NUMERICAL SIMULATION OF TRANSITION TO DETONATION IN A H_2-AIR MIXTURE DUE TO SHOCK WAVE FOCUSING IN A 90-DEG WEDGE (ID 249)

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Presentation plan

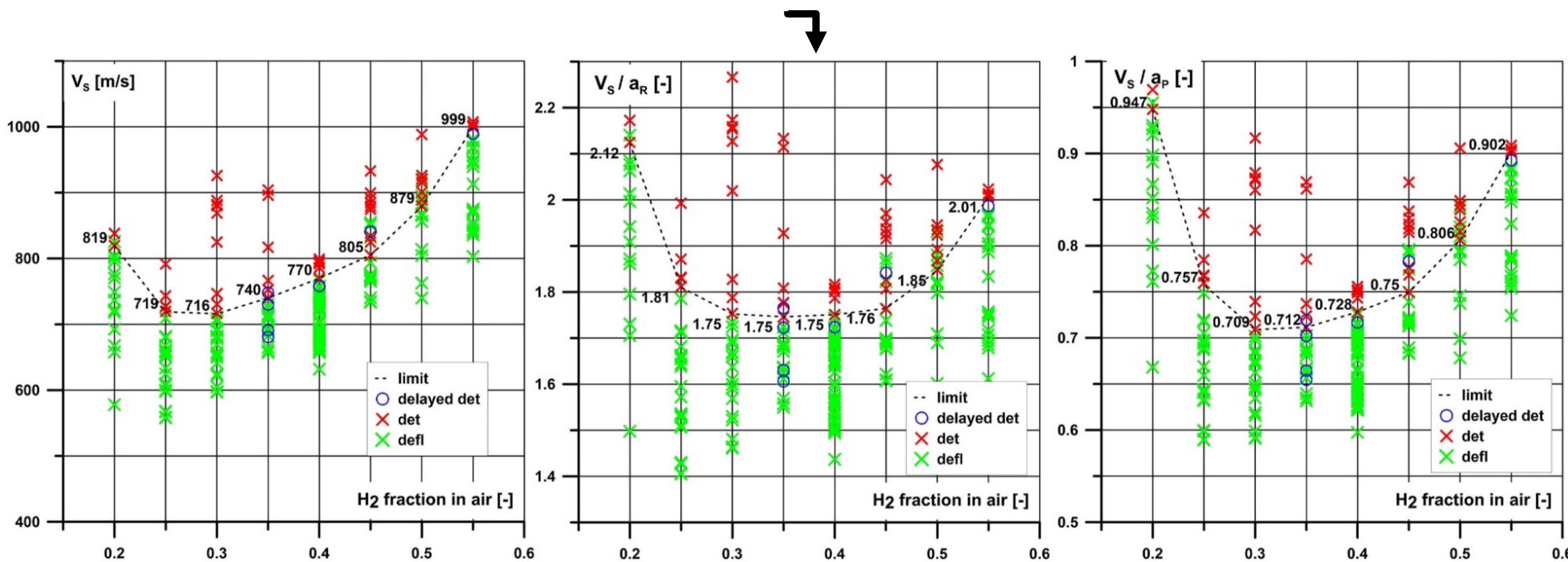
1. Introduction

- Hydrogen as future carbonless energy carrier → mass scale use → expected increase of unintended events of hydrogen release
- Hydrogen physical properties considered as advantages and disadvantages
- Detonation prevention (release → ignition → FA + TD) and support (RDE/PDE)
- Detonation is one of the most challenging combustion phenomenon by means of experimental equipment as well as numerical tools
- CFD → wide range of modelled scale → codes optimisation necessary for particular combustion regimes (e.g. sub-grid scale models, pre-calculated IDT data)
- Validated numerical codes should simulate more precise combustion processes → new tools to support R&D, risk assesment in process safety → safer and more efficient devices and processes

