VENTED EXPLOSION OVERPRESSURES FROM COMBUSTION OF HYDROGEN AND HYDROCARBON MIXTURES

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Background

Explosion Venting

- Venting is used to reduce the consequences of explosions
- The requirements for the venting have been specified in engineering standards
  - NFPA 68 (2007)
  - EN 14994:2007
- Standards based on empirical correlations of limited experiment data which may be off by an order of magnitude
- Hydrogen
  - Weak enclosures (rooms) – out of range of validity of correlations
  - Strong enclosures (equipment) – based on questionable $K_G = 550$
- There are other methods – V.Molkov – yet there are unresolved issues

Background

Research Program Objectives

- To generate a set of experimental data examining the effect of:
  - **mixture composition**
  - ignition location
  - vent size
  - obstacles
  - scale
  - …
- Use the experimental data to develop and validate a computational model
- Update technical recommendations and FM operating standards relevant to explosion hazards and to develop new models and engineering tools

Background

Hydrogen Mixtures

- Additional challenges
  - Hydrodynamic flame instability is enhanced by thermal diffusion effects in lean hydrogen mixtures
  - Effect of *Le* on the turbulent burning velocity
- Currently, these effects are not known well enough to be reliably modeled
- Comparisons with methane-air and propane-air mixtures should yield an insight on how to model them

Background

Objectives of this study:

- Examine the similarities and differences between three mixtures of similar laminar flame speed
  - 18% hydrogen–air
  - 9.5% methane-air and
  - 4.0% propane-air
- Test an extension to the numerical CFD model developed in the previous studies and identify its capabilities and deficiencies to describe the physics responsible for the pressure build-up

Experimental Setup

Chamber Details

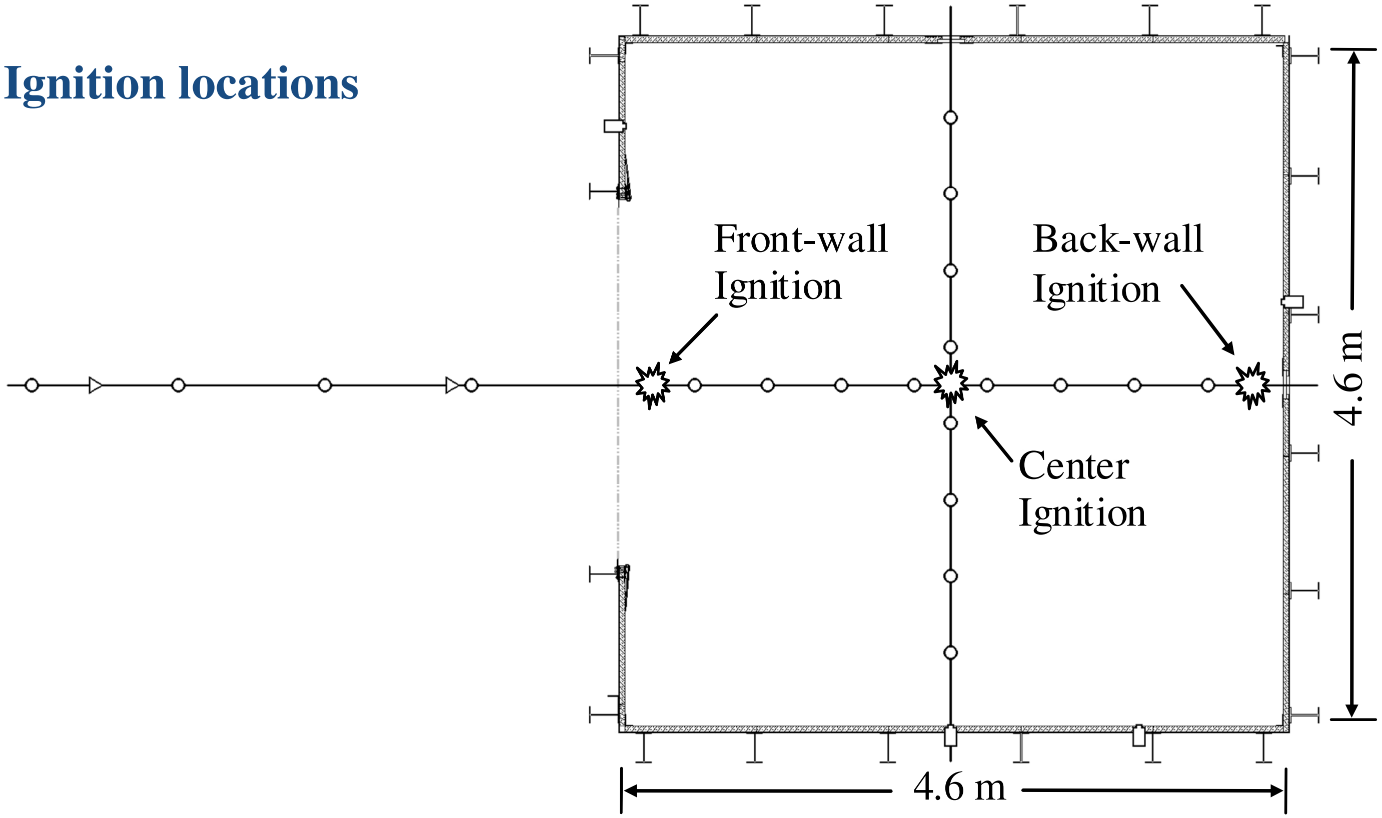
- Overall size:
  - 4.6 x 4.6 x 3.0 m
- Volume:
  - 64 m^3
- Vent Sizes:
  - 5.4 m^2 or 2.7 m^2
- Vent Material:
  - 0.02 mm Polypropylene Sheet

