

Investigation of non-uniform Hydrogen / Air mixture flame acceleration and transition to detonation

Reza Khodadadi Azadboni^a, Ali Heidari^a, and Jennifer X. Wen^{b,*}

^aFire, Explosion and Fluid Dynamics Research Team, School of Mechanical & Automotive Engineering,
Kingston University London, SW15 3DW, UK

^bWarwick FIRE, School of Engineering, University of Warwick, Coventry, CV4 7AL, UK

***Jennifer.Wen@Warwick.ac.uk**



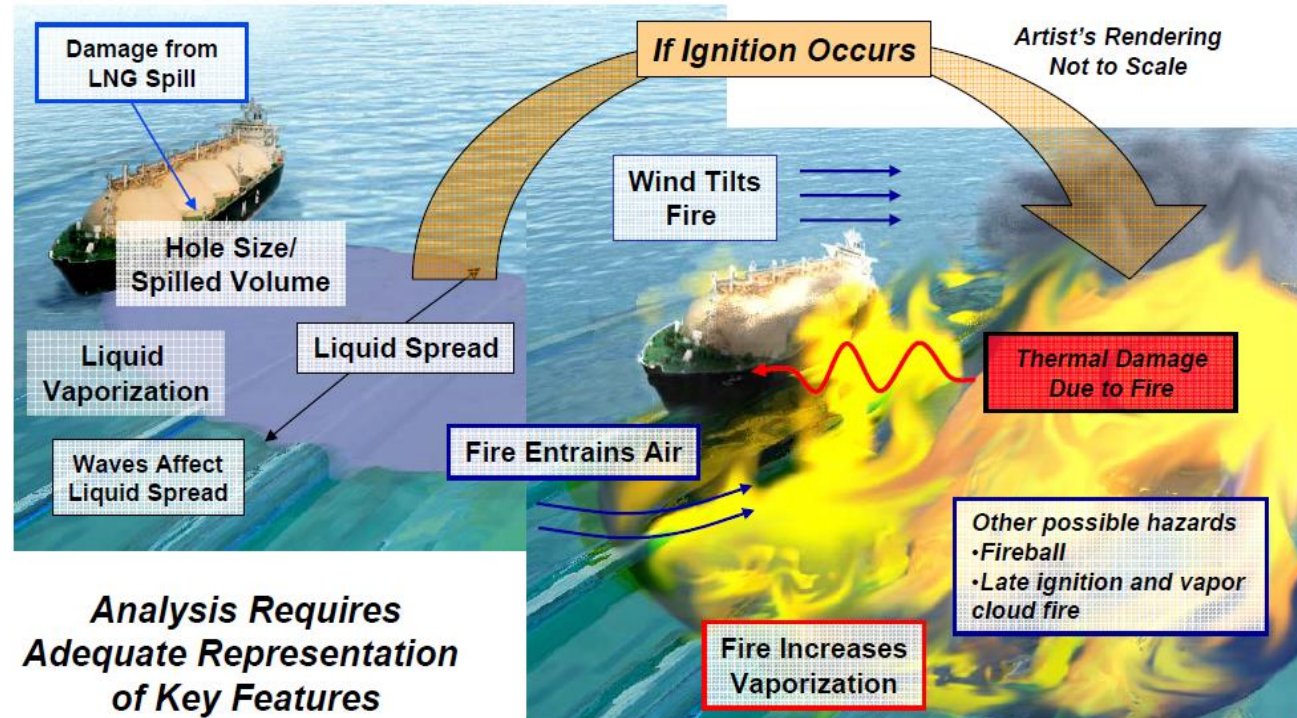
Contents

- **Introduction**
- **Problem description**
- **CFD approach**
- **Results**
- **Conclusion**

Problem Description

SafeLNG:>

Hazards of Liquid Fuel shipping



- Rollover
- Fuel cascade
- Spill and dispersion
- Flashing fuel jet fires
- pool fires

- Large scale vapour cloud explosions

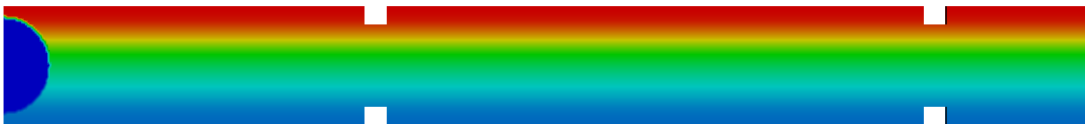
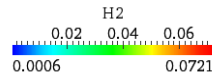
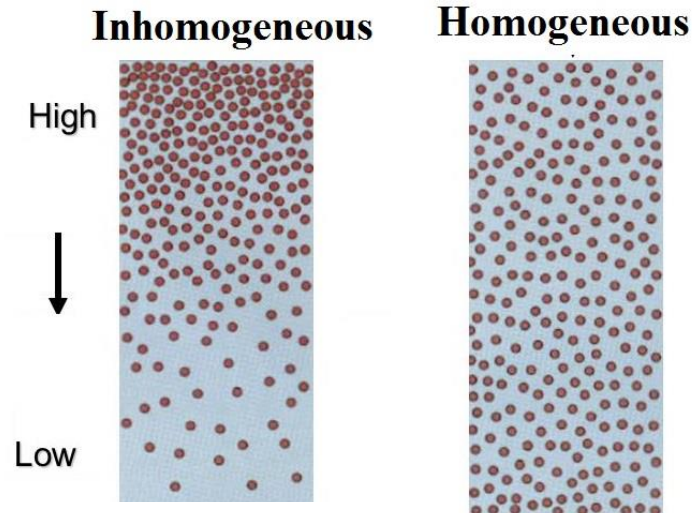
➡ Flame acceleration and interaction to obstacles and transition to detonation