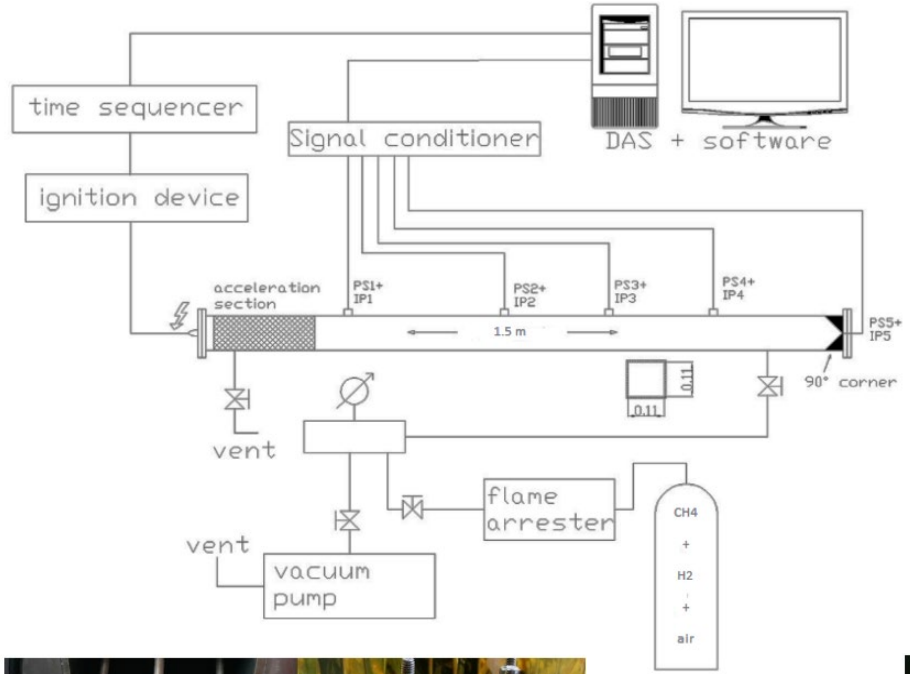
2. Objectives

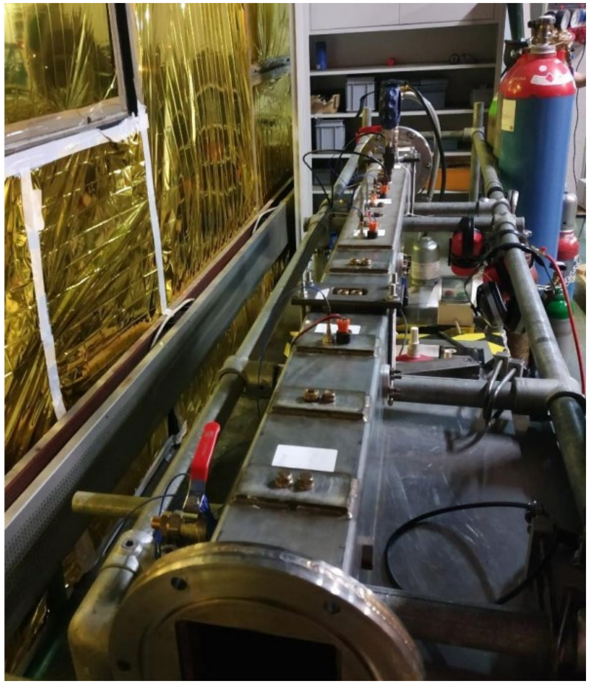
- Investigate numerically the detonation initiation process through shock reflection and focusing, to gather essential data on the TD process for different H_2 - air mixtures at initial pressure of 1 bara.

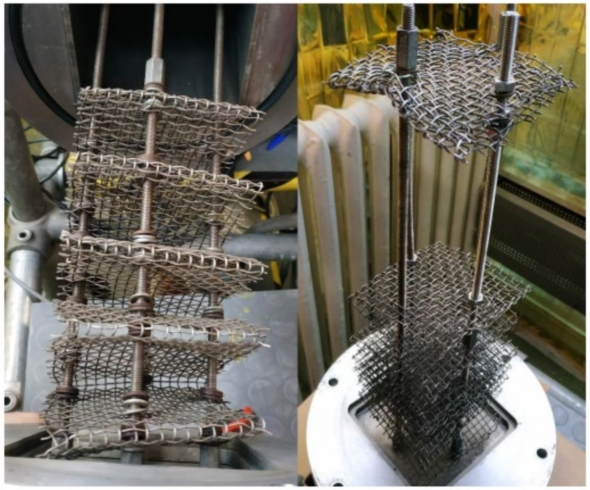
- Conduct numerical simulations using the ddtFoam code to replicate experimental conditions as described in paper: *Rudy, W., Transition to detonation in hydrogen-air mixtures due to shock wave focusing in the 90-deg corner, IJHE, 2023*