Experimental Setup

Ignition Locations:

Plan view:

3 Ignition locations



Experimental Setup

Test Parameters

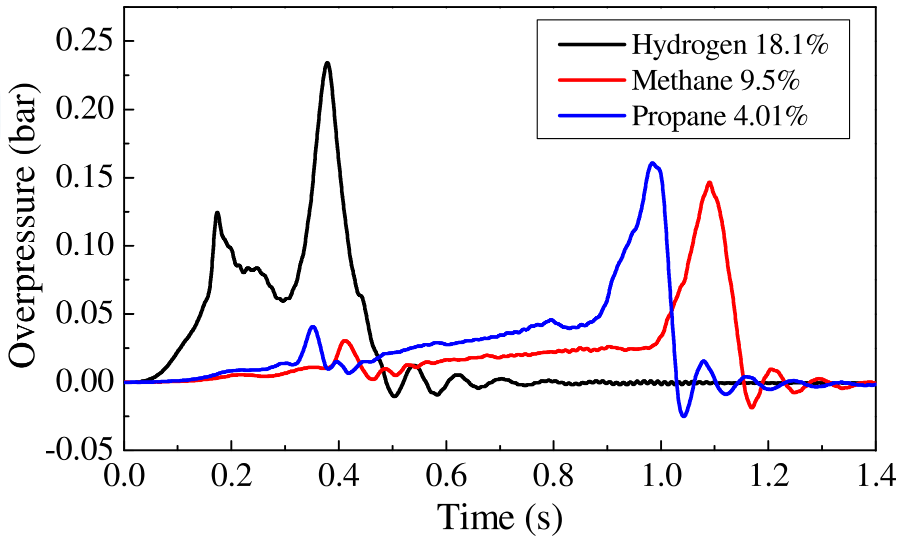
- 3 mixtures, 3 ignition locations, 2 vent sizes and no obstacles

Mixture	Laminar Burning Velocity, S_L (m/s)	Expansion Ratio, σ	Flame Speed, ($\sigma \times S_L$) (m/s)	Average Measured Initial Flame Speed, U_0 (m/s)
4.0% Propane	0.40	8.0	3.2	3.31 ± 0.06
9.5% Methane	0.38	7.5	2.9	2.90 ± 0.14
18% Hydrogen	0.64	5.2	3.3	6.47 ± 0.16