DDT experiment by Gexcon



Introduction

Concentration Gradient

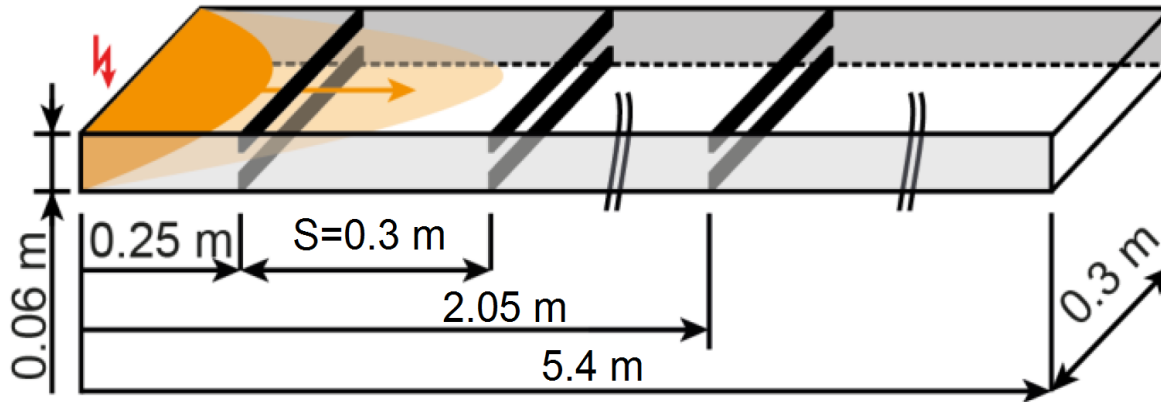


- ❑ Effect of Concentration gradient in DDT
- ❑ Effects of Blockage ratio in DDT

CFD Approach

- The density-based code developed under OpenFOAM solves the unsteady, compressible Navier-Stokes equation with single step Arrhenius chemistry.
- Cantera for the thermodynamic properties
- Harten–Lax–van Leer–Contact (HLLC) for accurate shock detonation capturing
- High capability of shock and detonation cell capturing
- Implemented Richtmyer Meshkov instabilities and Baroclinic vorticity effects in the solver
- Adaptive Refinement Mesh (AMR) method

The computational model



2-D calculations
Closed channel of 0.3 (W) 5.4 (L) 0.06 (H) (m)

Ignition:

Patch cells within a radius of 10 mm around the point of ignition ($x=0$, $y=0.03\text{m}$) to the burnt state (isobaric, adiabatic burnt mixture).

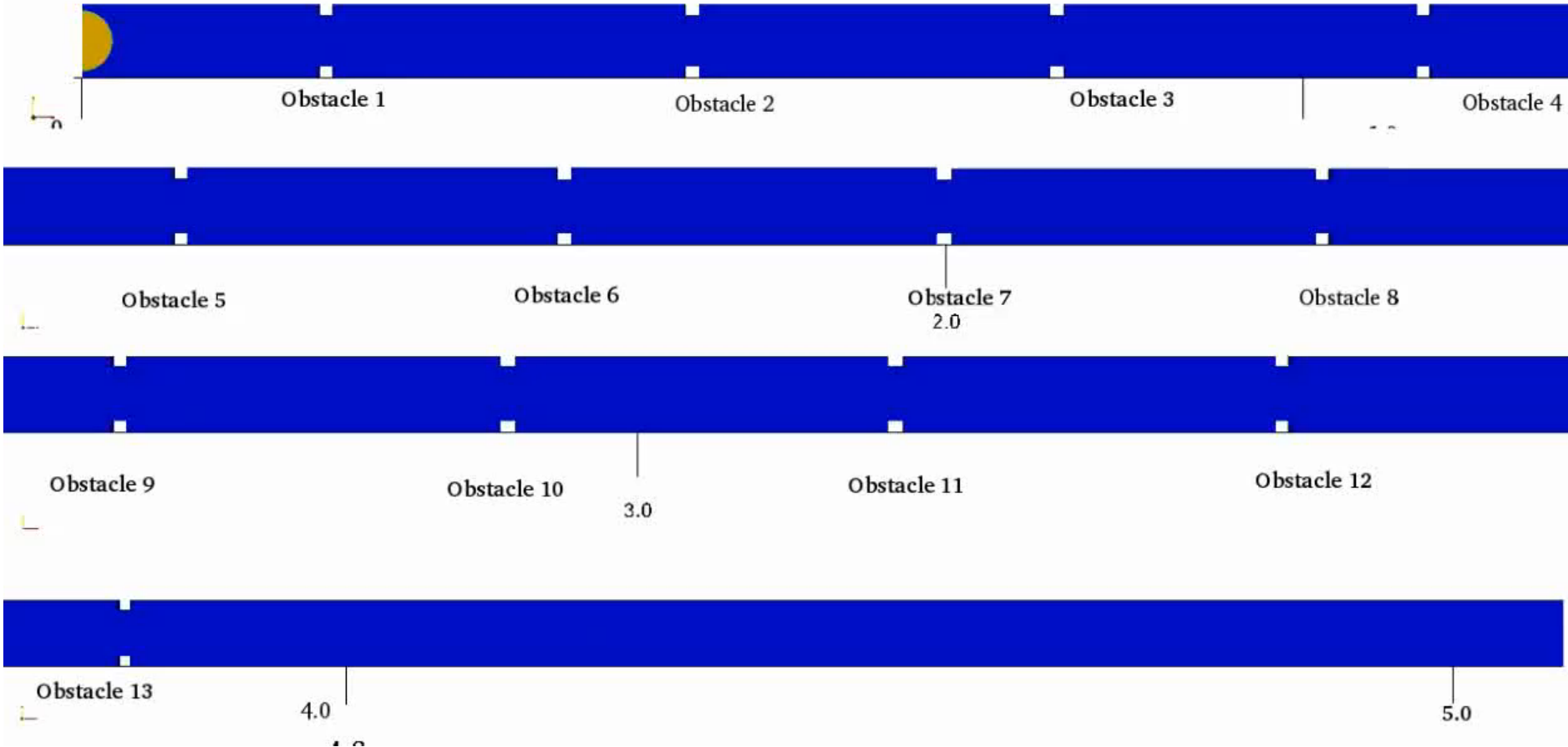
Boeck LR, Katzy P, Hasslberger J, Kink A & Sattelmayer T. (online 03/2016). The "GraVent DDT Database". Shock Waves, doi:10.1007/s00193-016-0629-0

Inhomogeneous 30% H₂/Air mixture BR60

Temperature Fields

Time: 0.000000 (Sec)

T (K)