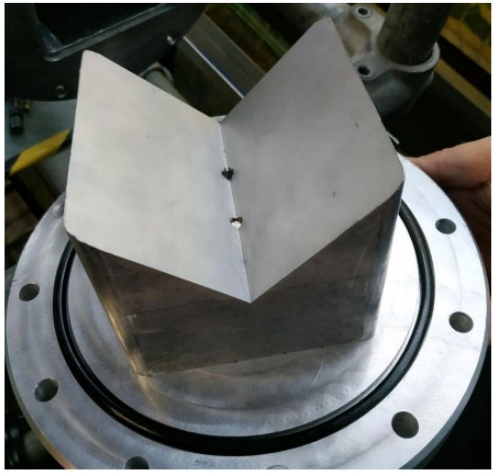


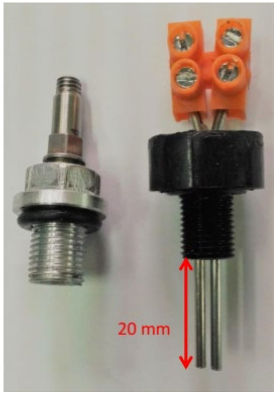
3. EXPERIMENTAL SETUP AND DATA





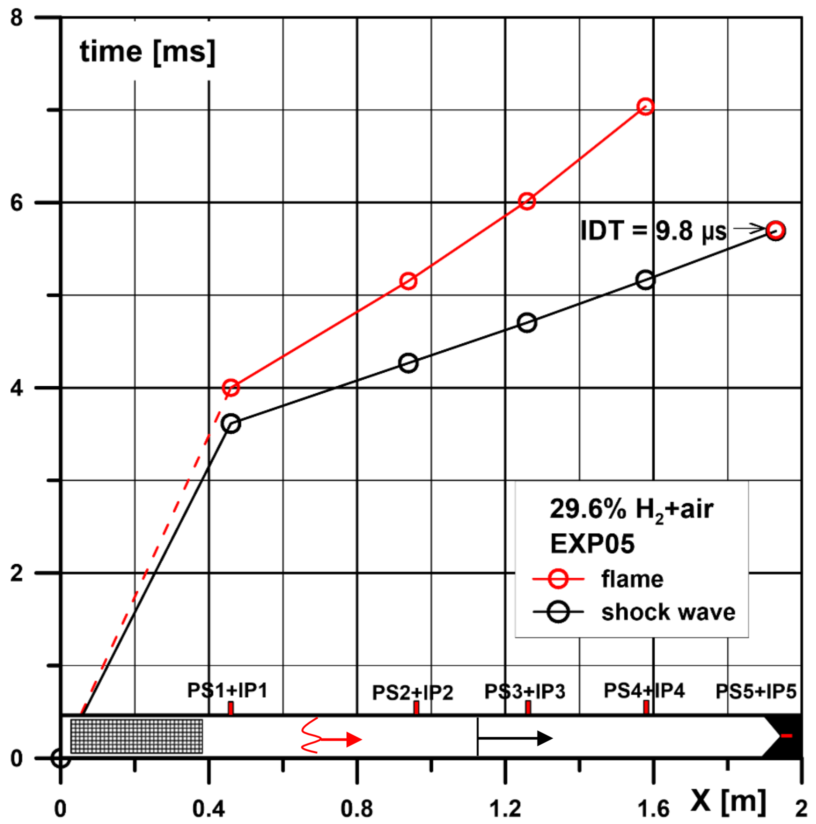


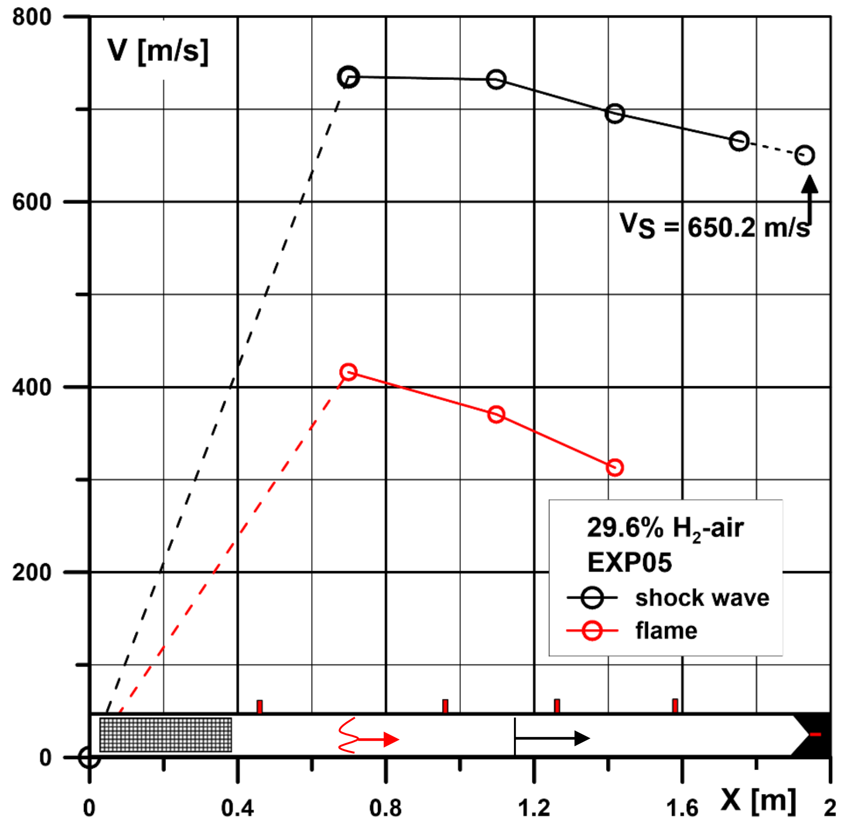




3. Experimental setup and data

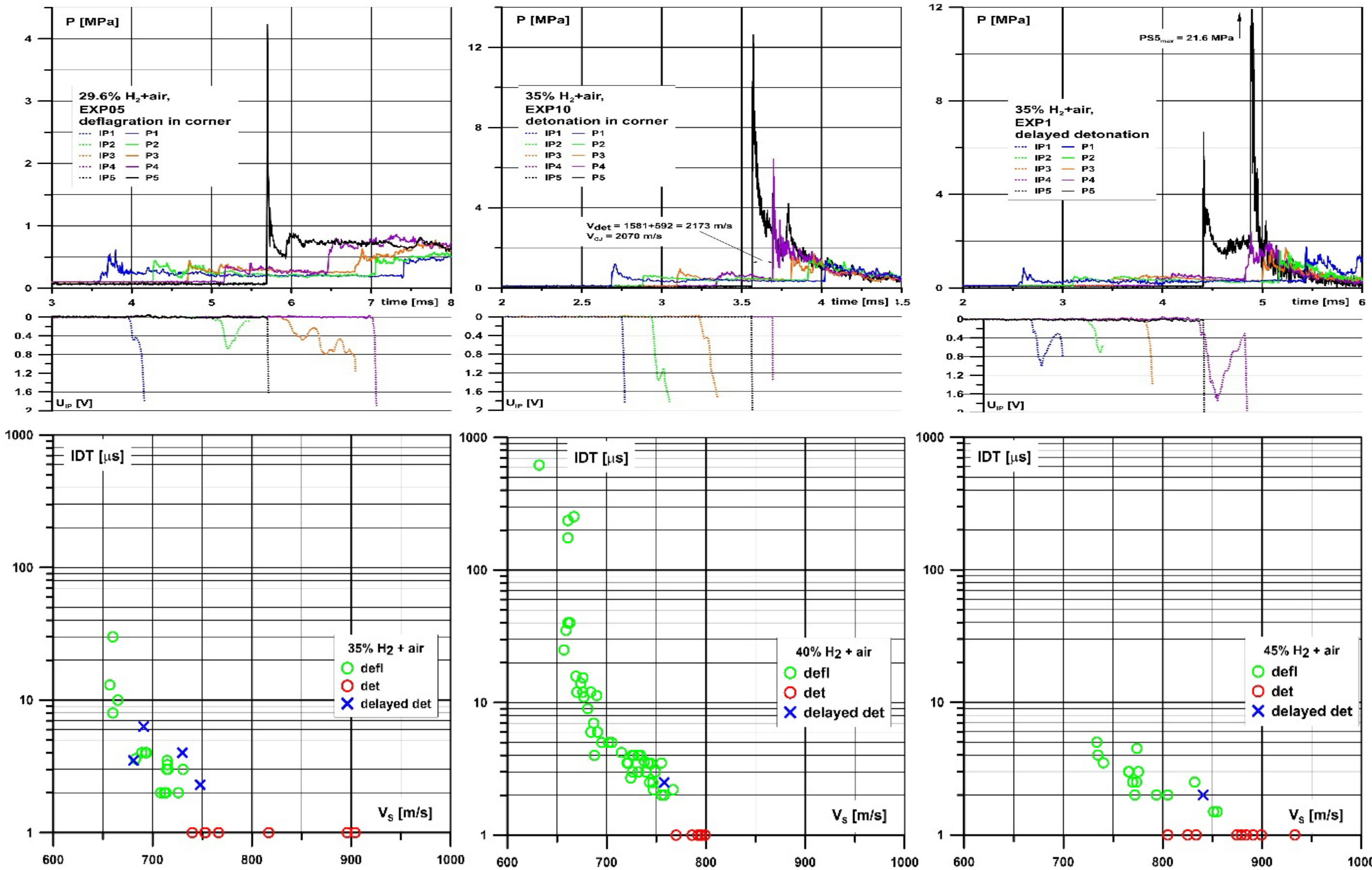
- ToA method for flame and shock wave velocity calculations
- Velocity of the shock wave at the reflection extrapolated
- Pressure in the corner obtained from max. PS5 value.
- Calculation of ignition delay time (IDT) in wedge tip





3. Experimental setup and data

3 ignition types recorded: deflagration, detonation and delayed detonation



4. Simulation description

- Utilized ddtFoam solver from OpenFOAM® developed by Ettner et al. (*Ettner, F. A., Vollmer, K. G., Sattelmayer, T., Numerical simulation of the deflagration-to-detonation transition in inhomogeneous mixtures, Journal of Combustion, 2014*)
- Based on unsteady, compressible Navier-Stokes Equations in Favre-Average sense
- Density-based solver, employs the HLLC scheme to determine all the convective fluxes.
- Turbulence modelled by k- ω- SST model
- Two source terms for ignition: deflagrative (Weller gradient combustion model) and detonative (autoignition)
- Autoignition model utilizes a pre-calculated ignition delay time (IDT) table based on O'Conaire's reaction mechanism (Cantera generated)
- Sub-grid scale modeling of shock wave to capture post-shock parameters → applicable for coarse grids ≤ 0.5 mm
- Thermo and transport data properties for hydrogen-air mixture obtained from the Chemkin database.
- ddtFOAM validated against variety of cases:

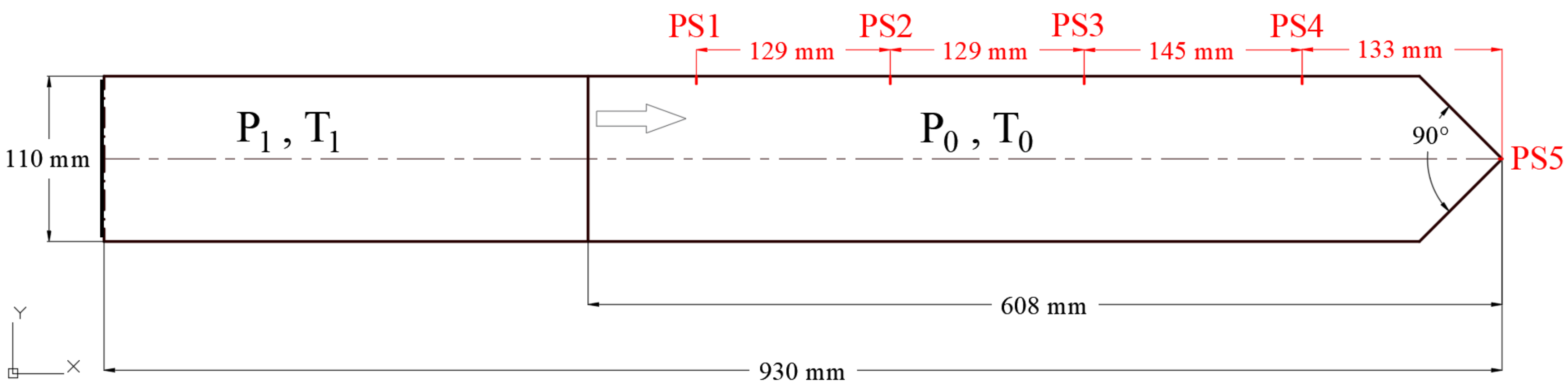
  - *Ettner et al., Journal of Combustion, 2014* - semiconfined detonative layer

  - *Rudy et al., Energies, 2019* – tube filled with obstacles

  - *Hasslberger et al., J. Loss. Prev. Proc. Ind., 2015* - RUT facility, simulations with AMR

4. SIMULATION DESCRIPTION CONT.

- Computational Domain: the final segment of a 0.11x0.11x2 m tube with a 90° wedge-shaped cavity filled with a hydrogen-air mixture with concentrations from 15% to 50% (equivalence ratio: 0.42 to 2.91)
- Shock tube problem: P_1, T_1: 8-15 bar 298 K, P_0, T_0: 1 bar, 298 K
- V_S = 650-800 m/s,
- Numerical sensors placed in positions as in experiments
- Hexahedra+prism mesh: 0.5x0.5 mm → 0.05x0.05 mm in the wedge area ~70 k cells
- BCs: Walls assumed to be non-slip and adiabatic



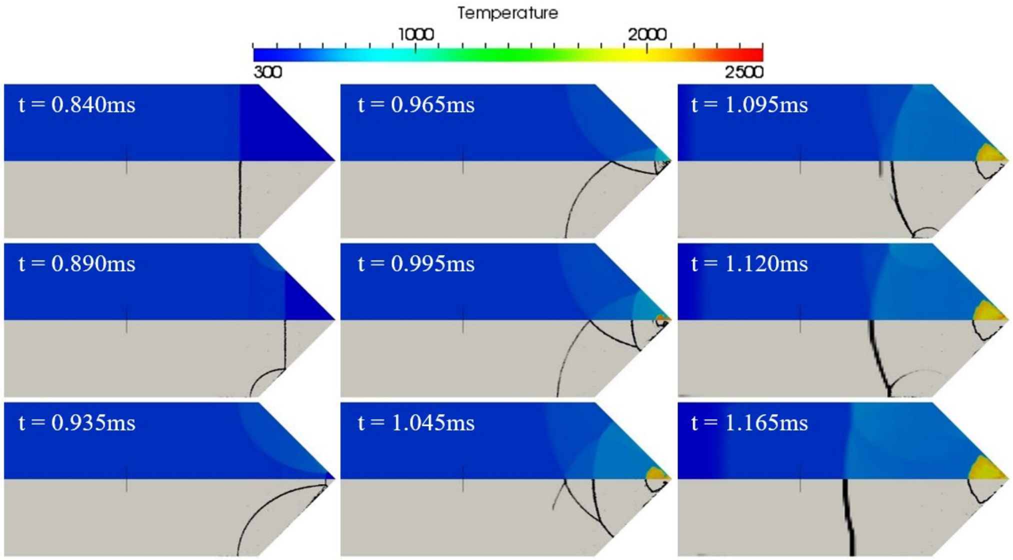
5. Results

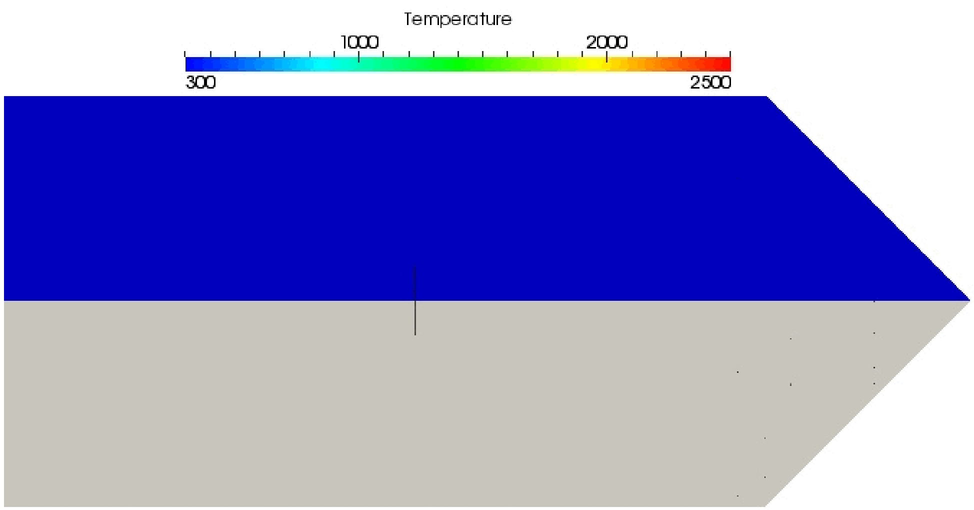
- Numerical results processed as in experiments:
  - velocity profiles extracted from pressure sensors using the Time of Arrival method
  - maximum pressure from PS5

