

***Detonations in risk assessment of
hydrogen systems***

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PROCESS SAFETY, COMBUSTION AND EXPLOSION RESEARCH GROUP

February 2023, PhD Candidate, USN

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RA4 Safety and material integrity

Table of Content

INTRODUCTION

1

Slide 4-5

- Accidental Explosions
- Hydrogen Properties
→ H₂ Safety

2

Gas Explosions

Slide 7-8

- Introduction to Gas Explosion
- Ignition, Deflagration, DDT, Detonation
- How do we study these mechanisms?

3

Explosion Experiments

Slide 9-13

- Small/lab scale
- Experimental setup
- Equipment
- Results

4

Explosion Modeling

Slide 14-18

- CFD/OpenFOAM
- Solver
- Numerical Setup
- Results

5

Conclusion & Future Research

Slide 20

- Conclusions
- Future Research
- Q&A

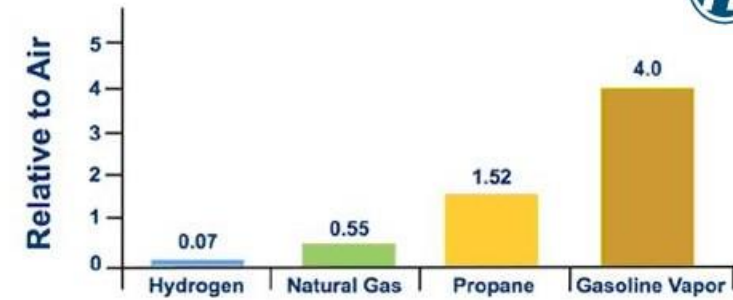
1

INTRODUCTION

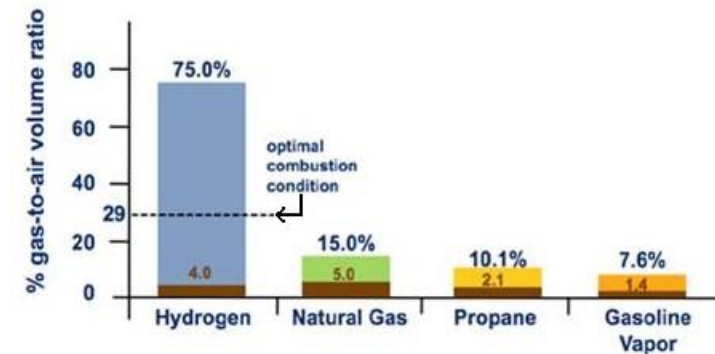
H₂ properties:

- LHV: **119.96 MJ/kg**
- $\rho = 0.0883 \text{ kg/m}^3$
- Minimum ignition energy: **0.017mJ**
- Flammability range in air: **4-75 %vol**
- $D = 120 \text{ pm}$ (atom) ; **74 pm** (molecule)
- Non-toxic and non-corrosive
- Flame visibility: low
- Colour and odour: non

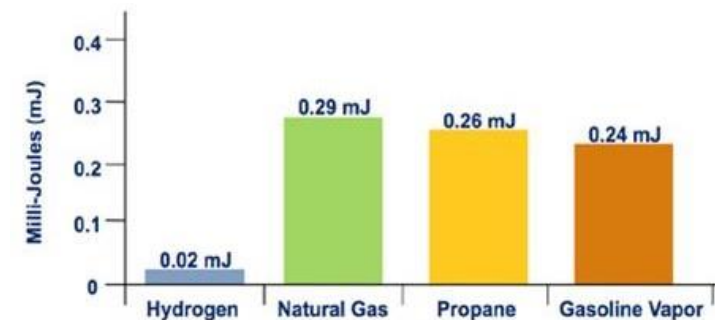
Property	Hydrogen	Methane
Laminar Flame Speed [m/s]	2.7	0.4
LHV [MJ/kg]	120	50
Detonation Energy	1 g TNT	1 kg TNT



Relative Vapour Density



Flammability Range in Air



Minimum Ignition Energy

Accidental Explosion

- June 10, 2019
- Blast from explosion felt miles away
- 75 kg wall elements found 40m from the main building
- No fatalities
- Possible fail: End flange of the high-pressure H₂ storage unit (composite tank)
- Possible DDT



Uno-X Station Explosion in Sandvika, Norway

- **Learning** from accidents
- Implement better **standards** and **regulations**