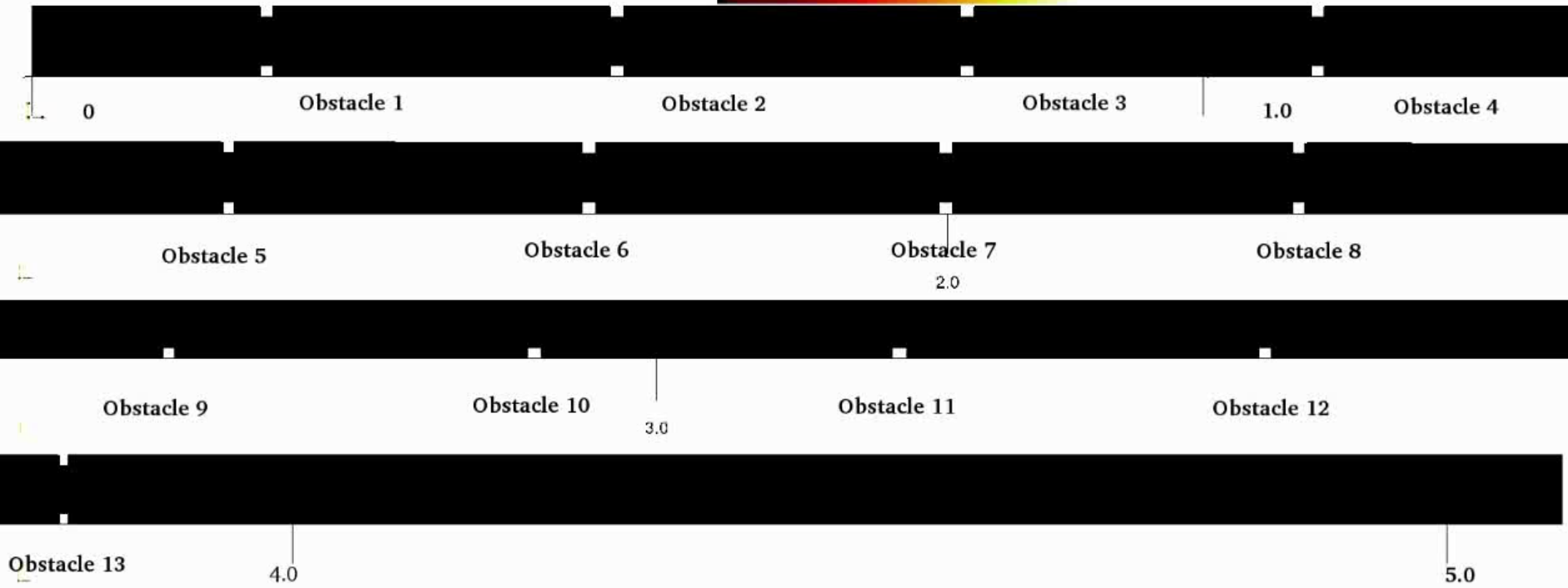


Inhomogeneous 30% H₂/Air mixture BR30

Pressure Fields

Time: 0.000000 (Sec)