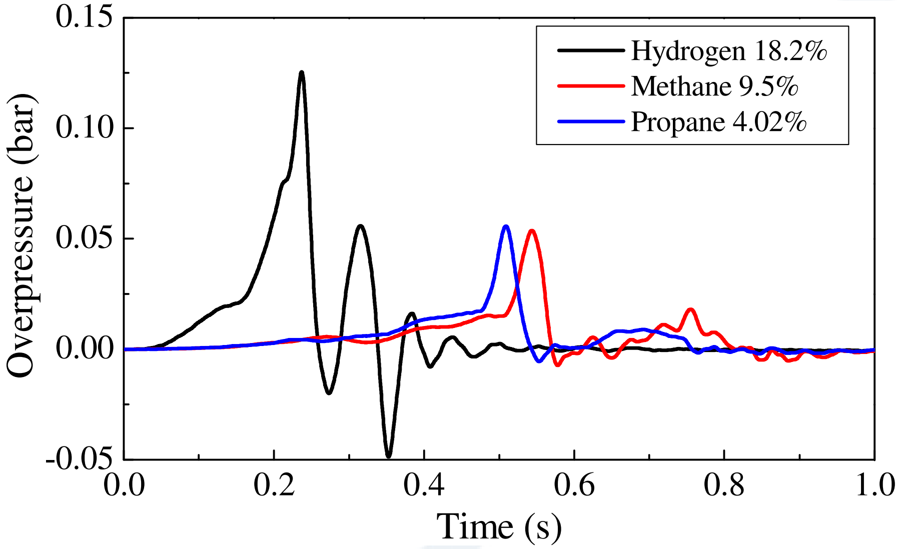
Experimental Results

Effect of Mixture composition

- Explosion overpressures



Center ignition 2.7 m^2 vent

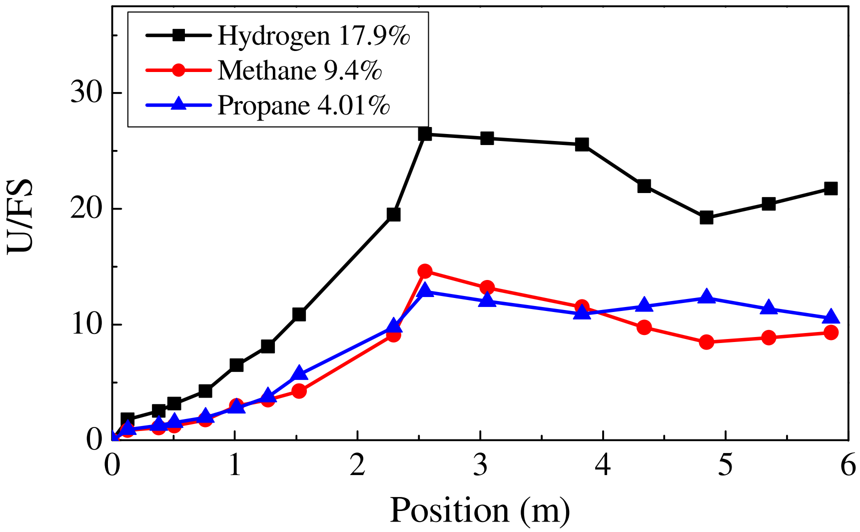


Back-wall ignition, 5.4 m^2 vent

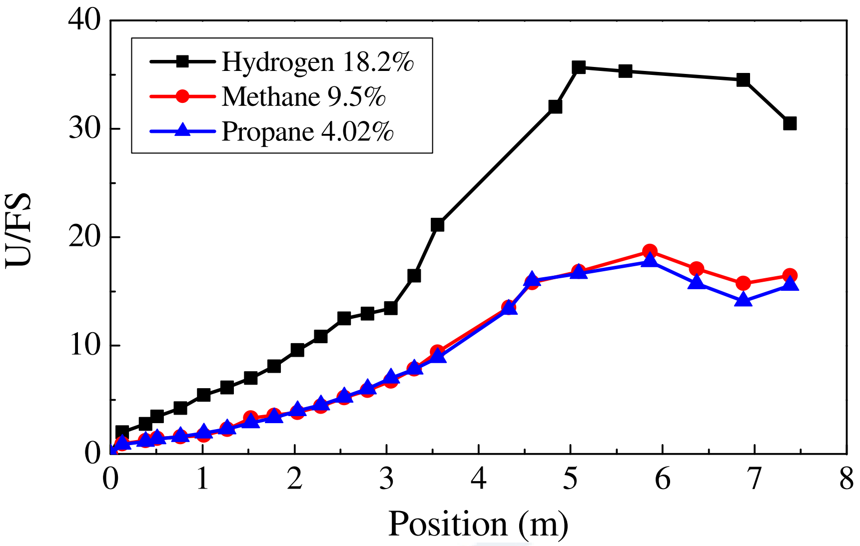
Experimental Results

Effect of Mixture composition

- Flame speeds normalized by LFS



Center ignition 2.7 m^2 vent

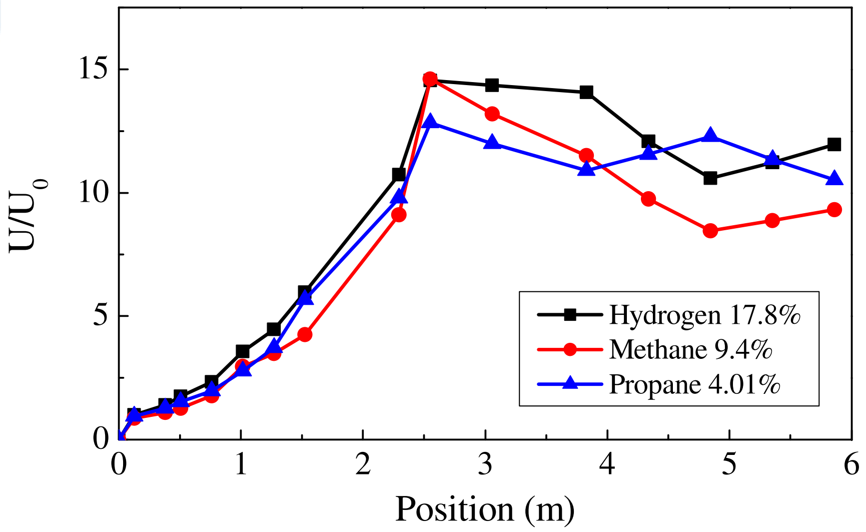


Back-wall ignition, 5.4 m^2 vent

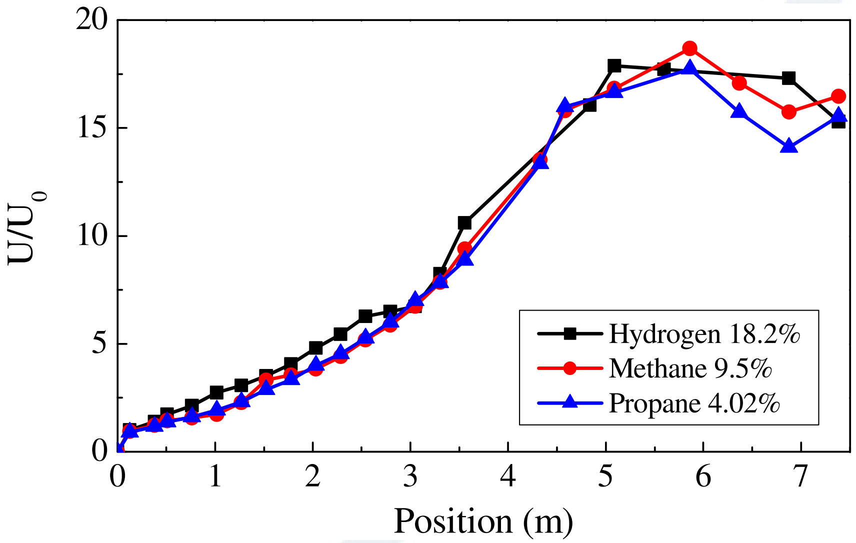
Experimental Results

Effect of Mixture composition

- Flame speeds normalized by initial flame speeds
- Enhancement of the hydrogen propagation speed caused by flame instabilities remains constant throughout the combustion process



Center ignition 2.7 m^2 vent



Back-wall ignition, 5.4 m^2 vent

Numerical Model

OpenFOAM

- OpenFOAM (Weller et al. 1998)
  - Open source Field Operations And Manipulation
- Solver details
  - Fully compressible implicit NS solver
  - 2nd order discretization schemes in time and space
- LES model
