Numerical Analysis of Flame Acceleration and Onset of Detonation in Mixtures with and without Concentration Gradients

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Contents

- Introduction

- Methodology

- Verification and validation with some classical cases
- Flame Acceleration (FA) and DDT in mixtures with and without concentration gradients

- Concluding remarks

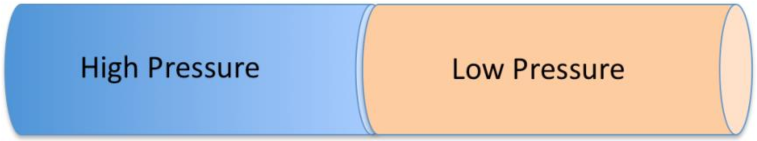
Introduction

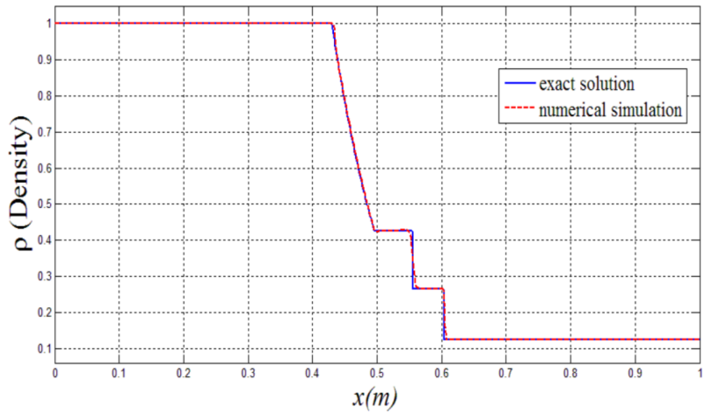
Methodology

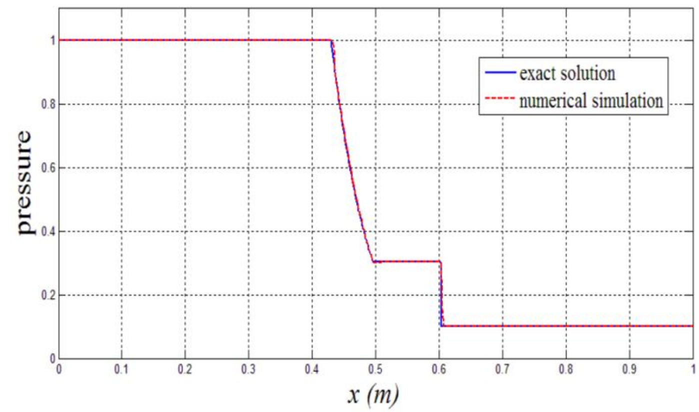
- VCEFoam, the density-based solver developed under OpenFOAM
- MILES (Monotone Integrated Large Eddy Simulation
- Cantera for the thermodynamic properties
- Harten–Lax–van Leer–Contact (HLLC) for accurate shock detonation capturing
- High capability of shock and detonation cell capturing
- Richtmyer Meshkov instabilities and Baroclinic vortices
- Adaptive Refinement Mesh (AMR) method