p (pa)
1.013e+05 4e+5 8e+5 1.2e+6 1.6e+6 2.100e+06



Effects of Concentration gradient

60 % Blockage ratio

30 % H₂

Homogenous

Inhomogeneous

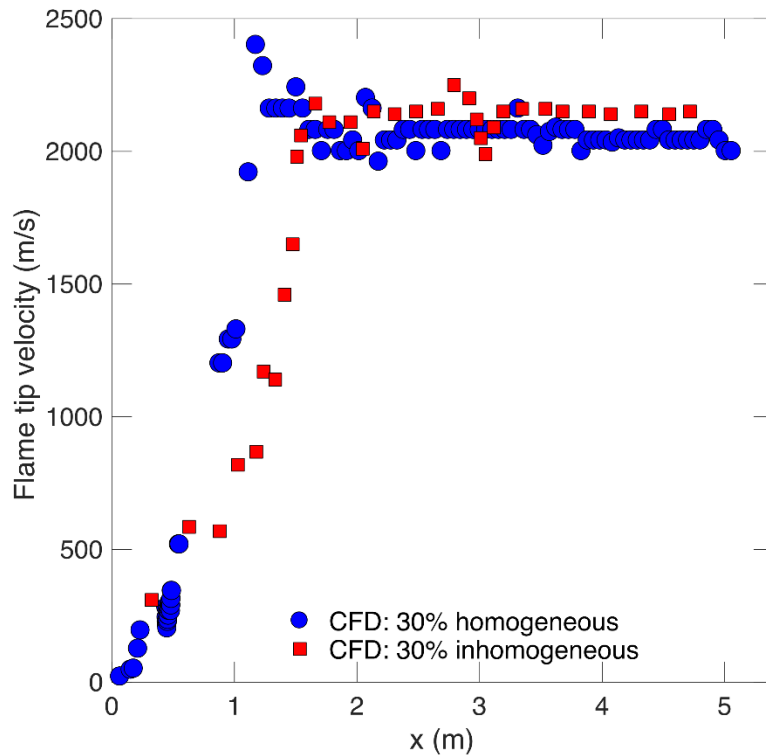
20 % H₂

Homogenous

Inhomogeneous

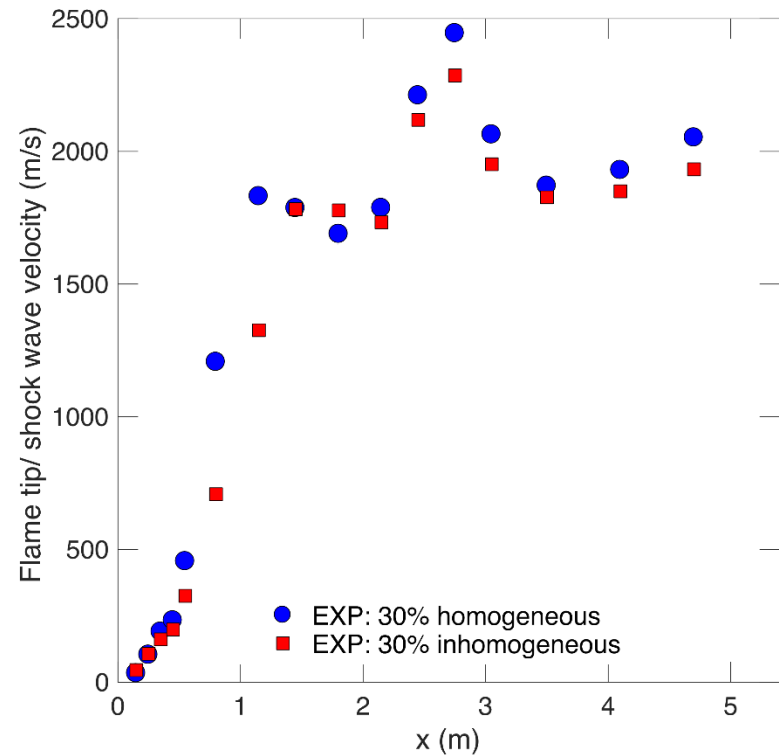
30% H₂/Air mixture BR60%

- Comparison between homogenous and inhomogeneous cases



Homogenous mixture

Inhomogeneous mixture

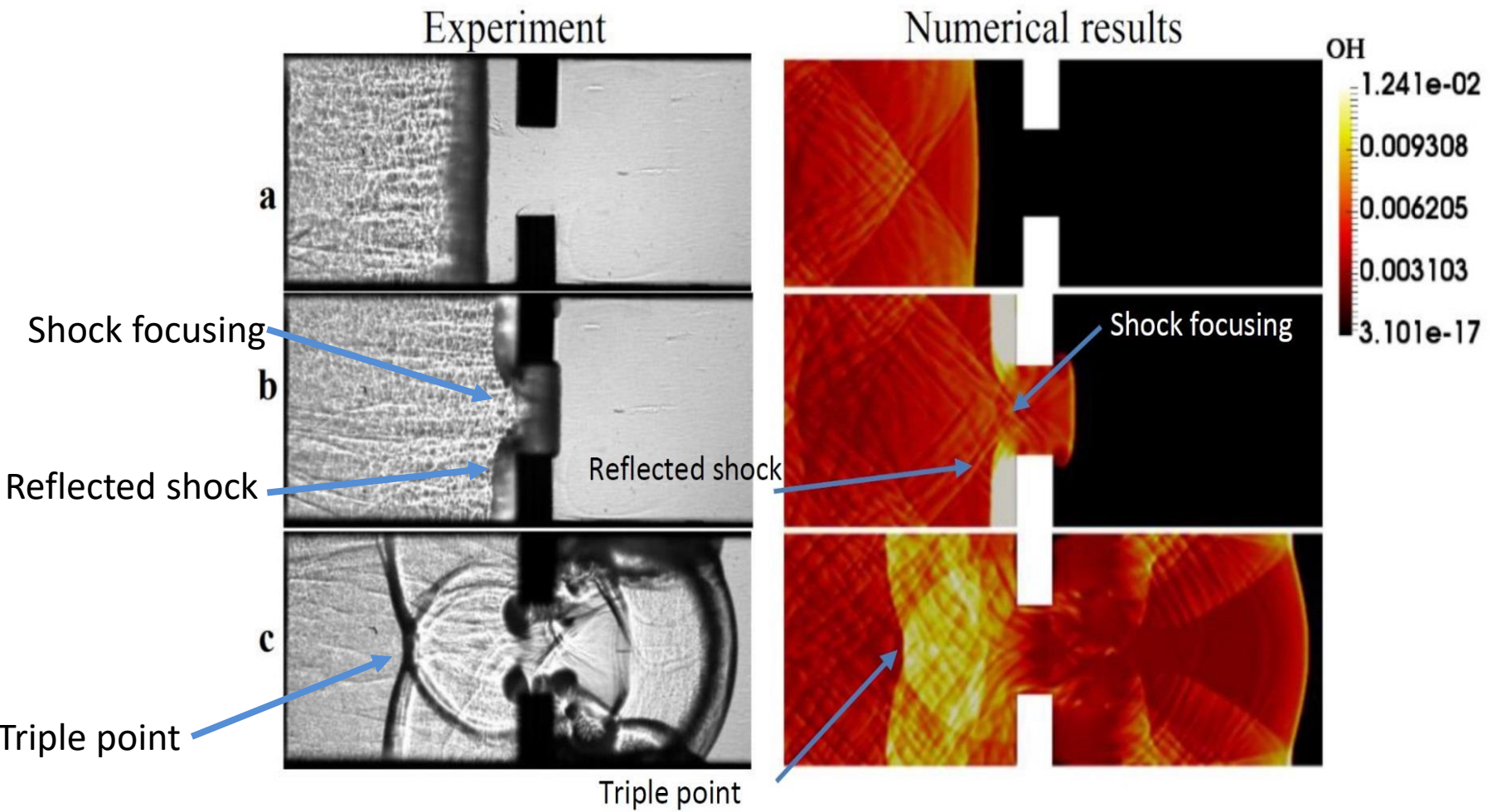


DDT happened at x=1.09

DDT happened at x=1.45 m

Homogenous 30% H₂/Air mixture BR60%

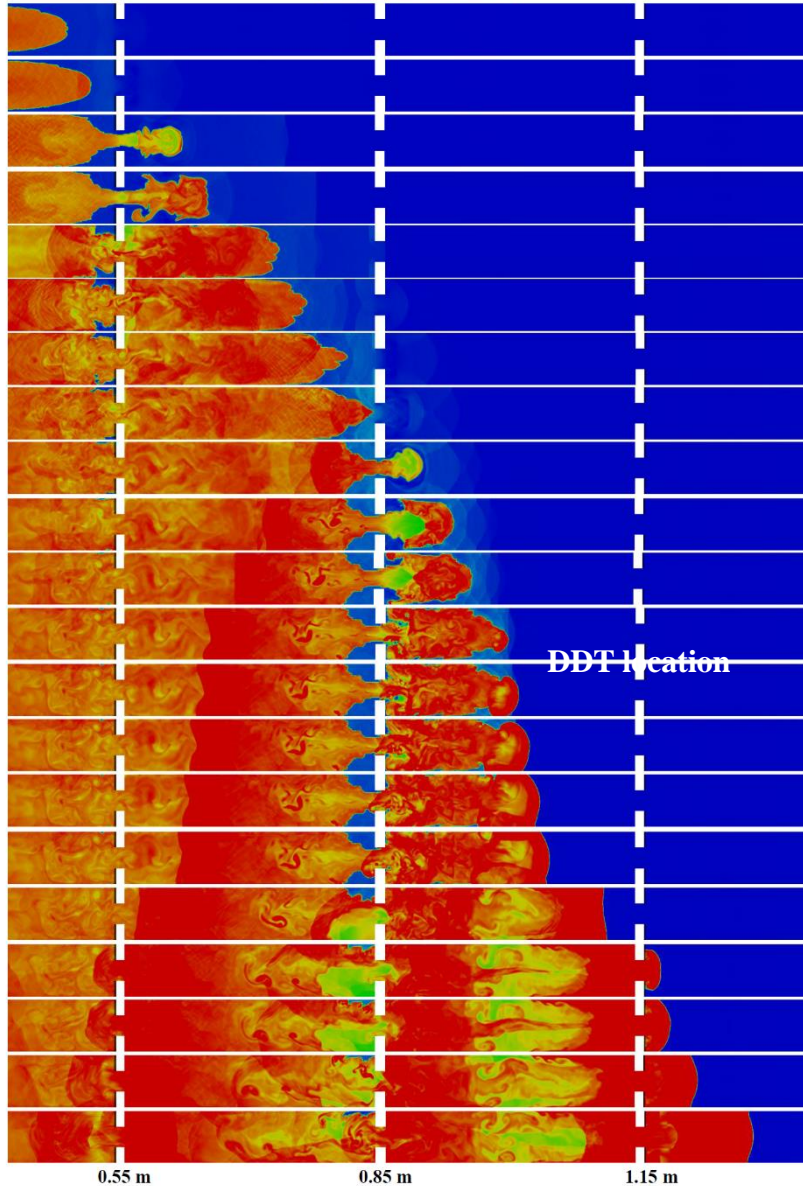
Qualitative comparison between CFD and Experiment