  - One equation eddy viscosity model for sub-grid turbulence

Numerical Model

Partially Pre-Mixed Combustion Model

- Regress Variable Combustion Model

$$\frac{\partial \bar{\rho}\tilde{b}}{\partial t} + \nabla \cdot \left(\bar{\rho}\tilde{\mathbf{U}}\tilde{b}\right) - \nabla \cdot \left(\bar{\rho}\mathcal{D}\nabla\tilde{b}\right) = -\bar{\rho}_u S_L \Xi \left|\nabla\tilde{b}\right|$$

- Sub-grid flame wrinkling, Ξ, is due to both turbulence and flame instabilities
- Taylor instability model important to resolve external explosion (ICDERS-2009)
- Separate transport equations for Ξ_{RT} and Ξ_T
  - Assumption of different dominant length scales

$$\Xi = \Xi_{HI} \cdot \Xi_{RT} \cdot \Xi_T$$

Numerical Model

Combustion Model - HI

- Flame surface area increase due to hydrodynamic instability

$$\frac{A}{A_0} = \left(\frac{\lambda_m}{\lambda_c}\right)^{1/3} = \left(\frac{\lambda_m}{\Delta}\right)^{1/3} \left(\frac{\Delta}{\lambda_c}\right)^{1/3}$$

$$\Xi_{HI} = \max\left[1, a_I \left(\frac{\Delta}{\lambda_c}\right)^{1/3}\right] = \max[1, \theta]$$

