United Kingdom Consortium
on Turbulent Reacting Flows
(UKCTRF)

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Collingwood college

CFD Modelling Of Non-Uniform Hydrogen Flame Propagating Across Obstacles And Inducing Detonation

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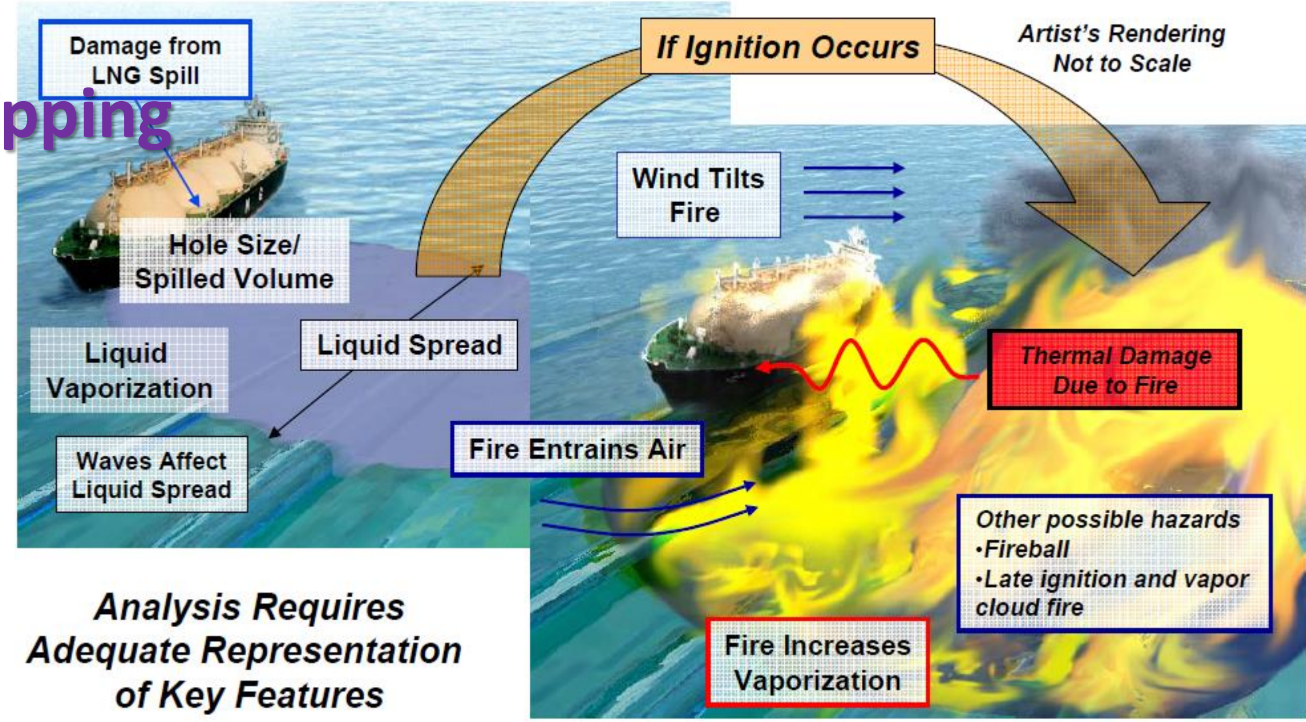
SafeLNG