Homogeneous 30% H₂/Air mixture BR60

Temperature (K)

2.930e+02 920 1547 2173 2.800e+03

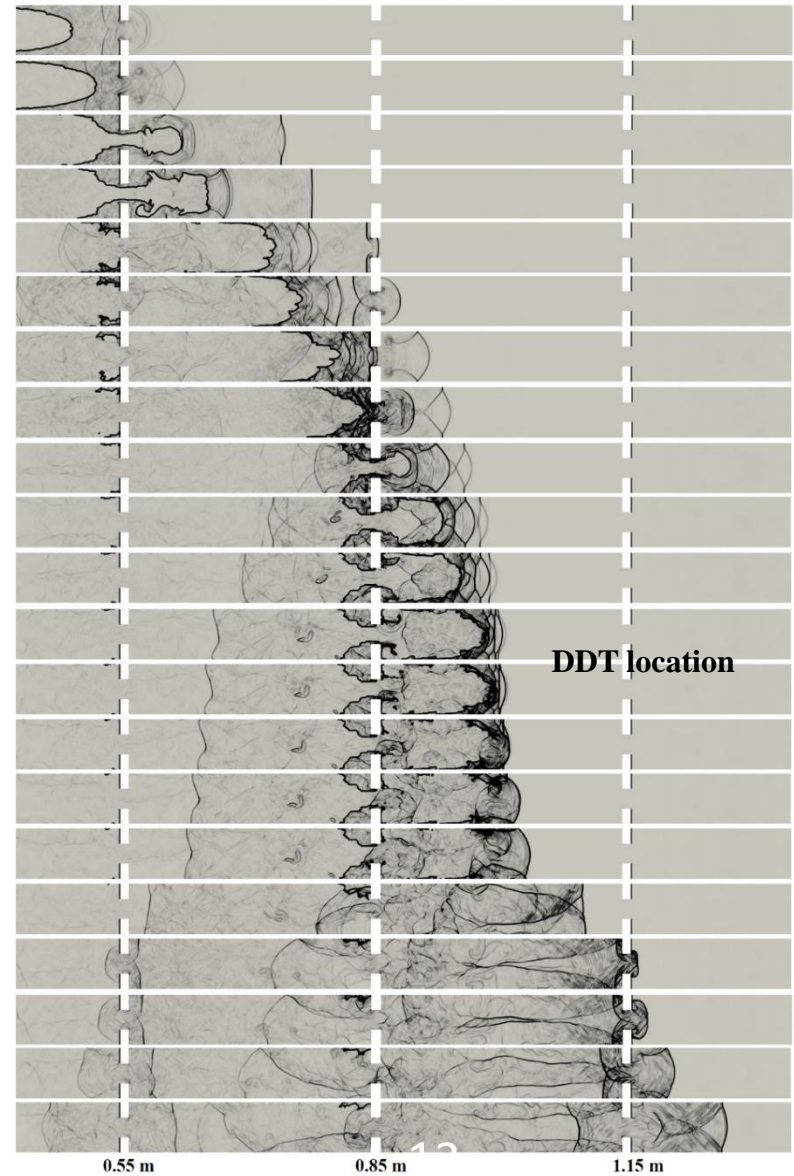


Numerical Schlieren

1.565e-11 119 239 359 4.774e+02

Time (sec)

0.006975
0.007050
0.007280
0.007335
0.007460
0.007500
0.007555
0.007600
0.007645
0.007680
0.007700
0.007720
0.007725
0.007730
0.007735
0.007740
0.007770
0.007800
0.007805
0.007820
0.007850



Time (sec)

0.006975
0.007050
0.007280
0.007335
0.007460
0.007500
0.007555
0.007600
0.007645
0.007680
0.007700
0.007720
0.007725
0.007730
0.007735
0.007740
0.007770
0.007800
0.007805
0.007820
0.007850

Homogeneous 30% H₂/Air mixture BR60

Numerical Schlieren



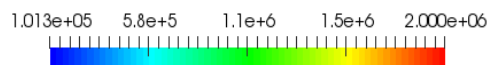
Time: 0.006950 sec

Temperature (K)



Time: 0.006950 sec

Pressure (pa)