RESEARCH AREAS

PRODUCTION

TRANSPORT &
STORAGE

END-USE

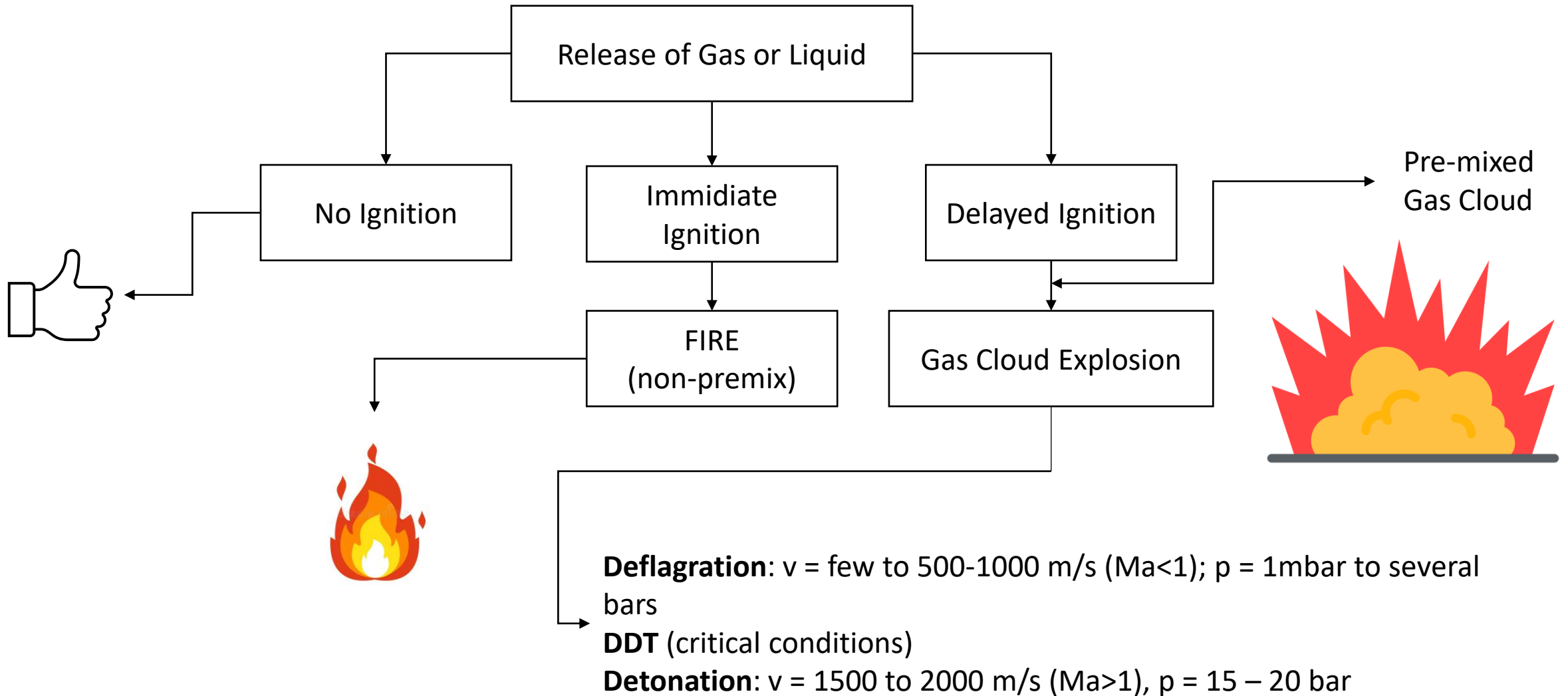
SAFETY & MATERIAL INTEGRITY

SUSTAINABLE
HYDROGEN
ECONOMY

2

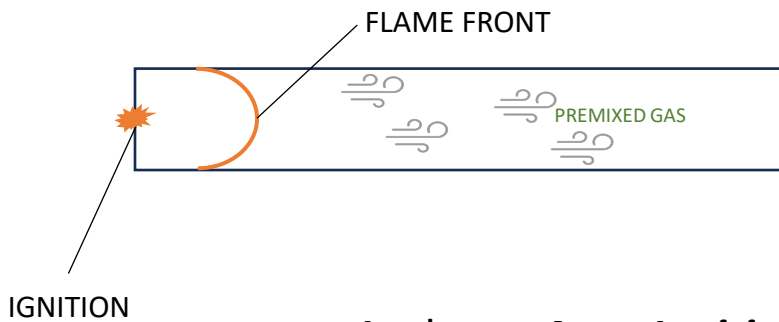
Gas Explosion

Combustion

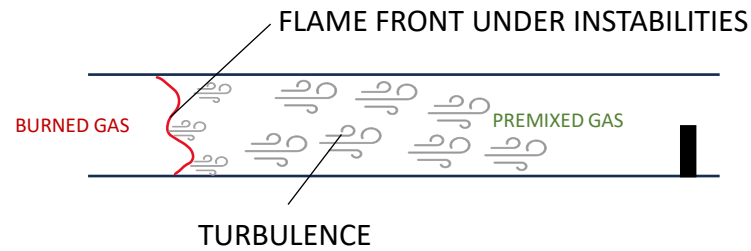


Process : Deflagration Detonation Transition (DDT)