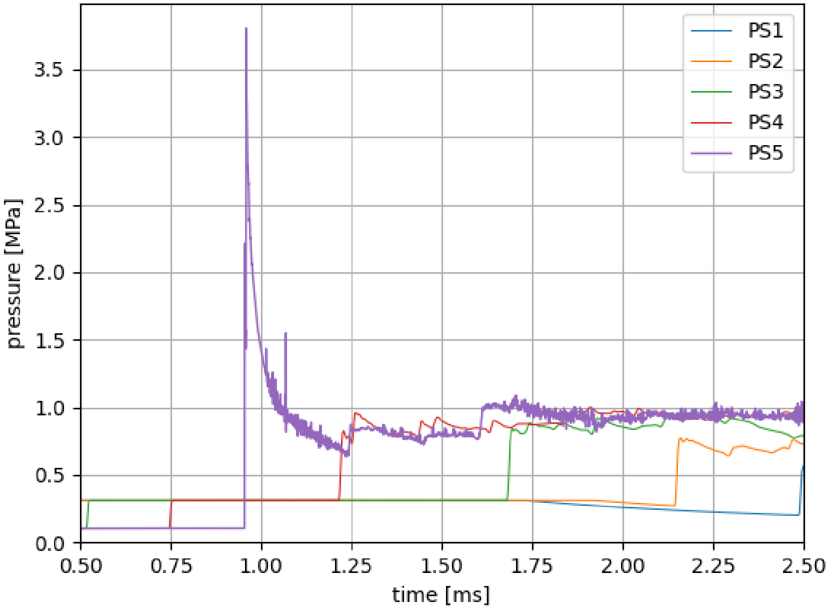
- Three ignition modes were observed, similar to the experiments:
  - Deflagrative ignition
  - Delayed detonation ignition
  - Transition to detonation

5. Results

Deflagrative ignition mode for 20% H2+air mixture and V_S = 643.7 m/s.