Contents

Problem Description

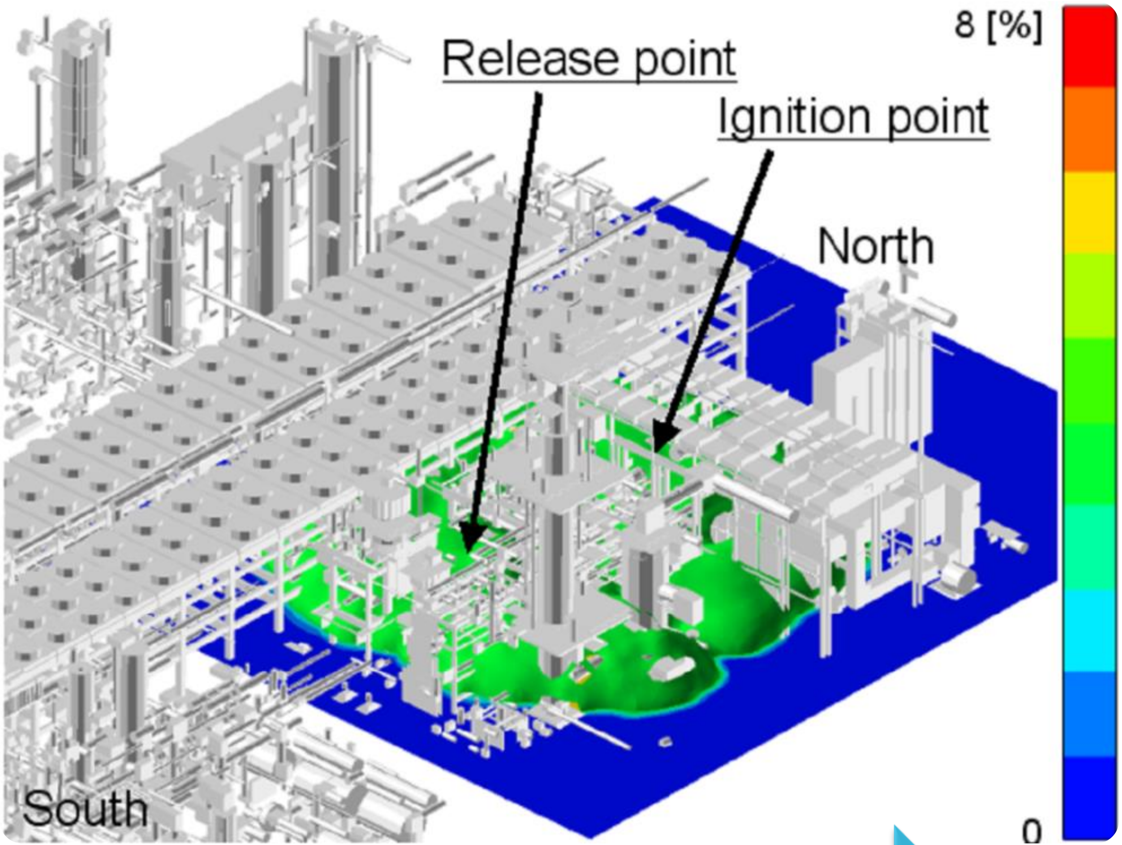
SafeLNG:>
Hazards of LNG shipping

- ❑ Rollover
- ❑ LNG fuel cascade
- ❑ LNG spill and dispersion
- ❑ Flashing LNG jet fires
- ❑ LNG pool fires



- ❑ Large scale LNG **vapour cloud explosions**

Brief Information about deflagration to detonation transition (DDT)



Releasing Flammable Gas → ignition → Explosion

DDT experiment by Gexcon

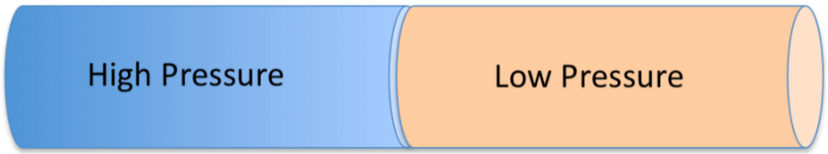
CFD Approach

- The **density-based code** developed under OpenFOAM solves the unsteady, compressible Navier-Stokes equation with single step Arrhenius chemistry.
- **High capability of shock and detonation cell capturing** (it has been verified with analytical solutions such as SOD's problem). (because of density-based approach)
- **Hydrodynamic instabilities** can be captured by this solver (implementing Richtmyer Meshkov instabilities and **Baroclinic vorticites effects** in the solver).
- **Using high order numerical schemes** like **Harten–Lax–van Leer–Contact** (**HLLC**) for accurate shock detonation capturing.
- Using **Adaptive Refinement Mesh (AMR)** method, for having high resolution simulations with less computational costs.

Code Verification

SOD's shock Tube problem

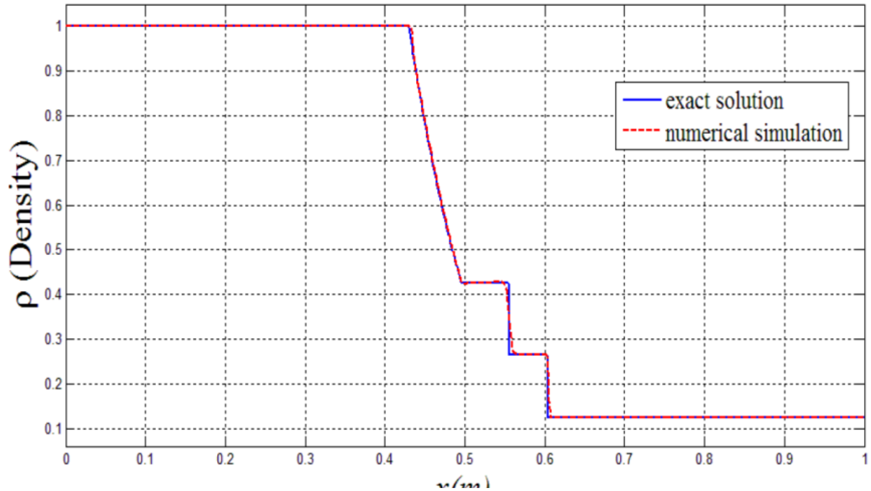
The Sod shock tube is a Riemann problem used as a standard test problem in computational hydrodynamics.