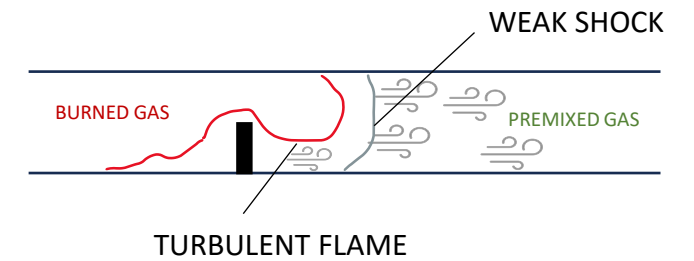
1. Phase: **Laminar Flame**



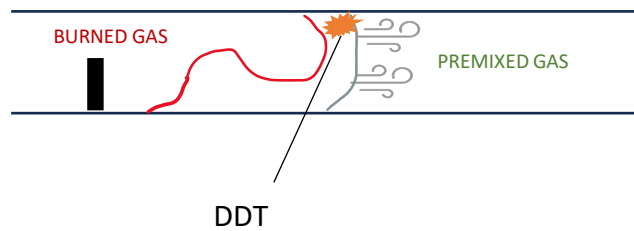
2. Phase: **Wrinkled Flame**



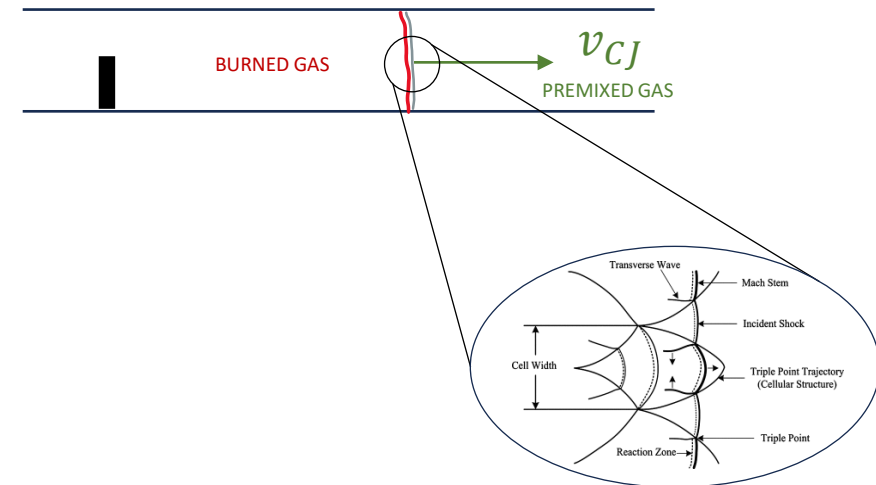
3. Phase: **Turbulent Flame Brush**



4. phase: **Auto-Ignition (DDT)**



5. phase: **Freely propagating Detonation Wave**

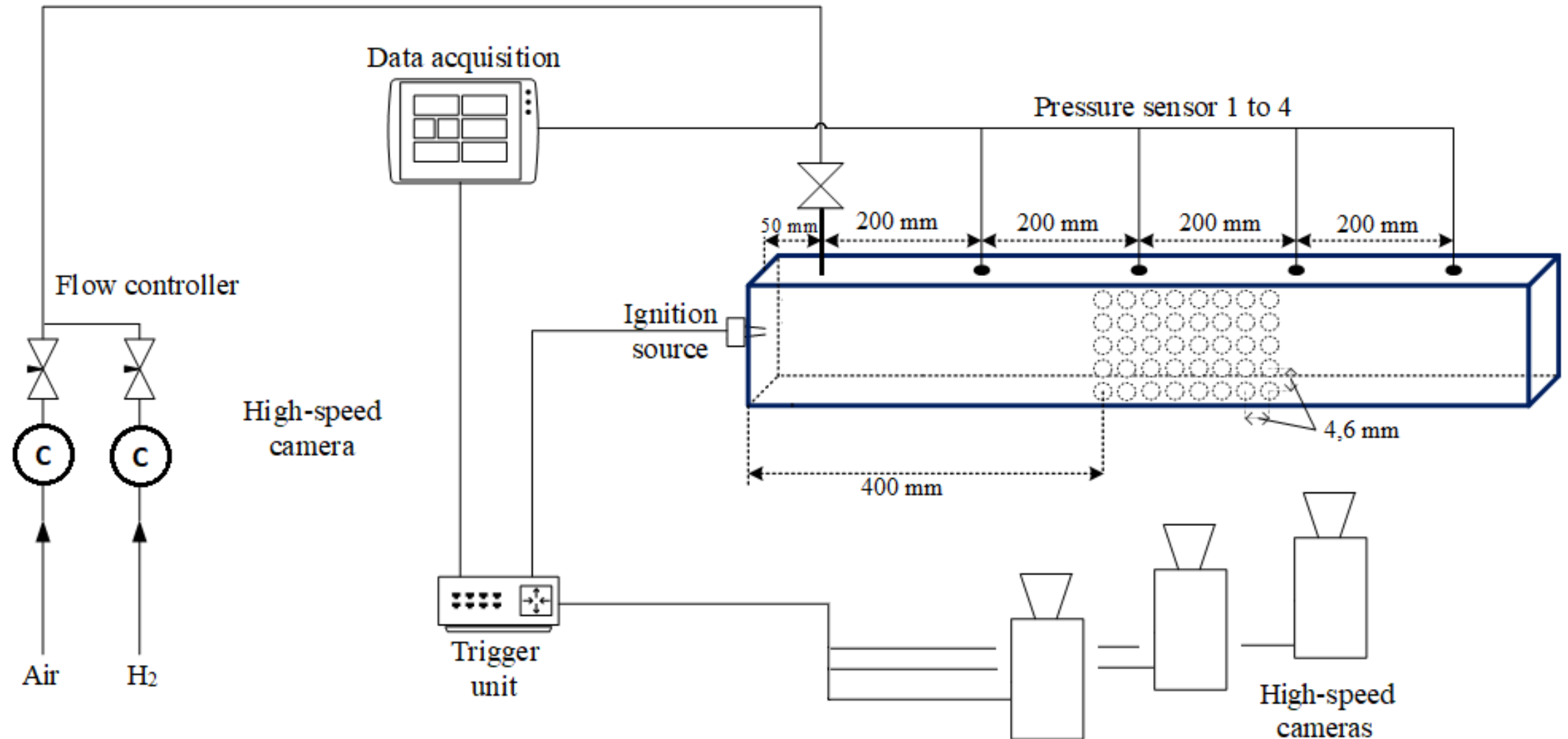


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Explosion Experiments

SMALL SCALE

1m Explosion Channel with Obstructions







Ref: Mathias Henriksen

4

Explosion Modeling

Numerical Model

- The solver *blastXiFoam* developed on the OpenFOAM platform by Synthetic Applied Technologies is an extension of the standard OpenFOAM *XiFoam* solver
- **Flame-wrinkling combustion model**
- **k-omega SST** turbulence model with wall functions
- **HLLC Riemann solver** is used to calculate numerical fluxes (DENSITY BASED SOLVER)



A. V. Gaathaug, K. Vågsæther, and D. Bjerketvedt, 'Experimental and numerical investigation of DDT in hydrogen–Air behind a single obstacle', *Int. J. Hydrog. Energy* (2012)