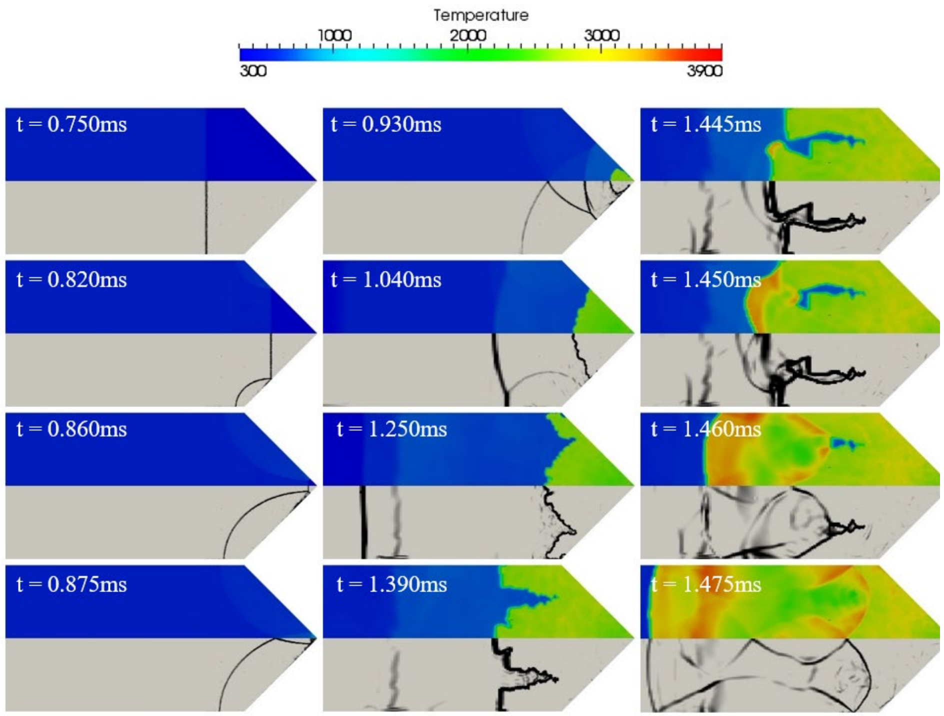


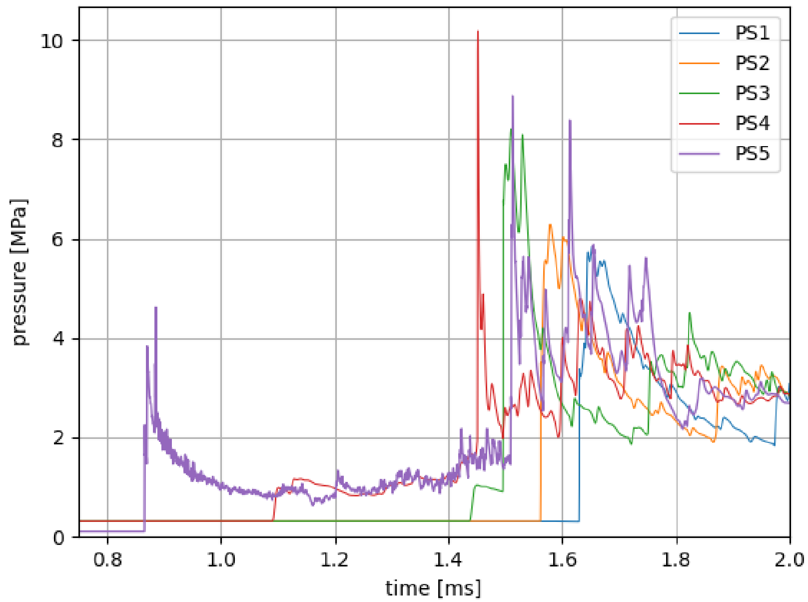


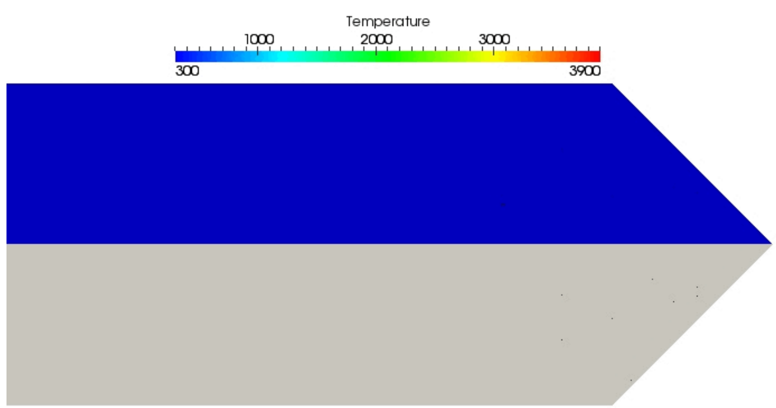


5. Results

Delayed detonation mode for 35% H_2+air mixture and V_S = 698.65 m/s.