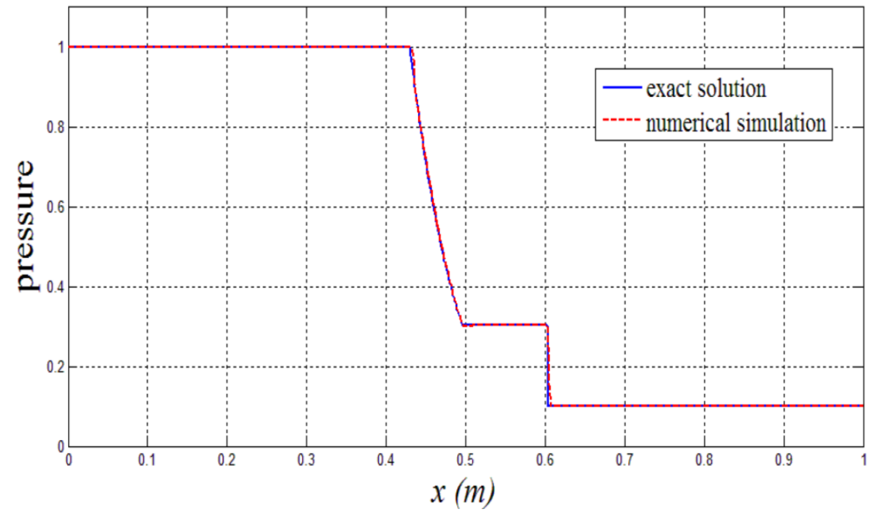


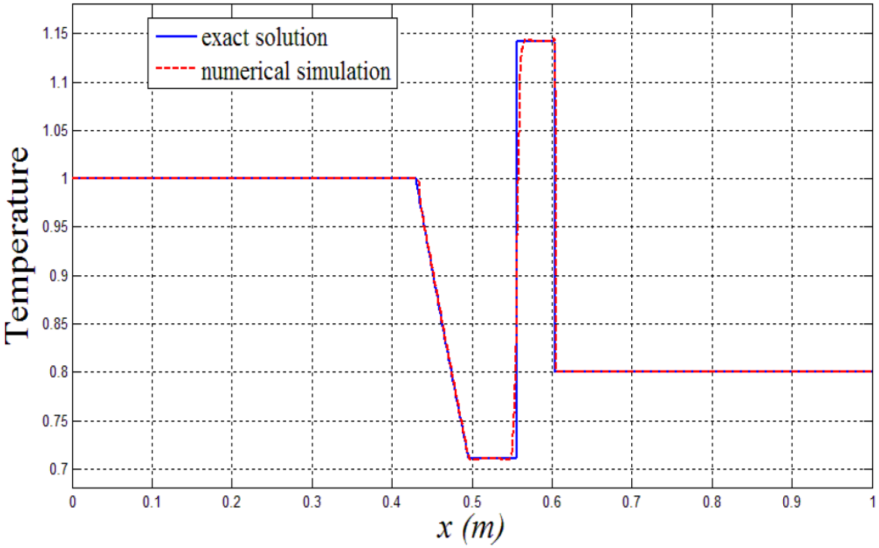
Compartment	$X > 0.5$ Left (driver)	$X < 0.5$ Right (driven)
Pressure	$p_L = 1$	$p_R = 0.1$
Density	$\rho_L = 1$	$\rho_R = 0.125$
Velocity	$U_L = 0$	$U_R = 0$

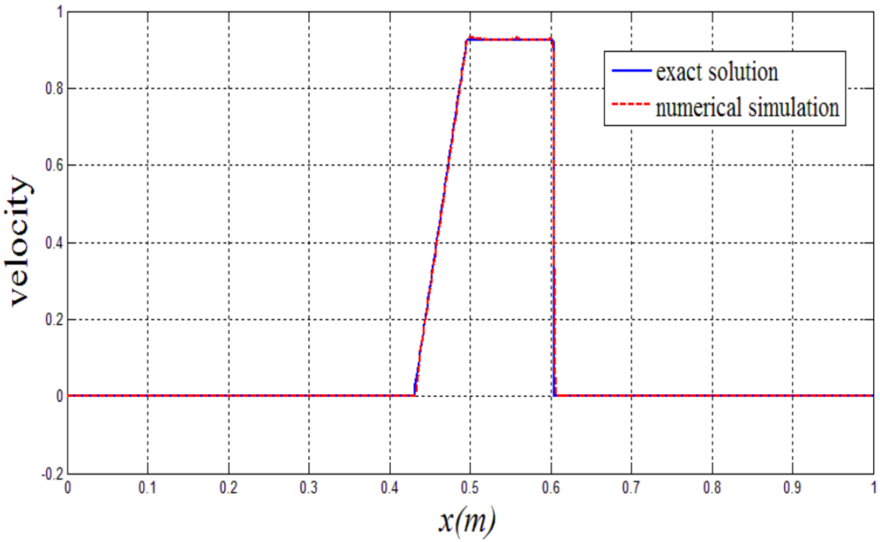
Code Verification

Validation with; Analytical solution

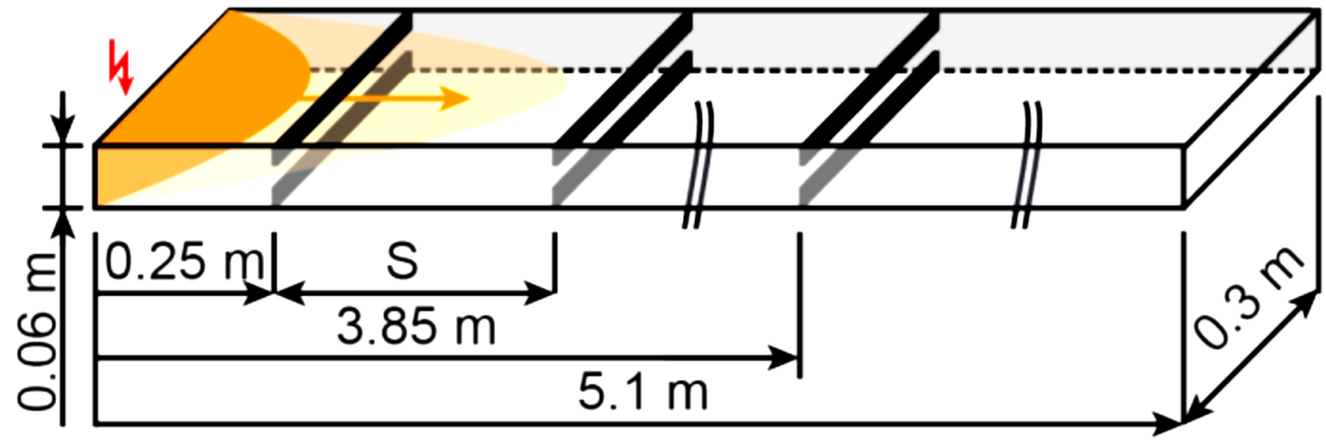








Experimental and Numerical Setup



Ref: L. R. Boeck et al., “The GraVent DDT Database,” in *25th International Colloq. on the Dynamics of Explosions and Reactive Systems (ICDERS)*, Leeds, UK, 2015.