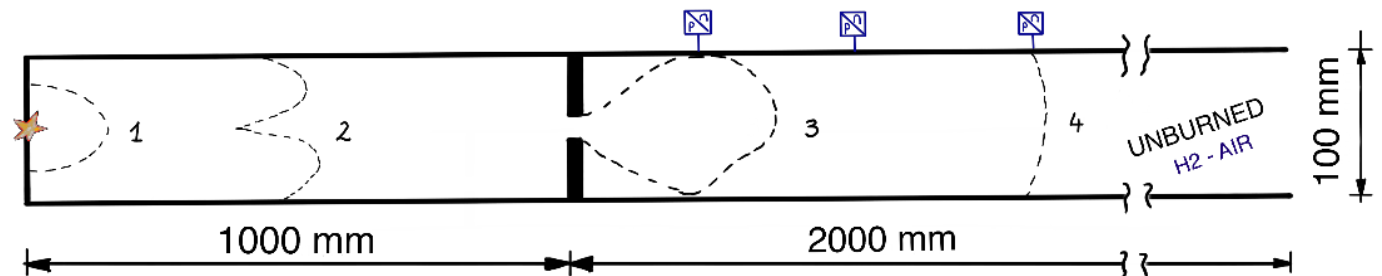
1. CASE

Model Validation

Numerical Setup

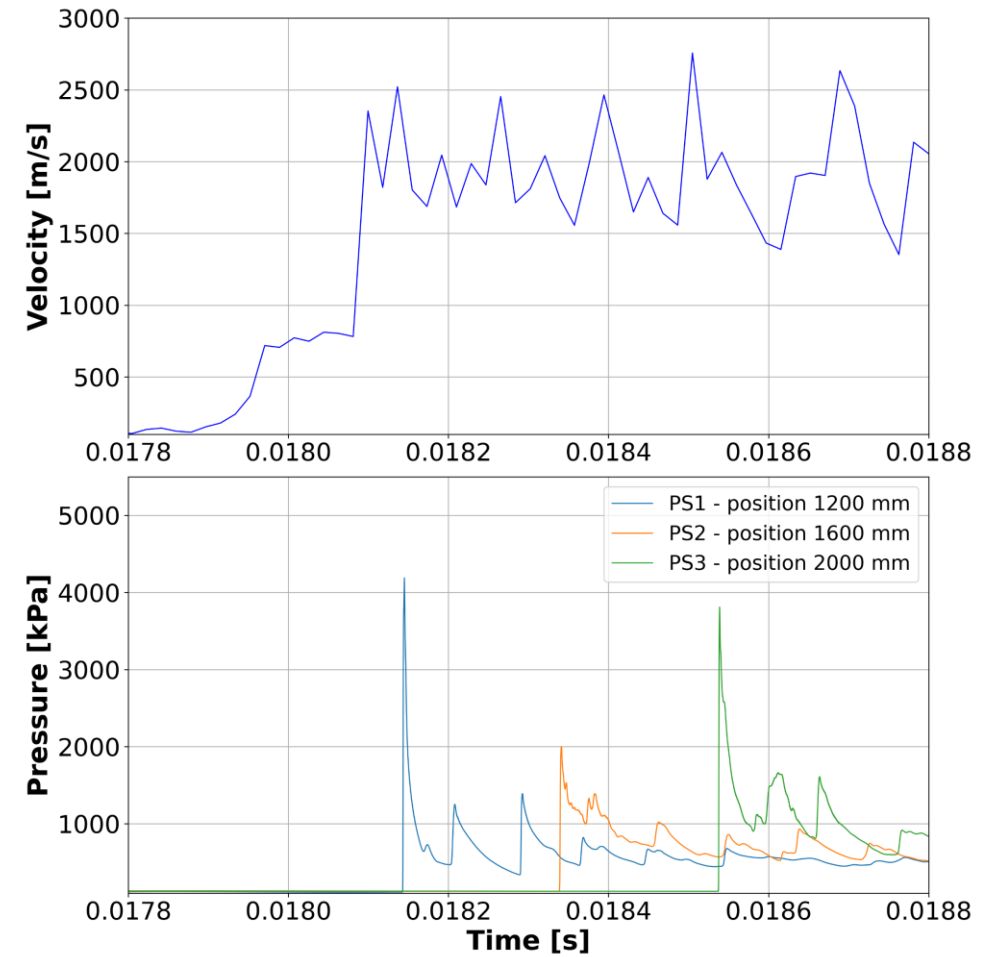
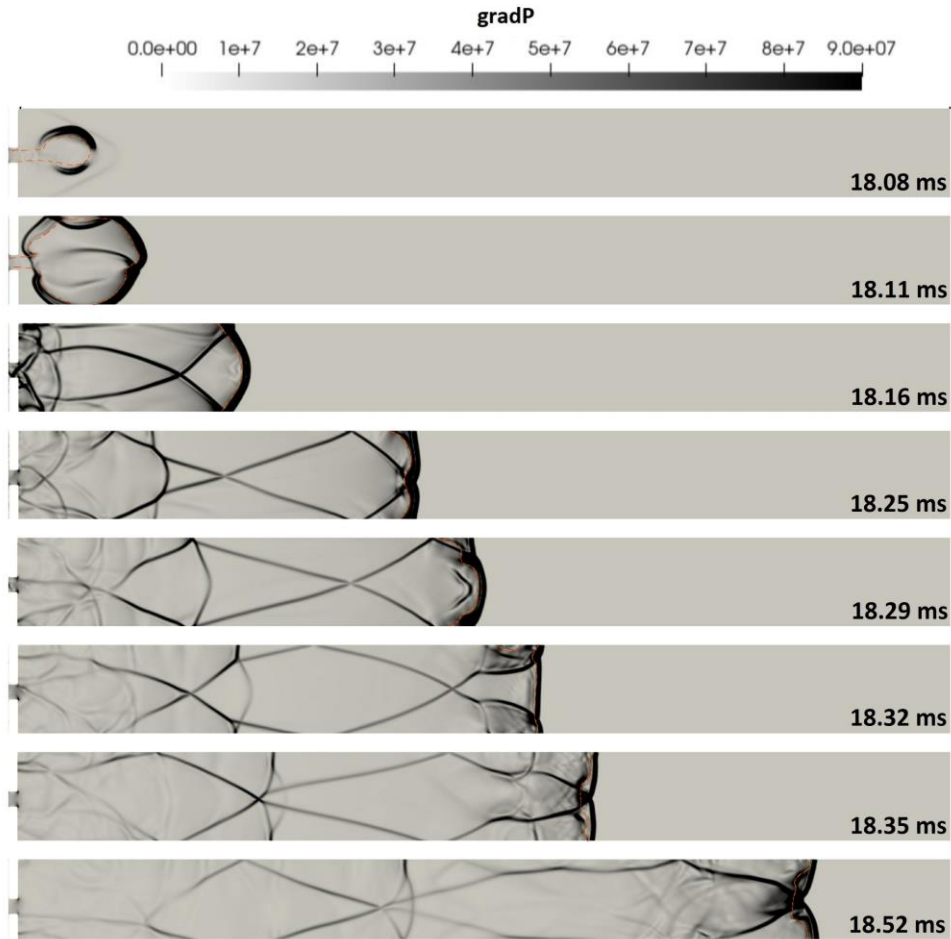
- The gas mixture → homogeneous blend of hydrogen and air with a hydrogen concentration of 35%
- 3 m long channel with a 0.1 x 0.1 m² square cross-section, where one end was closed, while a single obstacle was placed 1m from the close end (creating an 84% blocked ratio)
- The resolution of the 2D mesh is 1 mm per square cell, which comprises **299 160** orthogonal hexahedral elements with an aspect ratio of 1
- The thermophysical and transport properties of the gas mixture were obtained using the open-source code *mech2Foam* developed by Mathias Henriksen