- Constant for given grid size (Δ) and given mixture (λ_c)
- θ(hydrogen)/θ(methane, propane) $\approx$ 2.4 – consistent with known values of λ_c

Numerical Model

Combustion Model - Turbulence

- Sub-grid wrinkling due to Turbulence (Weller et al 1998, Bradley et al 1992)

$$\frac{\partial \Xi_T}{\partial t} + \mathbf{U}_s \cdot \nabla \Xi_T = G\Xi_T - R(\Xi_T - 1) - (\sigma_t - \sigma_s)\Xi_T$$

$$G = \frac{0.28}{\tau_\eta} \qquad R = G\frac{\Xi_{eq}}{\Xi_{eq} - 1}$$

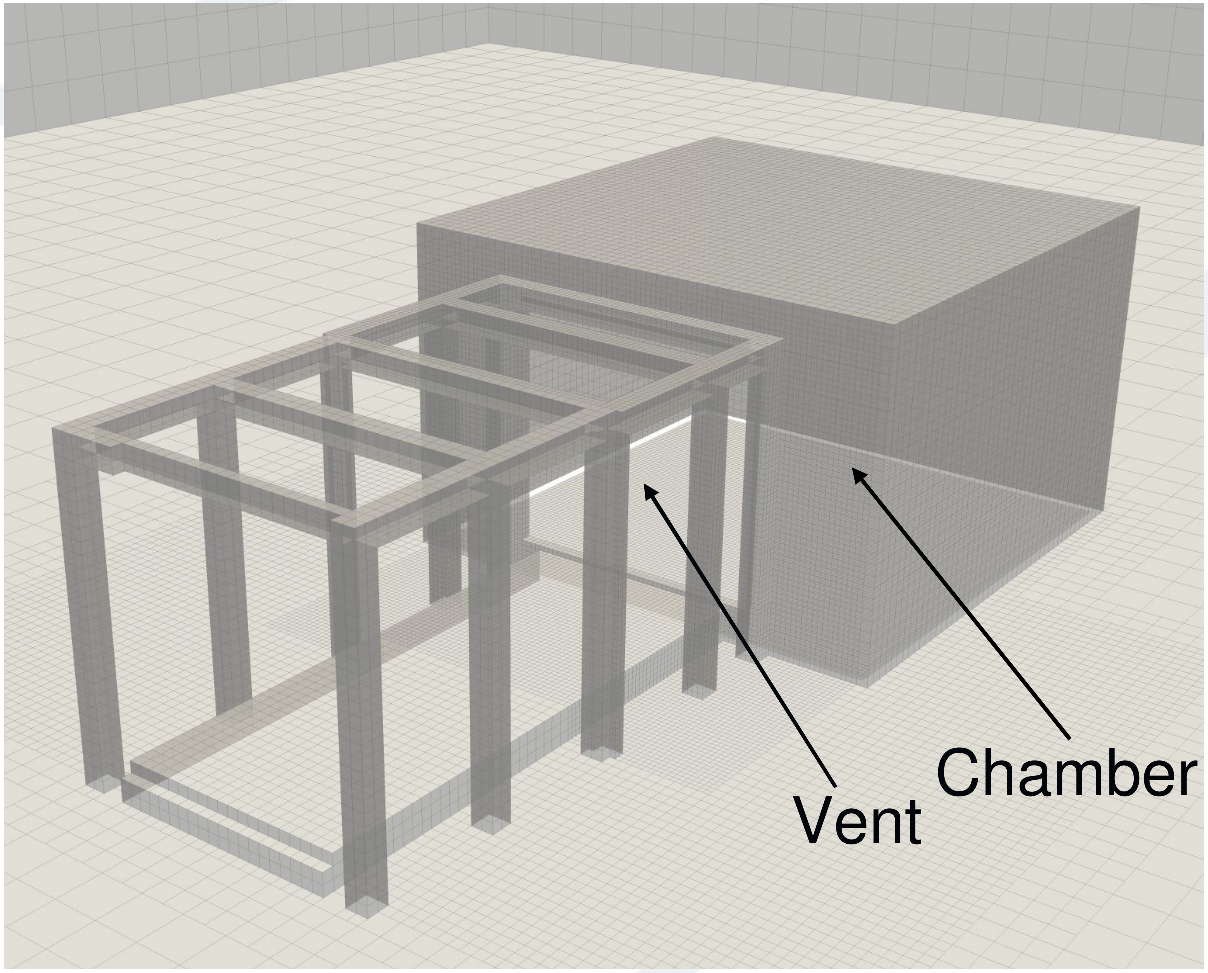
$$\Xi_{eq} = a_T \left(u' / S_L\right)^{\frac{1}{2}} \left(\Delta / \delta\right)^{\frac{1}{6}} Le^{-n}$$