Geometry (2D calculation):

- Channel height: 60 mm
- Channel length: 5.1 m
- (channel width): 300 mm (irrelevant for 2D)
- Smooth walls (no obstacles)
- channel entirely closed

Ignition:

- Weak spark ignition in the experiment
- For simulation, patch cells within a radius of 10 mm around the point of ignition (x=0, y=0.03m) to the burnt state (isobaric, adiabatic burnt mixture).

Numerical setup

Turbulence model:

LES: one eddy equation.

Eric Pomraning and Christopher J. Rutland. "Dynamic One-Equation Nonviscosity Large-Eddy Simulation Model", AIAA Journal, Vol. 40, No. 4 (2002), pp. 689-701

Reaction mechanism:

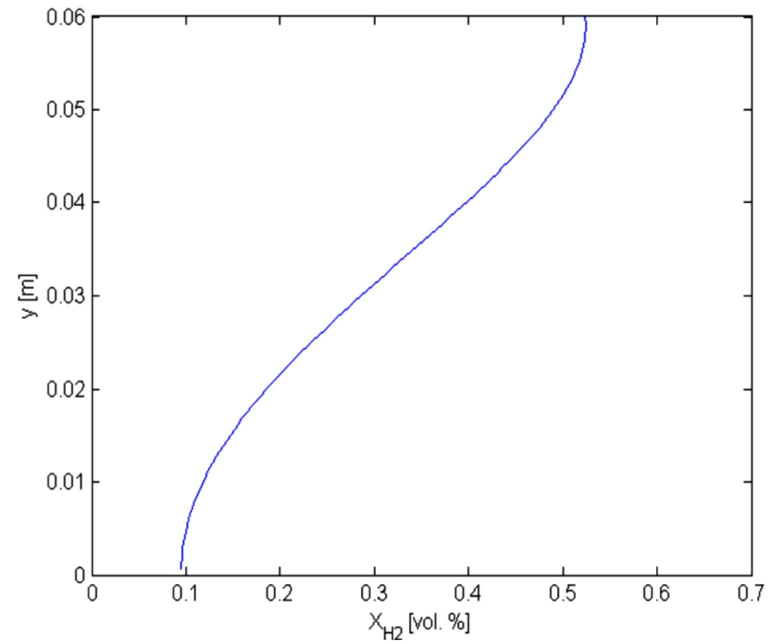
H_2-Air, Single step Arrhenius chemistry of Dr Wang & Jennifer Wen

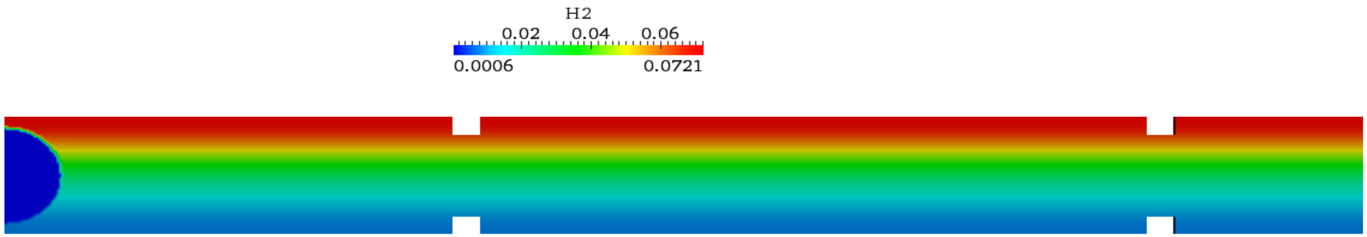
$H_2 + 0.5O_2 \Rightarrow H_2O$

- **Solver: Density Based Reacting**
- **Max Courant Number: 0.3**
- **Time step = 3.28084e-08**
- **Cell Size: dx=dy (cell size)=0.001953125 cm (10 point in HRL)**
- **Using Adaptive refinement Mesh (AMR) method.**
- **Half Reaction Length (HRL) of H_2=0.01927 cm**
- **Harten–Lax–van Leer–Contact (HLLC) 2nd order**
- **OpenMpi, method has been used for parallel**
- **Running Duration: 35 days, with using 128 cores in cluster**

