Further Studies on Spontaneous Ignition of Compressed Hydrogen Releases into Air

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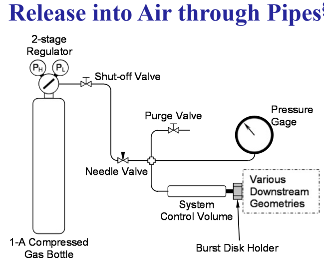
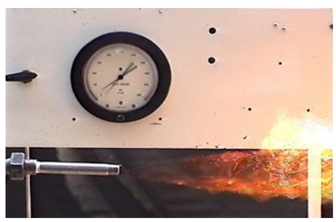
Motivation – Hydrogen use in industrial processing and as an energy carrier for transportation

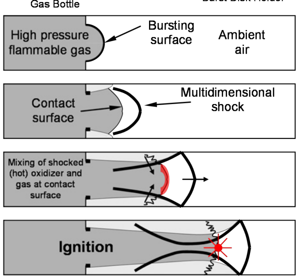
- Use of hydrogen as an industrial chemical in the manufacture of transportation fuels for upgrading of petroleum and non-petroleum feed stocks is expected to increase as we search for energy solutions in a carbon constrained world.
- Use of hydrogen as an energy carrier in stationary and transportation applications requires careful consideration of safety related matters and continuing evolution of design standards.
- Understanding the sources of and conditions that can lead to ignition is important to advancing safe operating criteria and application of design standards.
- One such ignition mechanism that is nearly unique to hydrogen is the release of compressed hydrogen into air.[1]

Spontaneous Ignition from Sudden Compressed Hydrogen Release into Air through Pipes§





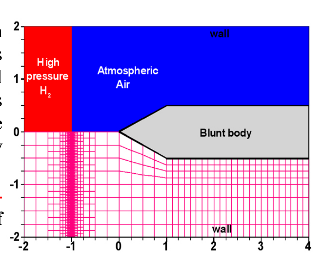
Video at http://www.princeton.edu/~combust/research/h2_safety/



- Gas release forms shock that heats air in contact with expanding H_2.
- Mixing regions near the contact surfaces must achieve temperatures sufficient for chemical ignition.
- Sufficiently heated regions must also achieve minimum critical volume of flammable H_2/Air mixture ratios to sustain transition from local ignition to inflammation.
- Turbulent burning characteristics control transition to sustained turbulent jet flame.
- In this configuration, transient boundary layer phenomena within the pipe are principally responsible for producing the required mixing.

- Partial shock reflections from reductions in pipe diameter can result in required spontaneous release heating at pressures as low as 300 psia.
- In all cases, a minimum pipe length is required to achieve sufficient mixing for spontaneous ignition to occur, even if H_2 release pressure is sufficiently high for heating requirement.
- Both initial compressed pressure and downstream geometry can be critical factors in promoting spontaneous ignition.[1]
- ***Controlling phenomena interact non-linearly and require more experimental and numerical study to determine geometry effects and scaling.***

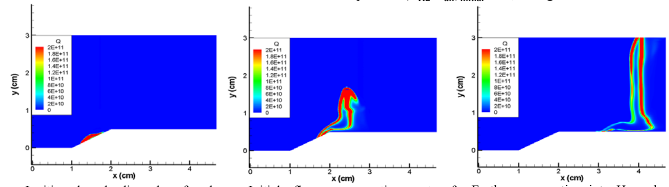
Spontaneous Ignition Induced by Compressed Hydrogen Release Interaction with Downstream Bodies



- Investigate transient shock interactions with simple two dimensional wedge geometries and fully-coupled, transient numerical simulations with detailed chemical kinetics and diffusive transport to investigate wide range of initial parameters and geometry effects.
- **Fully Coupled Numerical Modeling (A-SURF (1D, 2D) - (Adaptive Simulation of Unsteady Reacting Flow).**
- Methodology is adapted from prior laminar flame research.[3-5]
- Finite volume, unsteady, compressible N-S equations for multi-species reactive flow:
  - Reaction term: Strang splitting, VODE solver
  - Diffusion term: Finite difference scheme
  - Convection term: 2nd-order MUSCL-Hancock TVD Scheme
  - Time advancement: High order explicit TVD Runge-Kutta scheme
- Dynamically adaptive mesh refinement, (local mesh addition and removal), 8 to 10 levels with finest mesh size (16~4 μm) at contact surface.
- Detailed chemistry[2], multi-component transport, and radiation (optical thin & F-SNB-*ck* models).