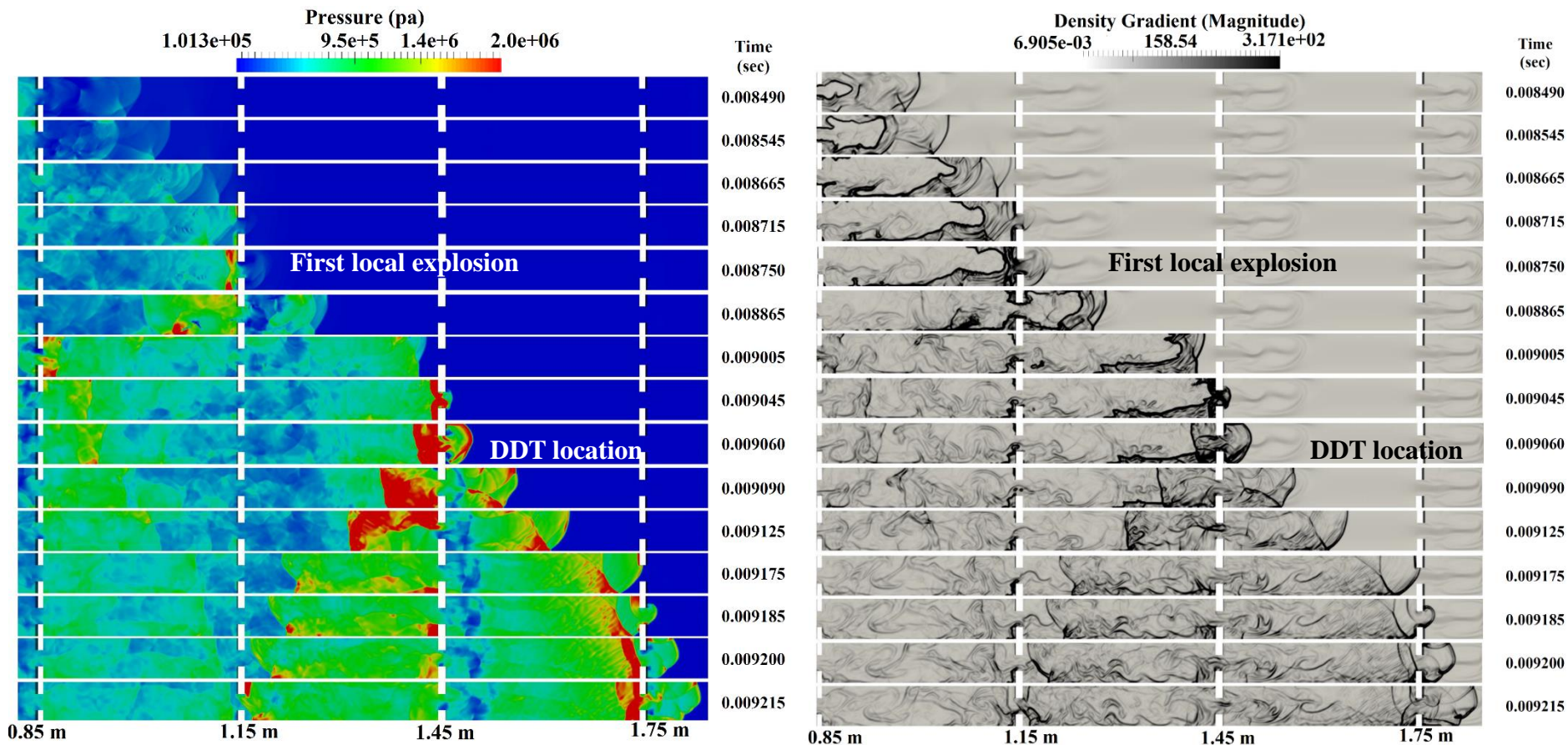
Time: 0.006950 sec

X=0.55m

X=0.85m

X=1.15m

Inhomogeneous 30% H₂/Air mixture BR60



Inhomogeneous 30% H₂/Air mixture BR60

Numerical Schlieren



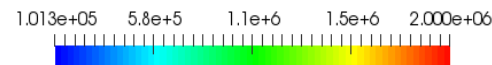
Time: 0.008475 sec

Temperature (K)



Time: 0.008475 sec

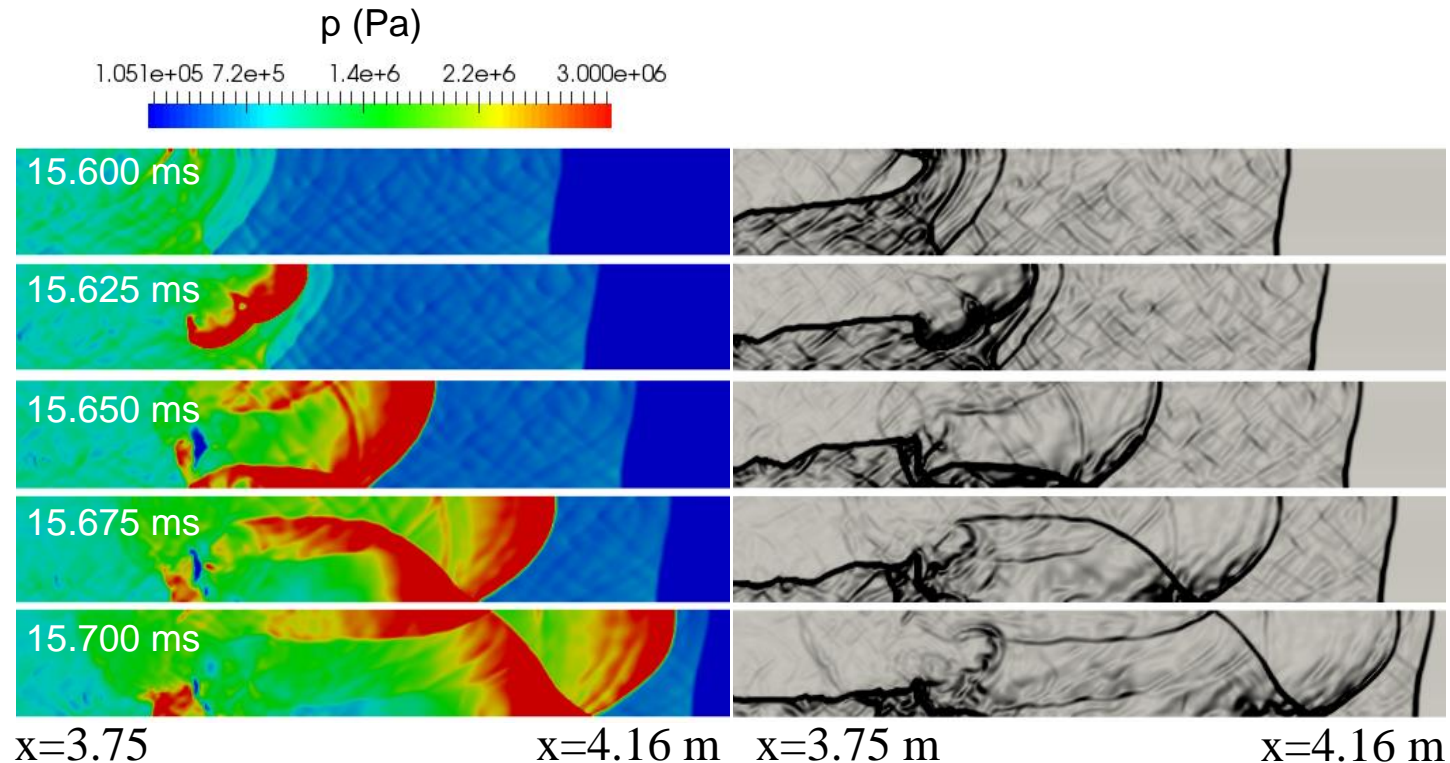
Pressure (pa)