Initial condition for non uniform mixture

Inhomogeneous:
vertical concentration gradient,





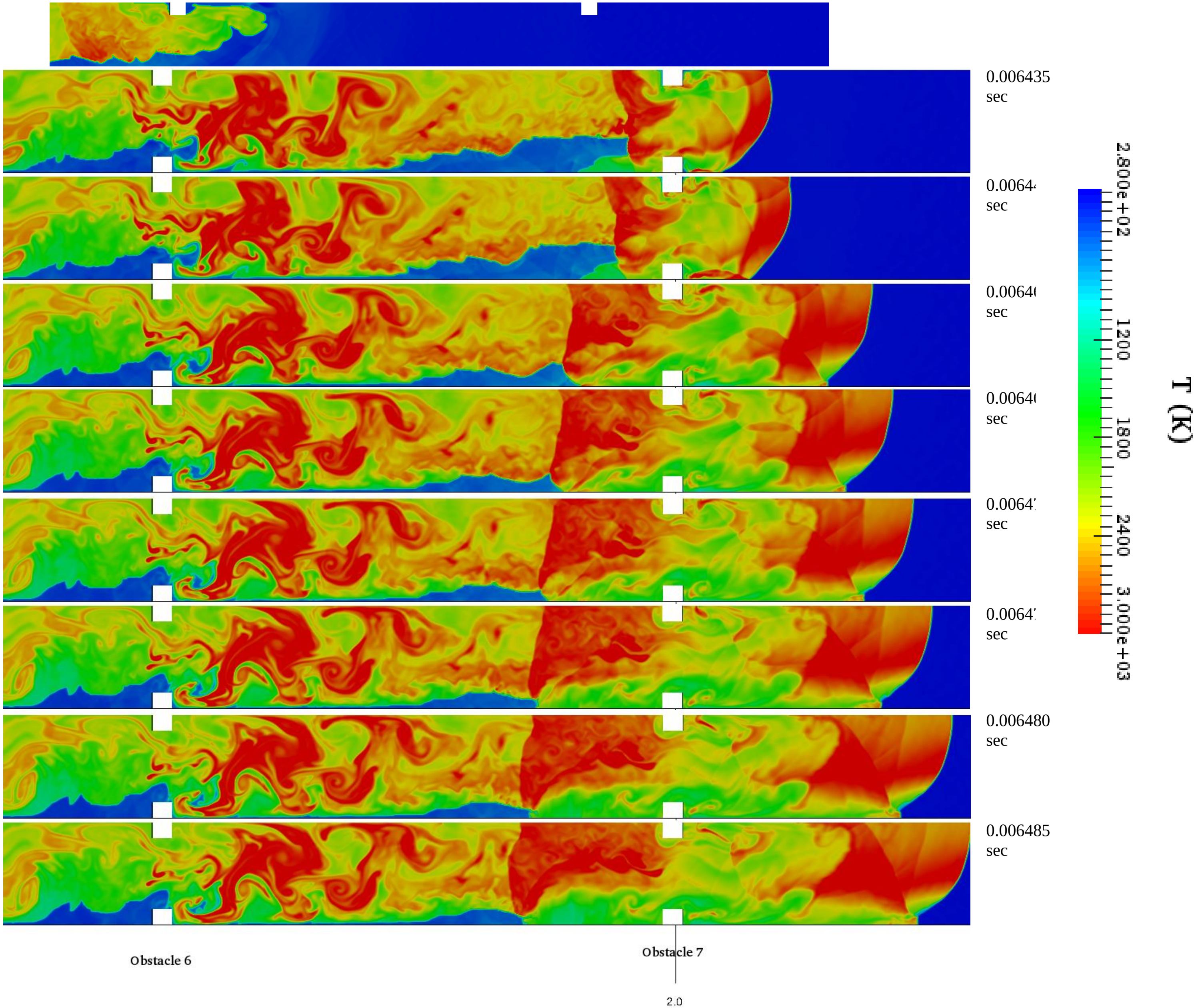
ignition point is assumed as a burned area