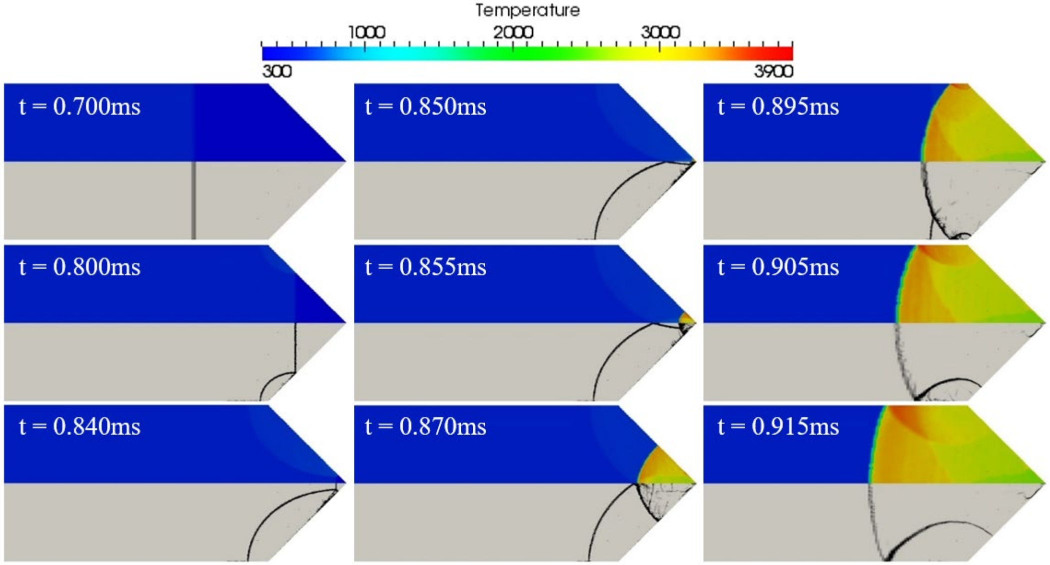


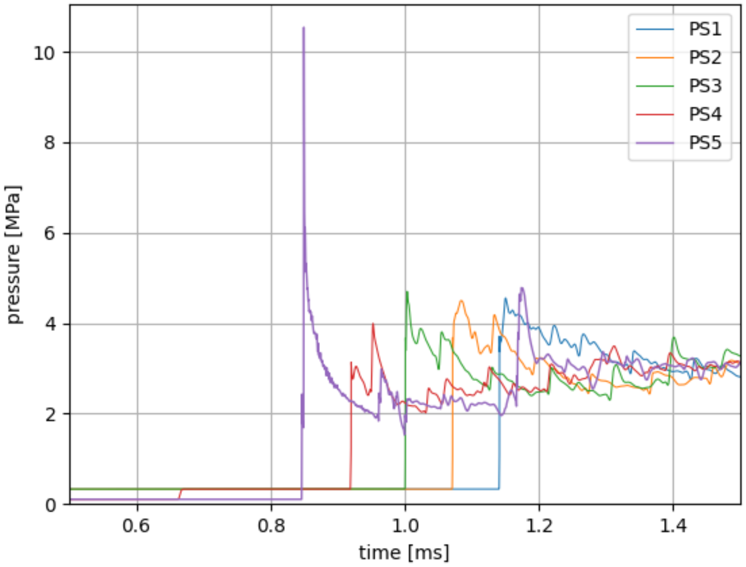


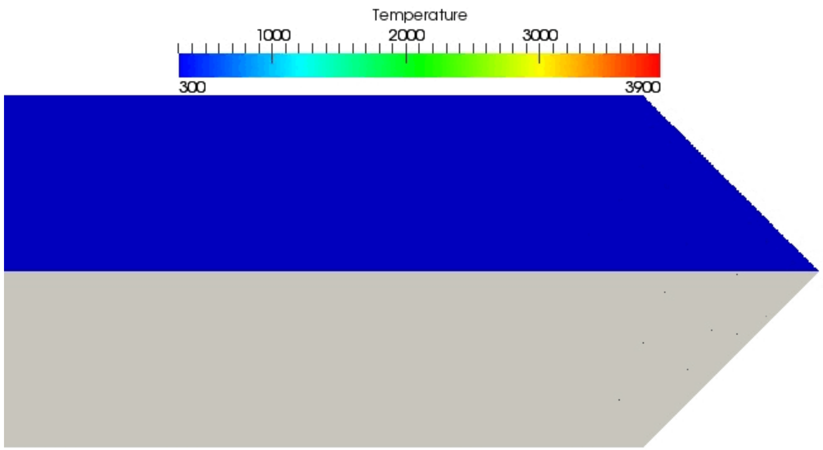


5. Results

Detonative mode for 35% H_2+air mixture and V_S = 714.88 m/s

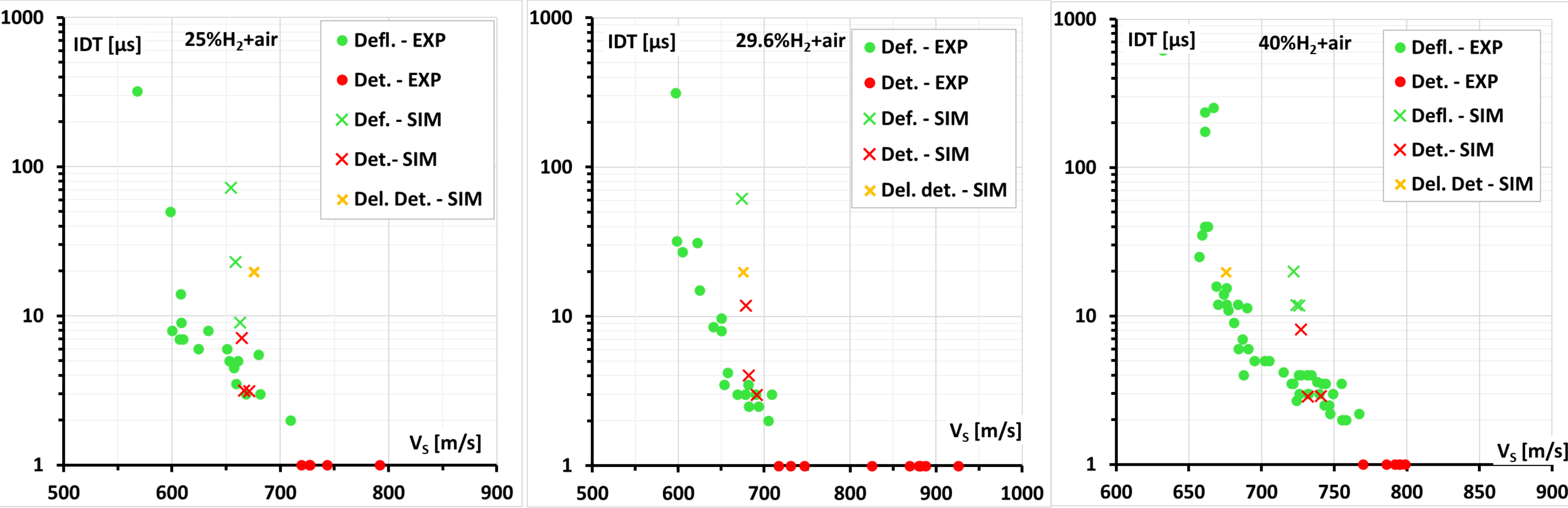






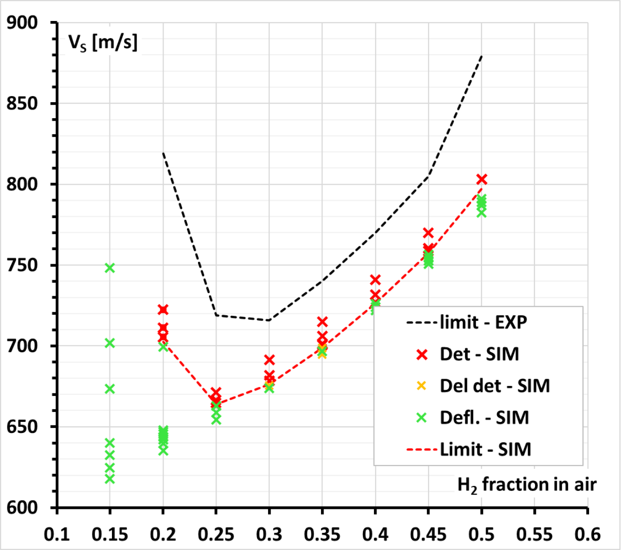
Detonation wave propagation velocity of 2225 m/s (V_{CJ} =2067m/s)

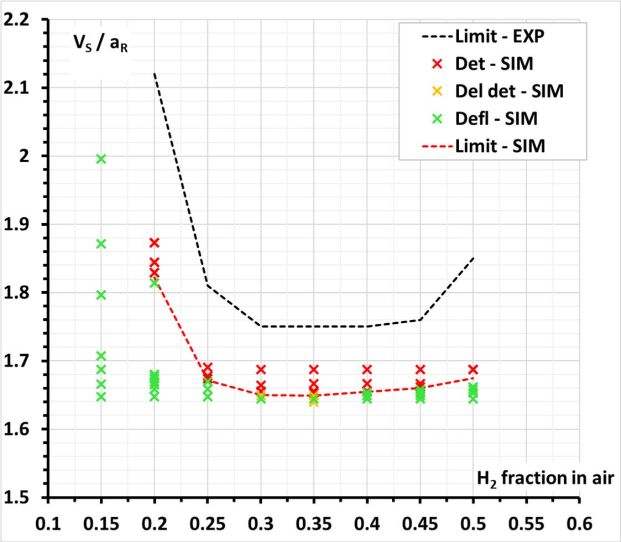
5. Results

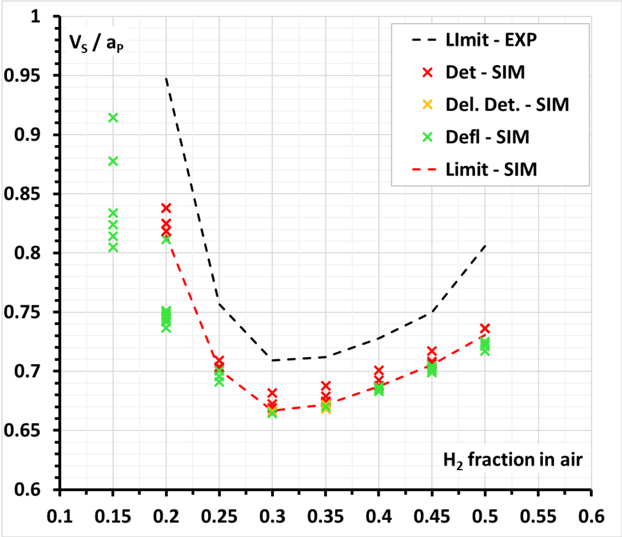


- The deviation from experiments is mainly due to the difference in IDT for direct transition to detonation → limit for SIM is of 10 µs whether limit for EXP is of 1 µs
- Simulations show stronger dependance of IDT = f(V_S) than in experiments