Open  FOAM



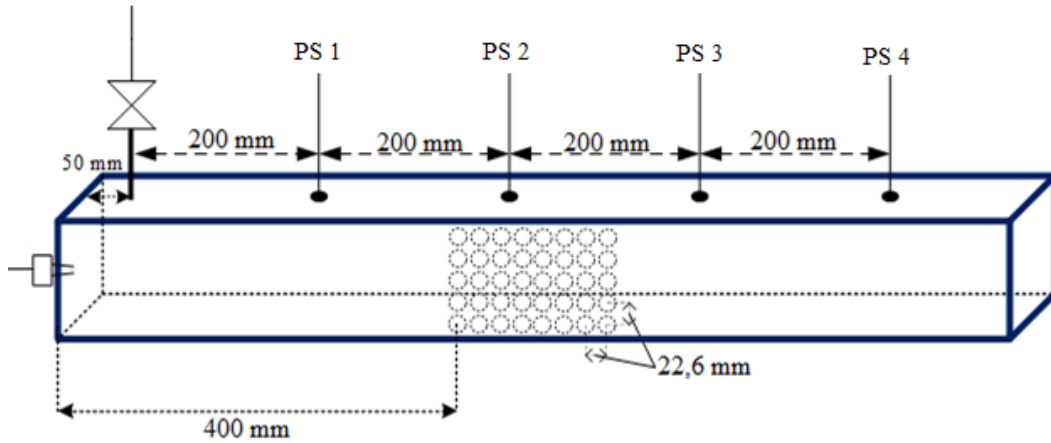
Experimental/Numerical configuration (the change from laminar to turbulent deflagration occurs in Regions 1-3, while detonation occurs in Region 4)

