Physics of spontaneous ignition of high-pressure hydrogen release and transition to jet fire

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QUANTUM Technologies WorldWide Inc. introduced “all-composite hydrogen storage tank that stores hydrogen at 10,000 psi (700 bar). At 10,000 psi, 80% more hydrogen fuel can be stored in a given space than at 5,000 psi” *

* QUANTUM Technologies WorldWide, Inc
Website: http://www.qtww.com/products/haft/hydrostorage.php
Motivation II

Activation of pressure relief device

High-pressure release of hydrogen

Possible ignition without any apparent reasons
Postulated mechanisms for spontaneous ignition*

- Reverse Joule-Thomson effect
- Electrostatic charge generation
- Diffusion ignition, ignition by shock waves
- Sudden adiabatic compression
- Hot surface ignition

Overall aim of the research

Aim of the research:
- To develop understanding of the physical phenomena underlying spontaneous ignition of hydrogen generated by shock waves resulting from sudden storage decompression (or activation of a PRD)
- To construct a model capable of reproducing experimental observations during transition of spontaneously ignited mixture into a jet fire

Planned contribution to knowledge:
Scientific
- Determination of critical conditions for ignition during high-pressure releases (i.e. ignited or not) and jet fire onset (sustained or not)

Applied. Recommendations for
- Hazard assessment
- Mitigation techniques
- Risk assessment
Spontaneous ignition of hydrogen following a storage decompression with a downstream confinement
Temperature in flame front

Contact surface separating gases
Regions of ignition onset
Atmospheric air

Cold expanding hydrogen
Shock heated air

2.06e+13
1.97e+13
1.88e+13
1.78e+13
1.89e+13
1.80e+13
1.50e+13
1.41e+13
1.32e+13
1.23e+13
1.13e+13
1.04e+13
9.16e+12
8.53e+12
7.31e+12
6.58e+12
5.75e+12
4.32e+12
3.89e+12
2.96e+12
2.03e+12
Calculation domain

Geometry was taken from experiments by Golub et al.
  High pressure chamber \( L = 145\text{mm}, d = 20\text{mm} \)
  Low pressure chamber (Tube): \( L = 140\text{mm}, d = 5\text{mm} \)
Meshed with total number of control volumes 431k in 3D
  Low pressure chamber – uniform mesh with cell size 0.2mm
Laminar Finite-Rate model + Dynamic S-L subgrid scale model

The initial conditions:
  Low-pressure chamber: air (mass fraction of O2 = 0.23, mass fraction of N2 = 0.77),
    pressure \( P = 1\text{ atm} \), temperature \( T = 300\text{ K} \).
  High-pressure chamber: hydrogen (mass fraction of H2 = 1), pressure \( P = 97\text{ bar} \),
    temperature \( T = 300\text{ K} \).
Boundary (burst disk) separating chambers was removed instantly.

Hydrogen auto-ignition during accidental or technical opening of high pressure tank. Journal of Loss Prevention in the Process Industries,
20, 439-446.
Dynamics of temperature
Temperature movie

Shown tube length corresponds to 13cm
Hydroxyl mole fraction

Shown tube length corresponds to 13cm
Transition of spontaneous ignition into a jet fire
Geometry was taken from experiments by Mogi et al.
Tube: \( L = 185\text{mm}, d = 5\text{mm} \) was uniform mesh with cell size 0.4mm
Outside mesh was adapted as the process evolved
Maximum number of control volumes was 479k,
but only the first 0.05s of the process were simulated
Eddy-Dissipation Concept model + RNG subgrid scale model

**The initial conditions:**
Low-pressure chamber: air (mass fraction of O2 = 0.23, mass fraction of N2 = 0.77),
pressure \( P = 1 \text{ atm} \), temperature \( T = 300 \text{ K} \).
High-pressure chamber: hydrogen (mass fraction of H2 = 1), pressure \( P = 145 \text{ bar} \),
temperature \( T = 300 \text{ K} \).
Boundary (burst disk) separating chambers was removed instantly.

Dynamics of the velocity, temperature and mole fractions of hydrogen and hydroxyl in 2D slice along the tube axis.
Velocity distribution in the underexpanded jet during development stage

Formation of barrel-like shock structure is followed by the formation of annular vortex, which moves downstream
Mole fraction of hydrogen distribution

Annular vortex induces mixing

Combustible mixture is formed as the vortex propagate downstream
Temperature distribution

Cocoon of combusting mixture is broken by developing vortex

Upstream part is pushed back to the tube exit
Hydroxyl mole fraction distribution

Downstream combustion regions are extinguished, while in the upstream region flame is stabilized.
Comparison of simulation results against experimental photographs from experiments by Mogi et al
Conclusions

- Mechanism of spontaneous ignition of high-pressure hydrogen discharges into downstream confinement (tube) was investigated.
- It was demonstrated that ignition occurs in the boundary layer.
- Dynamics of the spontaneous ignition process was demonstrated.
- Mechanism of initial stage of transition of combusting mixture into a jet fire was investigated.
- The transition largely depends on initial jet formation stage, where vortices push combusting mixture in recirculation zone. Once the flame is stabilized near the tube exit, it acts as a pilot flame and ignites jet fire later on (according to experimental observations by Mogi et al, 2008).
Thank you for your attention!
Questions?

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