- All mixtures: $\alpha_T = 0.7$
- Factor Le^{-n} undistinguishable from Ξ_I ($n = 0.5$)

Numerical Model

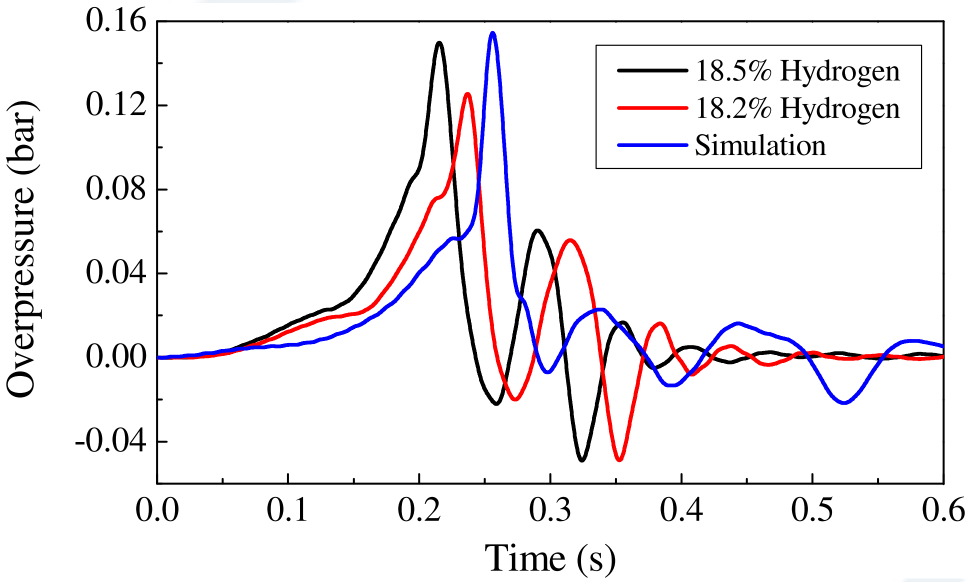
Computational Grid

- Unstructured Grid
- 0.05m cell size
- 1.2M cells

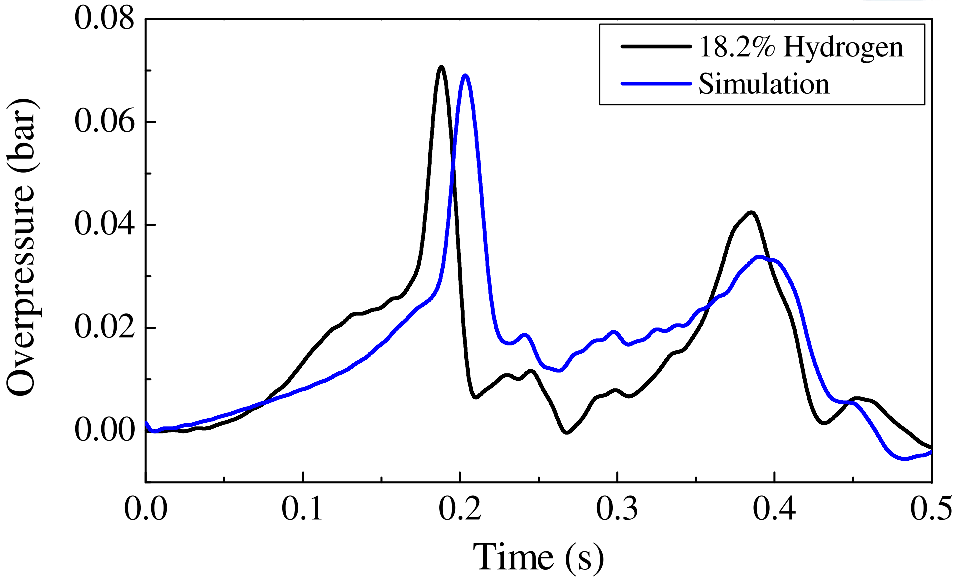


Results – Simulations

Back Ign. 5.4 m^2 vent 0 obs.:

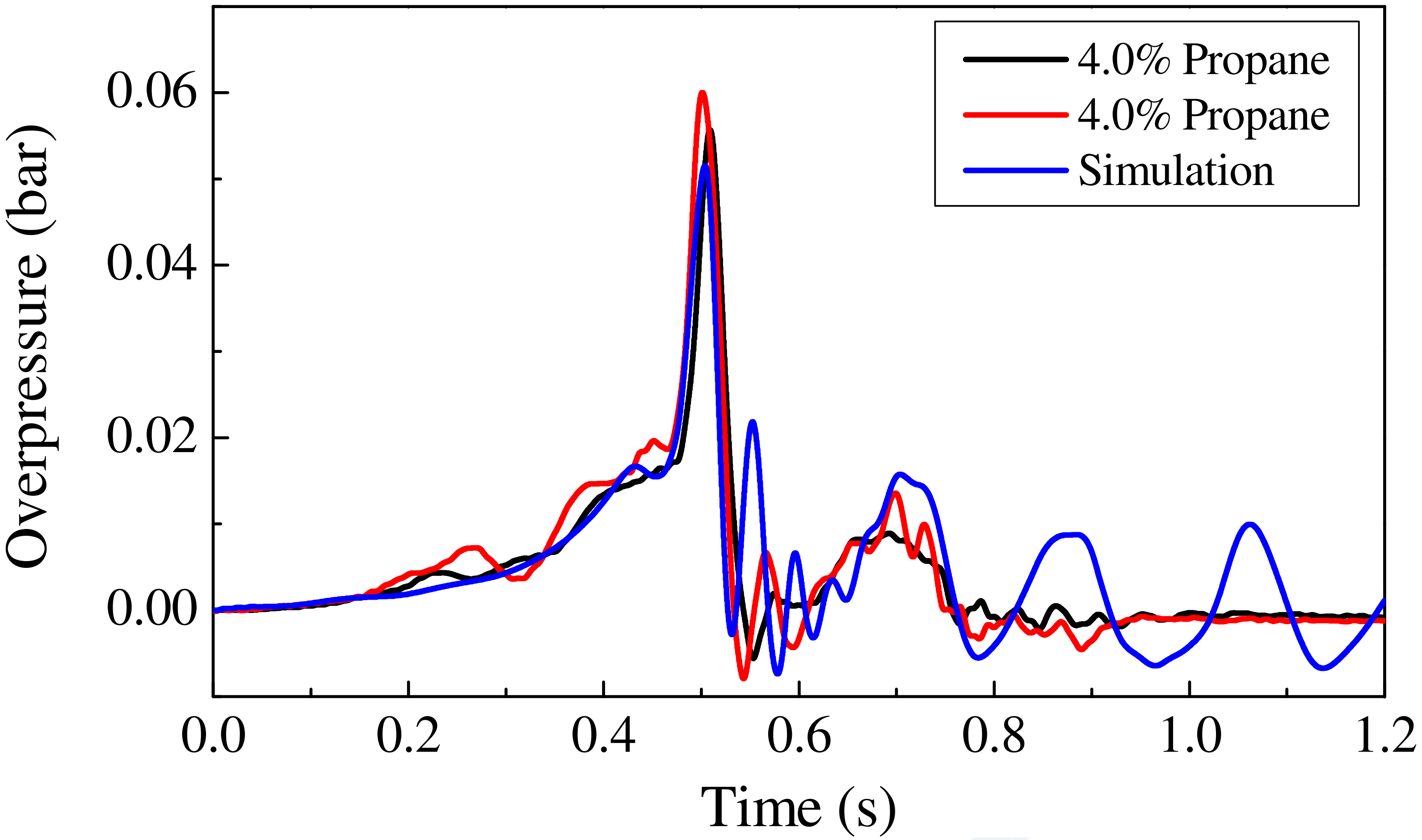


Center Ign. 5.4 m^2 vent 0 obs.:



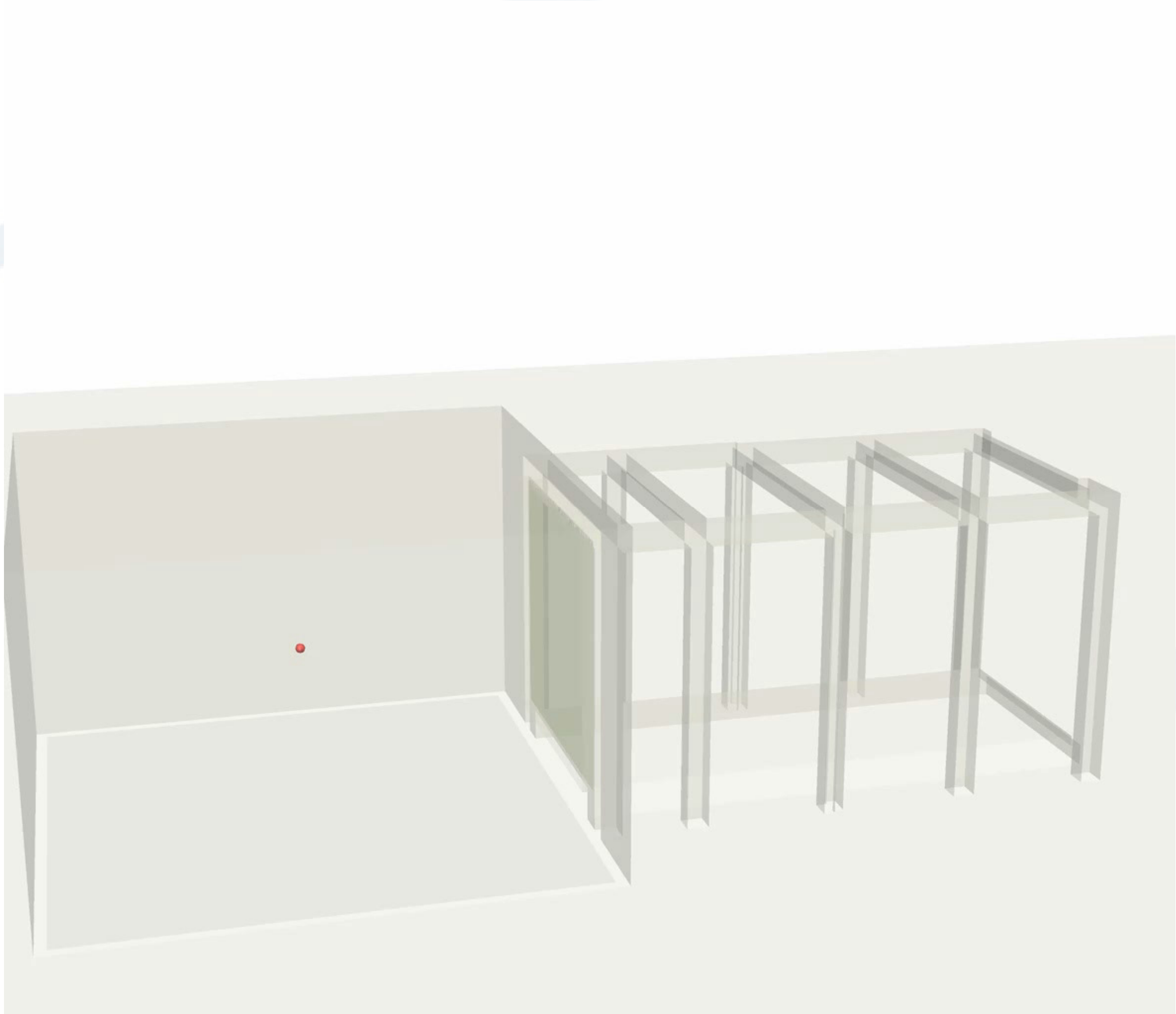
Results – Propane

Back Ign. 5.4 m^2 vent:



Results – Simulations

Movie



Conclusions

- Experiments showed that flame speeds and overpressures in H_2 mixtures were much higher than that in methane and propane due to flame instabilities, despite close laminar values
- Laminar flame speeds are not sufficient to characterize mixture reactivity in vent-sizing for hydrogen mixtures
- CFD model was tested that takes into account mixture properties, flame instabilities and turbulence
- Numerical results reproduce basic features observed in experiments, such as overpressures and flame speeds for the range of parameters studied
- Further studies are planned to include effects of scale and obstacles in the model validation exercises