Results - after the obstacle

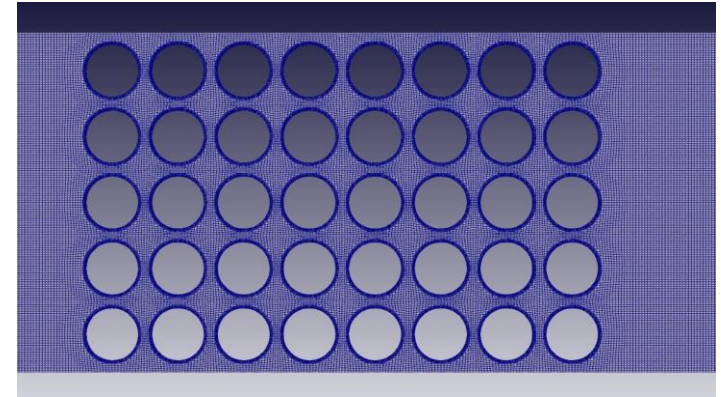


2. CASE

BLIND-PREDICTION

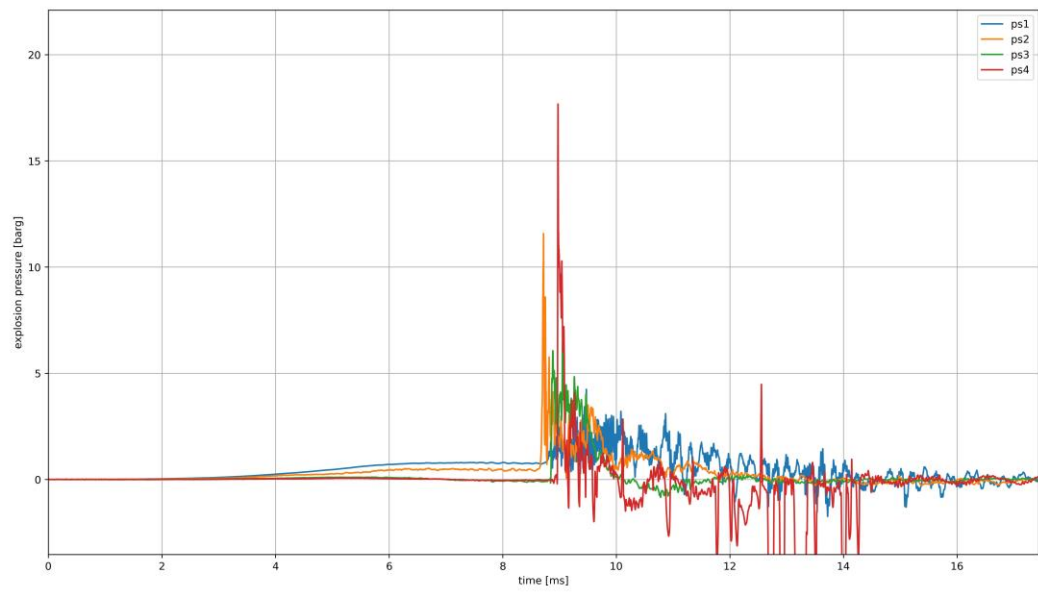


Filling time: 300 s
 H2 vol%: 32%
 H2 mass: 2.7 g
 AIR mass: 83.3 g

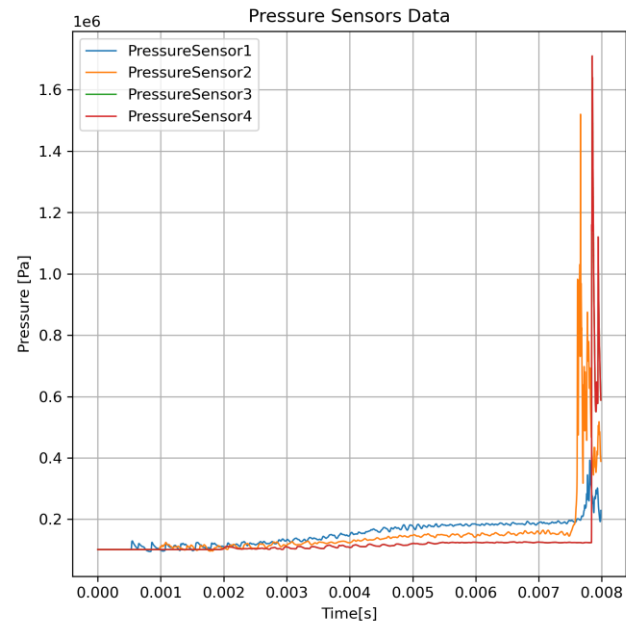


Mesh: 165 974 cells (2D)
 Numerical Setup: same as 1. CASE
 Simulation Time: 6 core → 23h

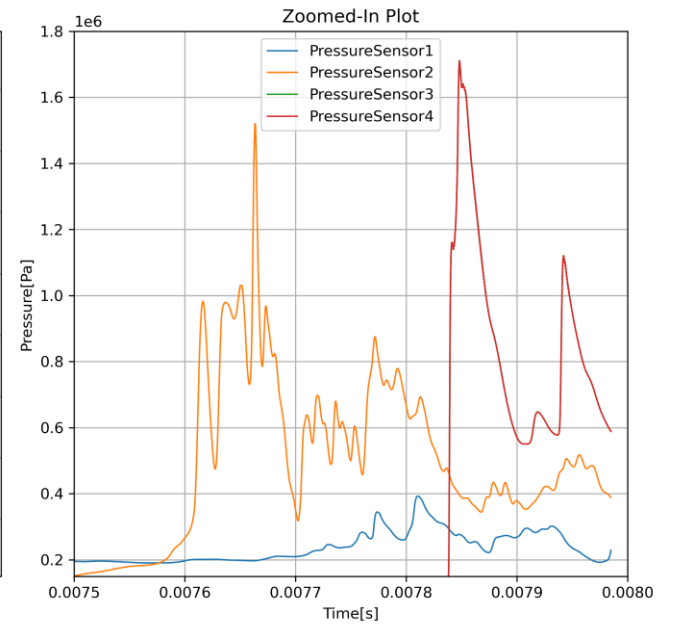
	Concentration	max PS 1 [barg]	max PS 2 [barg]	max PS 3 [barg]	max PS 4 [barg]
Experiment	1.129	4.2	11.6	6.9	17.7
Simulation	1.1	2.9	14.3	/	16.1



Experiment Data



Simulation Data



5

Conclusion

& FUTURE RESEARCH DIRECTION

CONCLUSIONS:

- **blastXiFoam** solver on the OpenFOAM platform to study flame dynamics
- Flame acceleration and Deflagration to Detonation Transition (**DDT**)
- Premix homogeneous hydrogen-air mixture within channel with an obstacle
- Benchmarked against two setups (CASE 1: model validation; CASE 2: blind prediction)
- **Shock/Flame Front interaction** → **Local "explosions"** that **lead** to transition to detonation
- Good **agreement** with **experiments** regarding **overpressure** and flame front **velocity** predictions
- **DDT** occurs in the numerical analysis
- **Understanding modeling of DDT in blastFOAM (reaction rate model)**

FUTURE WORK

- Experimental Research: addressing the stochastic nature of DDT through 180 random concentration experiments ranging from 24vol% to 40vol% of H₂ → hot-spot initiation probability, DDT probability, flame propagation inside obstructed geometry and channel mapping
- Numerical Research: Understanding reaction rate modeling in blastXiFoam and implementing new approaches to calculate turbulent flame speed ($Xi = S_{turbulent} / S_{laminar}$)

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Thank you!



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