_v > 4.6$
Experimental results

- Influence of the vent area and the ignition location on the internal overpressure for a small confined volume ($H_2/\text{air}$, $\Phi = 1$, $V = 3375 \text{ cm}^3$)
- 3 pressures peaks: vent failure pressure, external combustion, internal combustion with flame-acoustic interaction
- $\Delta P_{\text{max}}$ obtained with center ignition for $K_v \geq 9$ and back wall ignition for $K_v \leq 4.6$
- $P_2$ is dominant for small vent areas ($K_v \geq 9$)

Molkov 1999 correlation and Bauwens model

- Approximately similar results when comparing with experimental maximal overpressures (either $P_1$ or $P_2$) for center and back wall ignition
- Models results close to experimental data (Bauwens 26%, Molkov 31%) for a safe approach.
Thanks for your attention

Any questions?