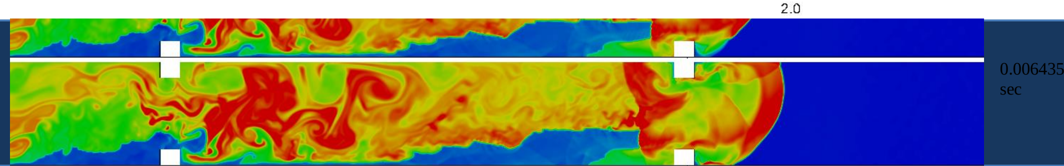
High temperature and combustion product

Results

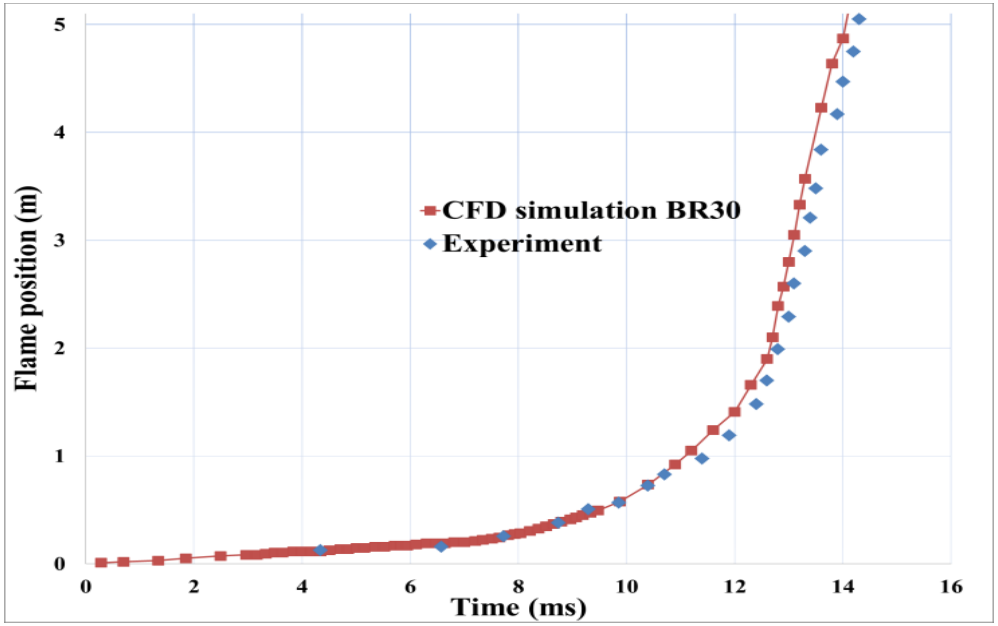
Temperature contours During DDT

average 30% Vol H_2, BR30



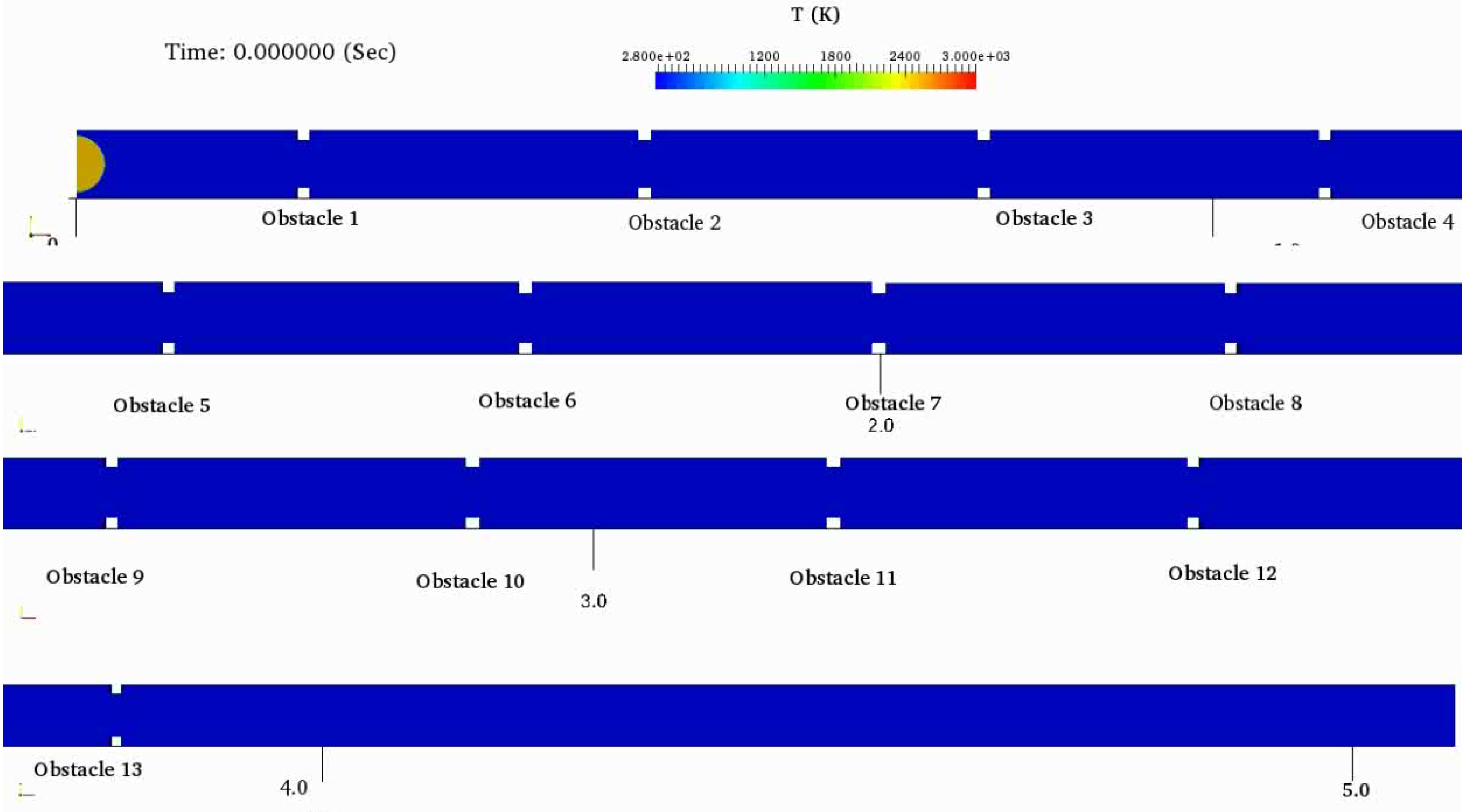


Validation with Experiment



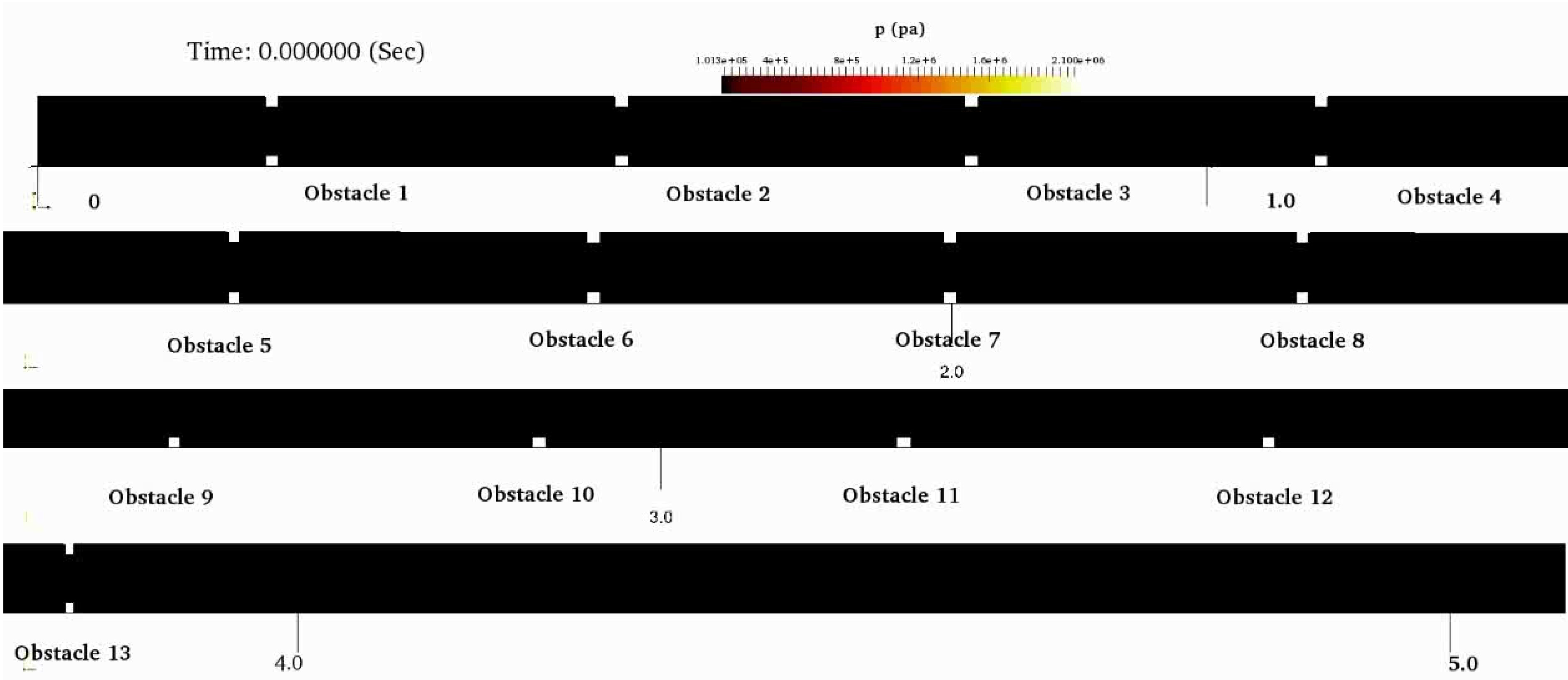
Temperature Results

BR60S300
30% H2

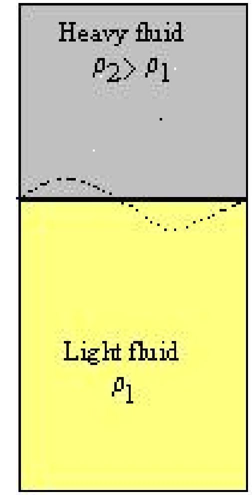


Pressure Results

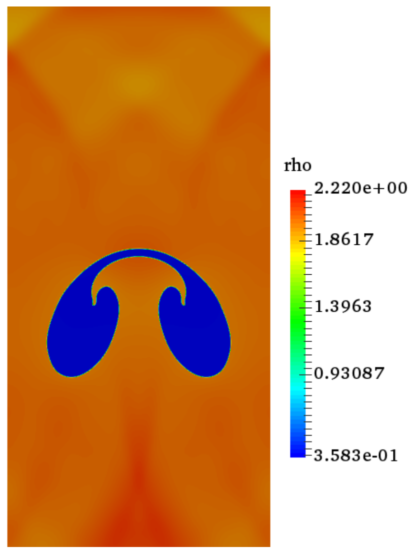
BR60S300
30% H_2

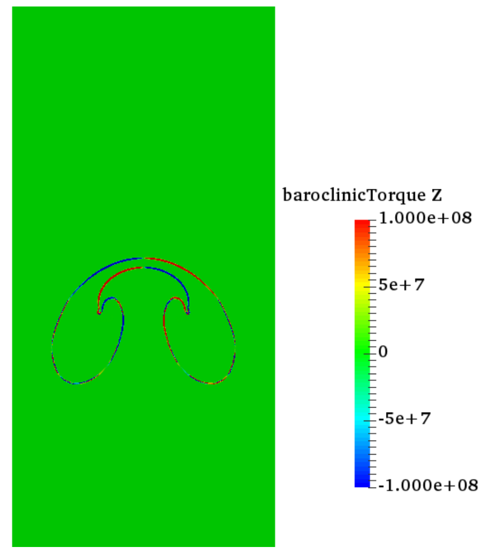


Richtmyer-Meshkov Instability (RMI)