Numerical Results

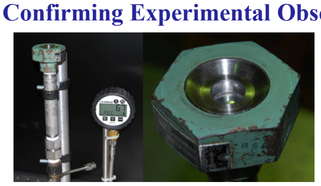
Movie Frame Sequence: $(P_{H2}/P_{air})_{initial}$ =70, Wedge thickness = 1 cm



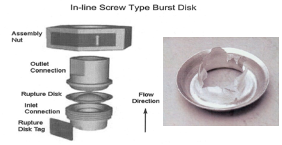
Ignition along leading edge of wedge. Initial flame propagation out of boundary layer into heated H_2 and air. Further propagation into H_2 and air mixture along contact surface.

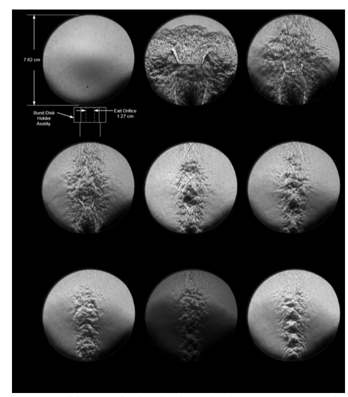
- Lower pressure ratio results in weaker ignition and flame does not propagate into free stream.
- Higher pressure ratio results in higher temperatures, stronger ignition and flame propagates along contact surface.
- Increased wedge angle enhances mixing downstream of wedge shoulder and promotes flame propagation.
- Reduced wedge angle results in reduced temperatures near wedge surface and delayed ignition.

Confirming Experimental Observations



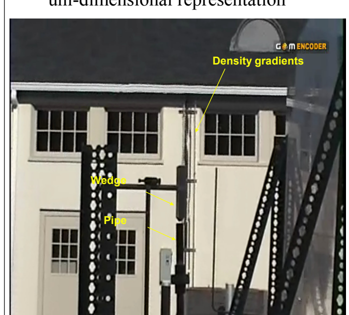
In-line Screw Type Burst Disk





Test conditions: 4" pipe length, 1/2" wedge, burst pressure 1715 psig. Refraction of light due to density gradients indicates sustained burning after spontaneous ignition event.

- Transient shock properties are affected by the pressure boundary rupture characteristics
- Shock structure is not modeled accurately by a thin discontinuity, uni-dimensional representation



Test conditions: 4" pipe length, 1/2" wedge, burst pressure 1715 psig. Refraction of light due to density gradients indicates sustained burning after spontaneous ignition event.
Video at http://www.princeton.edu/~combust/research/h2_safety/

- Combinations of pipe length and wedge geometries downstream of the pipe exit have been investigated

Test No.	Burst Disk	Configuration	Burst Pressure (Psig)	Result
1	0.007" Cu	4" pipe	1728	No Ignition
2	0.007" Cu	12" pipe	1743	Ignition
3	0.007" Cu	4" pipe, wedge 1/2" downstream	1762	Ignition
4	0.007" Cu	No pipe[1], wedge 1/2" downstream	1733	?
5	0.007" Cu	4" pipe, wedge 1/2" downstream	1715	Ignition

[1] ~1" female pipe threaded region downstream of burst disk

- Blunt body interactions with transient shocks formed by compressed hydrogen release can result in spontaneous ignition.
- Shock must be sufficiently strong and/or focused by the interaction to result in temperatures exceeding local autoignition temperatures.
- Critical mixing at the contact surface must also be induced by the shock/body interaction.

References

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3. Chen, Z., Qin, X., Ju, Y.G., Zhao, Z.W., Chaos, M. and Dryer, F.L. (2007c). *Proc. Combust. Ins.* **31**: 1215-1222.
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Acknowledgements

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