5. RESULTS

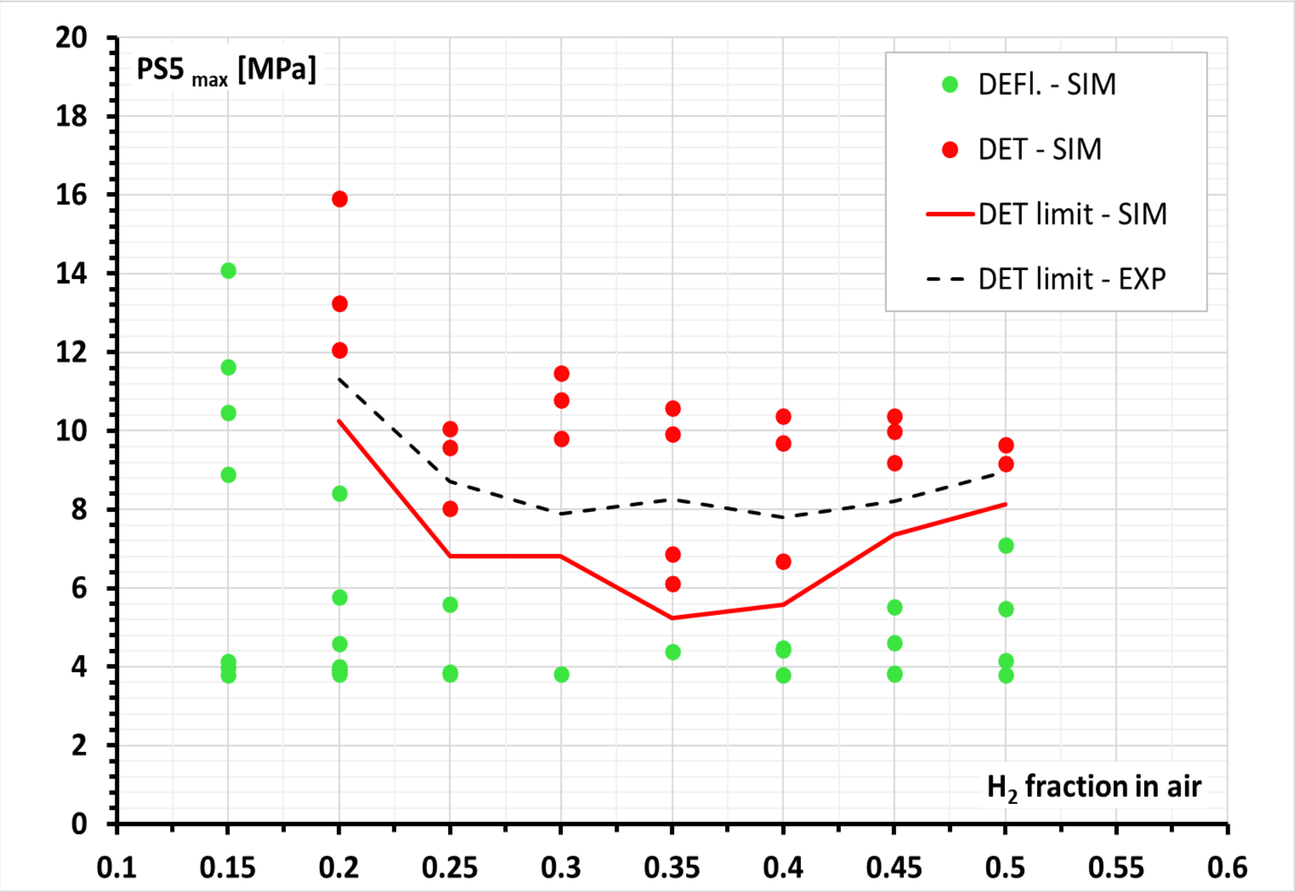






- Numerical results follow the experimental U-shape pattern with the lowest deviation for near stoichiometric mixtures (~5%)
- In geenral difference between numerical and experimental data stayed within range 5-8% below the exp. data for mixtures 25% - 45% H_2
- The highest deviation from experimental data was within range 14 - 17% for 25% and 50% H_2, respectively

5. RESULTS



- Pressure for direct detonation initiation ranges from 5-10 MPa for 25%-50% H_2 in air.

→ exp. Sensor averaging?

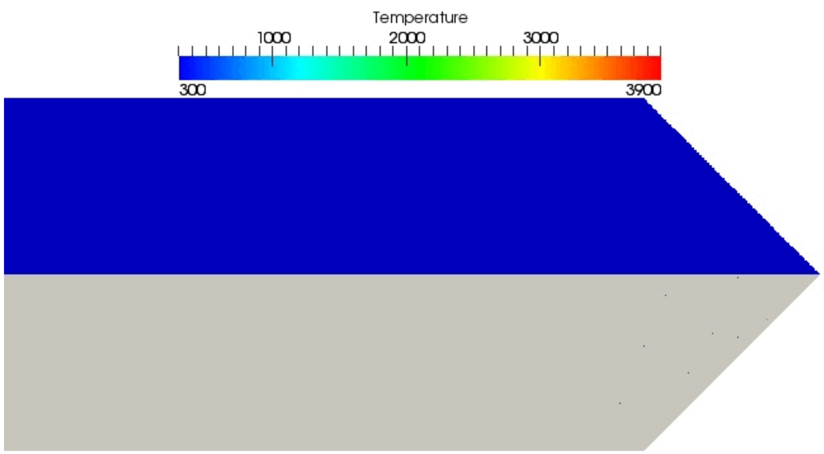
- Numerical limits deviated by 10-36%, largest differences in 30-40% hydrogen mixtures.

6. Conclusions

- The study was aimed to replicate experiments and assess ddtFoam code ability to predict TD limits due to shock focusing in a 90-deg wedge
- Numerical results revealed three ignition scenarios - deflagrative ignition, deflagrative ignition with delayed transition, and immediate transition to detonation.
- A notable deviations exist between numerical and experimental data by means of limiting velocities, IDT and maximum overpressures.
- In general the difference in limiting shock wave velocities ranged 5-8%, with the largest discrepancies observed for mixtures < 25% and > 45% hydrogen in air, up to 17%.
- IDT overestimated in simulations → underestimation of limiting shock velocities
- Numerical underestimation provides some safety margin within acceptable level

7. FURTHER RESEARCH

- Conduct simulations of leaner (H_2 < 25%) and richer (H_2 > 45%) hydrogen-air mixtures
- Perform 3D simulations of 3-wall 90-deg corner reflector → exp. research in progress
- Extend the research to HC-air and CH_4-H_2-air mixtures
- Test different chemical reaction mechanisms for IDT table?



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Thank you for your attention!

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