- **also called Rayleigh-Taylor Instability (RTI) (incompressible)**
- **shows the competition between surface tension and gravity.**
- **Occurs anytime a dense fluid is accelerated by a light fluid e.g. a heavy fluid over a light fluid.**
- **Baroclinic Torque triggers RMI**





Ref: R. KhodadadiAzadboni, K. Mazaheri, "two dimensional modelling of reacting shock bubble interaction", Master Thesis, 2012

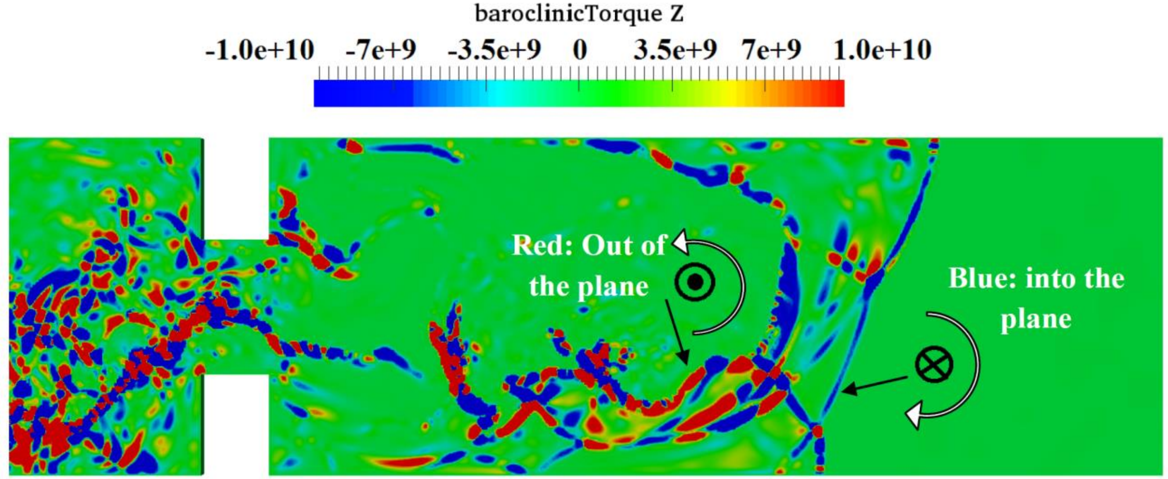
$$\frac{1}{\rho^2}[\nabla\rho \times \nabla P] = \frac{1}{\rho^2}[\nabla\rho \times \nabla p_D] - \frac{g}{\rho}\frac{\partial\rho}{\partial r}$$