Time: 0.008475 sec

Inhomogeneous 20 % H₂/Air mixture BR60

Transition to detonation



Homogenous mixture

DDT did not happen

Inhomogeneous mixture

DDT happened at x=3.95 m

30 % Blockage ratio

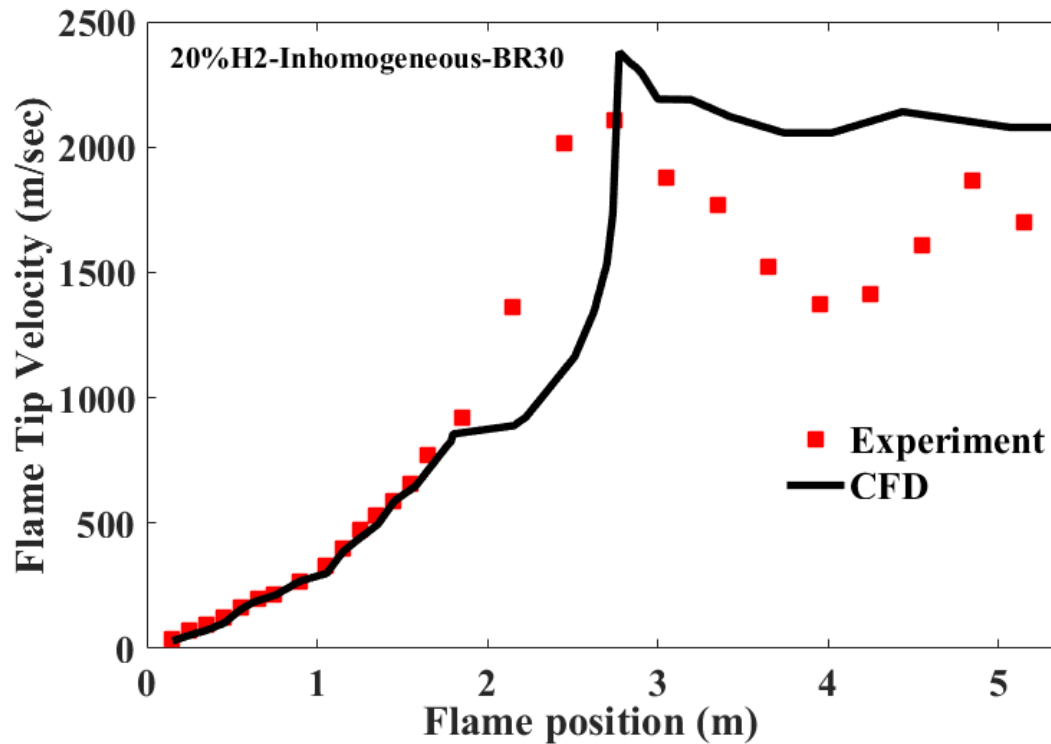
20 % Inhomogeneous H₂/Air

30 % Inhomogeneous H₂/Air

35 % Inhomogeneous H₂/Air

20% H₂/Air mixture BR30%

- Comparison between CFD and Experiment



DDT happened at $x=2.89$ m

20% H₂/Air mixture BR30%

Numerical Schlieren



Time: 0.016540 sec

Pressure



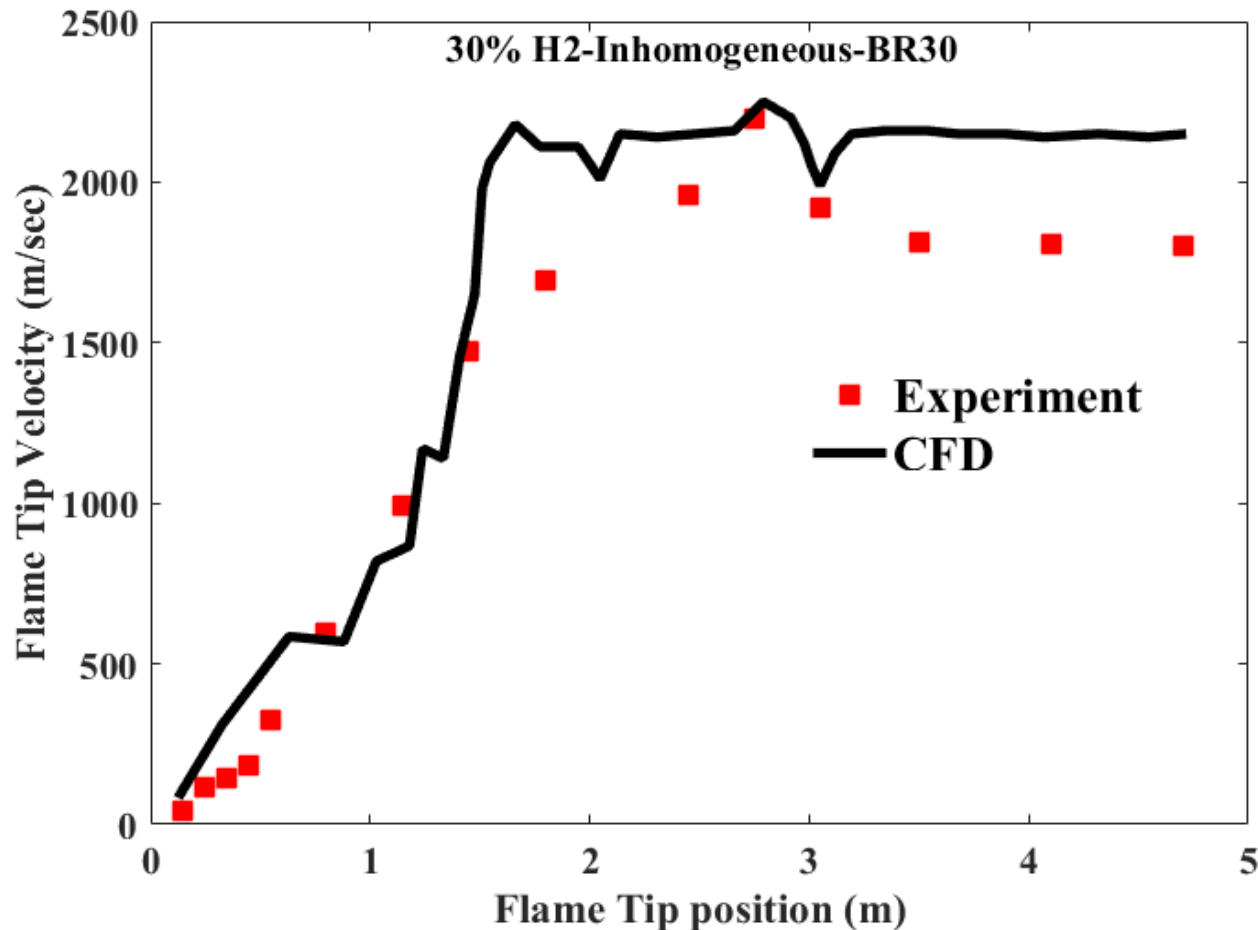
Time: 0.016540 sec

Temperature



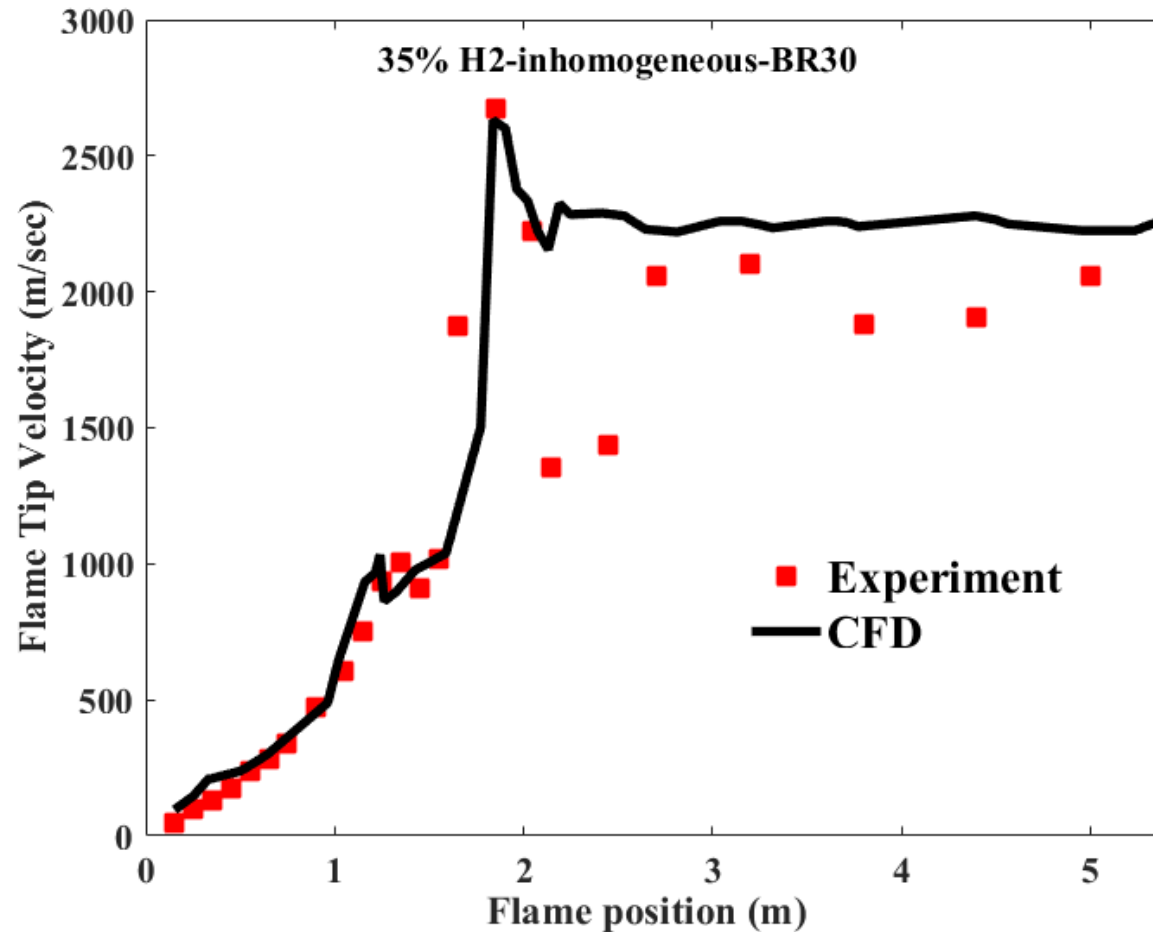
Time: 0.016540 sec

30% H₂/Air mixture BR30% comparison between CFD and Experiment



DDT happened at x=2.05 m

35% H₂/Air mixture BR30% comparison between CFD and Experiment



DDT happened at x=1.8 m

35% H₂/Air mixture BR30%

Numerical Schlieren



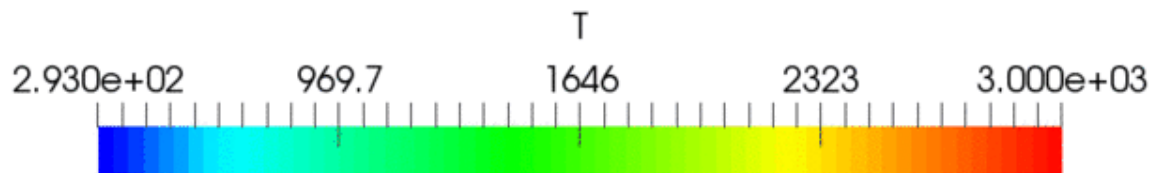
Time: 0.011810 sec

Pressure



Time: 0.011810 sec

Temperature



Higher resolution results

- Max Courant number: 0.3
- Time step = $3.28084e-08$
- **Minimum cell size 10 μm (30 grid points per HRL)**
- Running duration: 60 days, with using 128 cores in cluster

Unobstructed channel

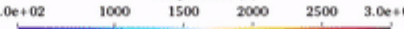
Transition to detonation

Concentration	Homogeneous	Inhomogeneous
20 % H ₂ /Air	No DDT (maximum flame speed = 45 m/sec)	No DDT (maximum flame speed = 200 m/sec)
25 % H ₂ /Air	No DDT (maximum flame speed = 150 m/sec)	DDT at x=4.55 m
30 % H ₂ /Air	No DDT (maximum flame speed = 1000 m/sec)	DDT at x=4.6 m
35 % H ₂ /Air	DDT at x=4.9 m	DDT at x=4.78 m

Time: 20.000000 ms

BR00-Inhomogeneous 35% H2/Air

Temperature (K)



4.60

4.80



Inhomogeneous
H2/Air mixture,
BR00 35%H2,
BR00

Temperature field

4.60

4.80



3.00e-2
2.00e-2
1.00e-2
0.00e+0
-1.00e-2
-2.00e-2
-3.00e-2

5.00

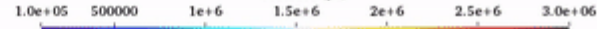
5.20

5.40

Time: 20.000000 ms

BR00-Inhomogeneous 35% H2/Air

Pressure (pa)



4.60

4.80



Pressure field

4.60

4.80



3.00e-2
2.00e-2
1.00e-2
0.00e+0
-1.00e-2
-2.00e-2
-3.00e-2

5.00

5.20

5.40

Conclusion

- The **flame position and flame tip speed** are in reasonably good agreement with the experimental measurements.
- For both homogeneous and inhomogeneous **30% hydrogen** cases, onset of **detonation** occurs within the **obstructed channel section**. The homogeneous mixtures shows slightly faster flame acceleration and earlier DDT.
- For the **20% case**, transition to detonation is observed only for the **inhomogeneous** mixture, where the concentration gradient enables stronger flame acceleration, especially in the **unobstructed channel** section, compared to the homogeneous mixture.
- Increase **in the fuel concentration** was found to increase the FA and faster transition to detonation.
- **High resolution** study captured the **keystone feature** as well as hydrodynamic instabilities, such as **Kelvin Helmholtz and Richtmyer-Meshkov instabilities**.

Acknowledgement



Numerical characterization and simulation of the complex physics underpinning the Safe handling of Liquefied Natural Gas (**SafeLNG**) (2014-2017) is an Innovative Doctoral Programme (IDP) funded by the **Marie Curie Action** of the 7th Framework Programme of the **European Union**.

Thanks for your attention!

Any questions?