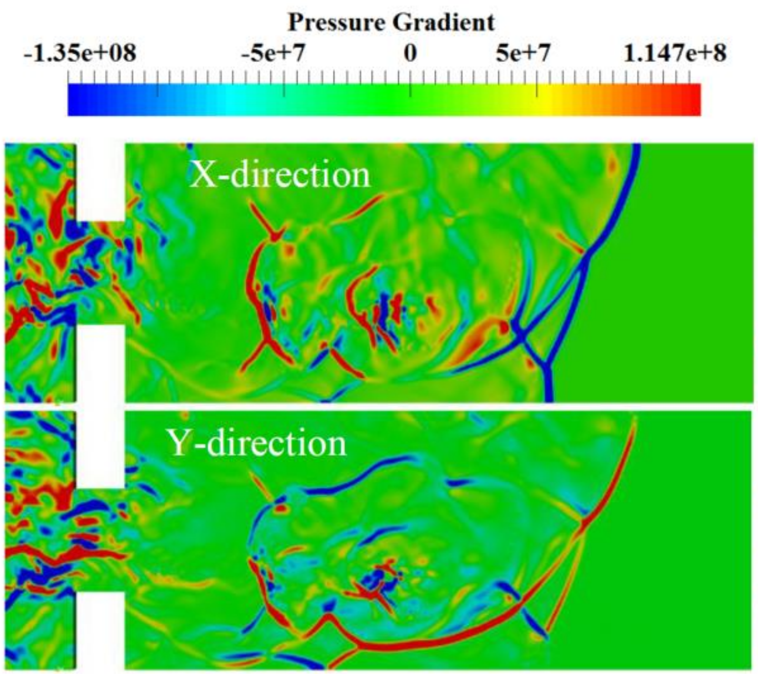
higher density fluid is accelerated toward the lighter density fluid

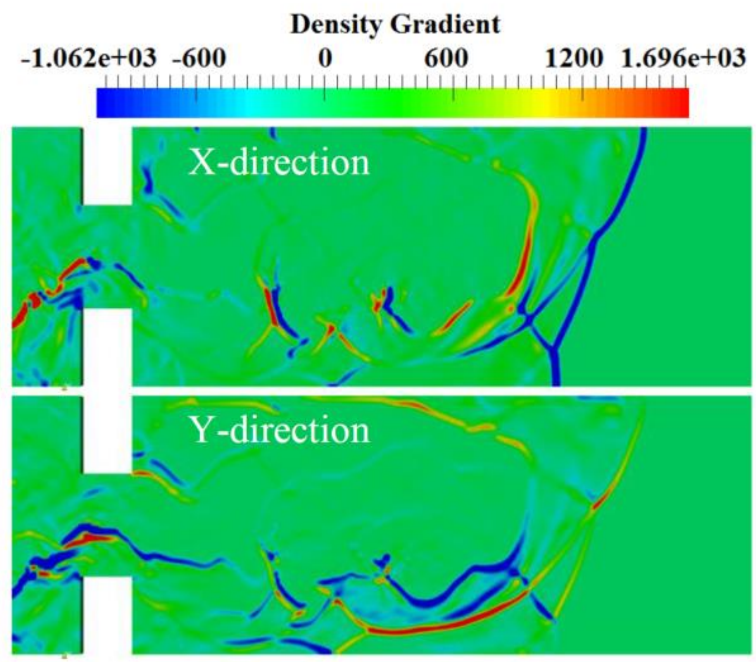
Results-Hydrodynamic Instabilities

baroclinic vorticity

$\left(\nabla\rho\times\nabla p/\rho^2\right)$







Conclusion

- Numerical studies have been conducted to investigate the **role of hydrodynamic instabilities in the DDT** of non-homogenous hydrogen-air mixture.

- **Pressure based** solver is good for **flame deflagration** but it is not suitable for Detonation.

- With **increasing baroclinic torque** there is a **possibility** for having **RM instability**, but in the case of having **Detonation**, this instability triggers more.

- The flame position and flame tip speed are in reasonably **good agreement** with the measurements of Boeck et al.'s **experiment**.

- The **first localized explosion** occurred near the **bottom wall** where the shock and flame interacted and the **mixture was most lean** and then the **second localized explosion** is occurred at the **top wall due to reflection of shock and flame front** which is in region and later develops to form the **leading detonation wave**.

- The **Richtmyer-Meshkov instability** is found to be the **primary source** of **turbulence** generation in **Deflagration to detonation transition** phenomena in **non-homogenous** mixture.

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**.

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Thanks for your attention!

Any questions?