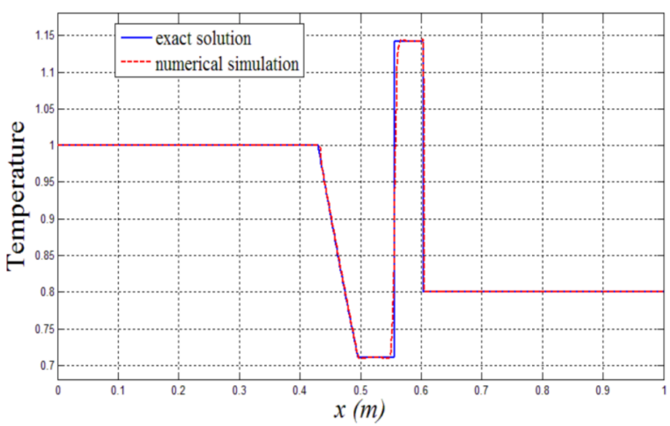
Code Verification

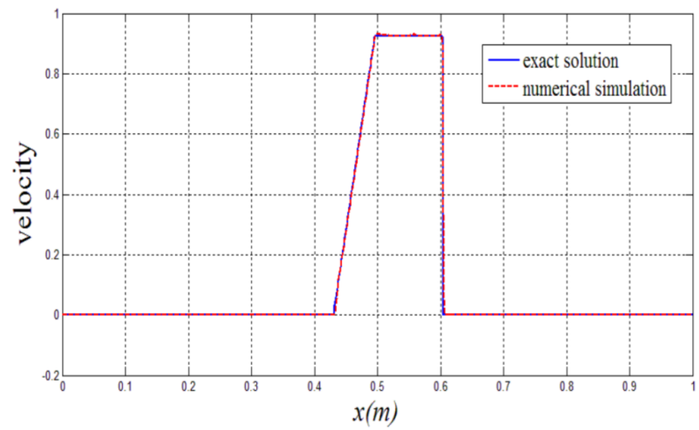
SOD's shock Tube



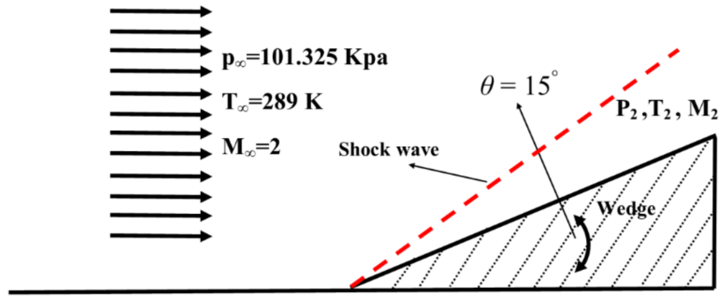


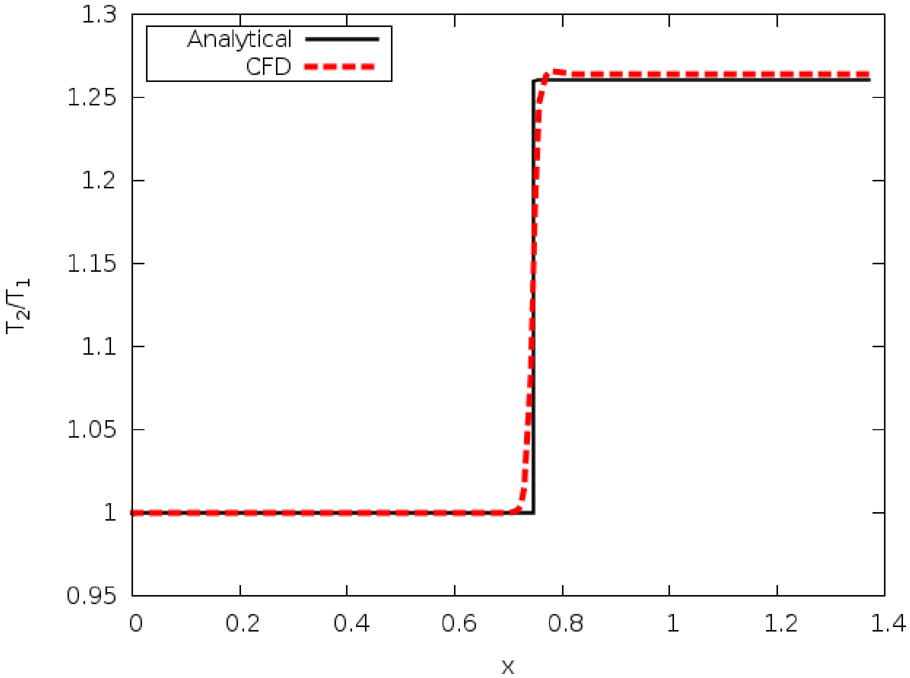


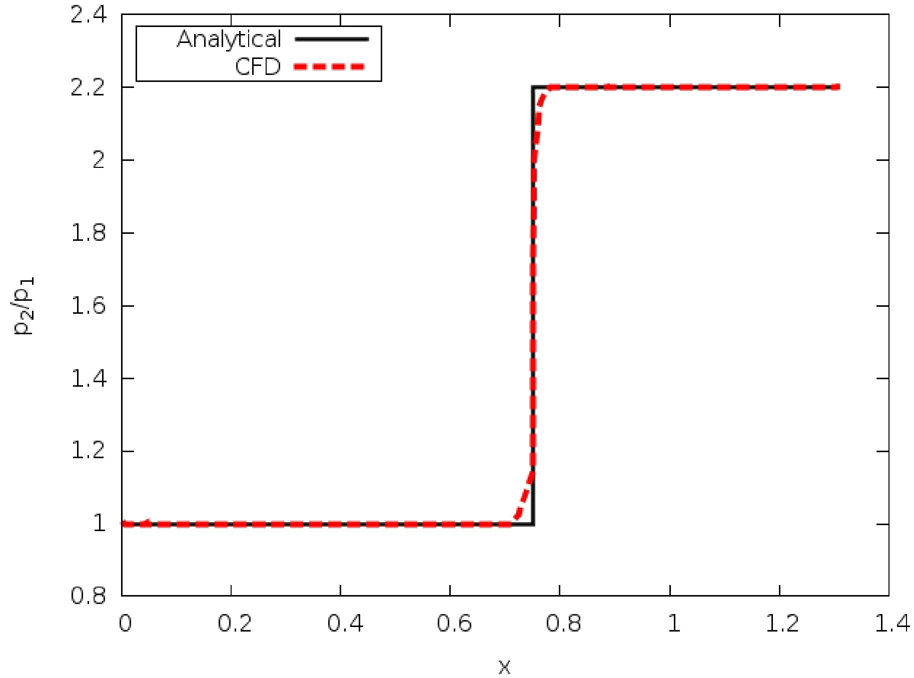




Oblique Shock Test Case



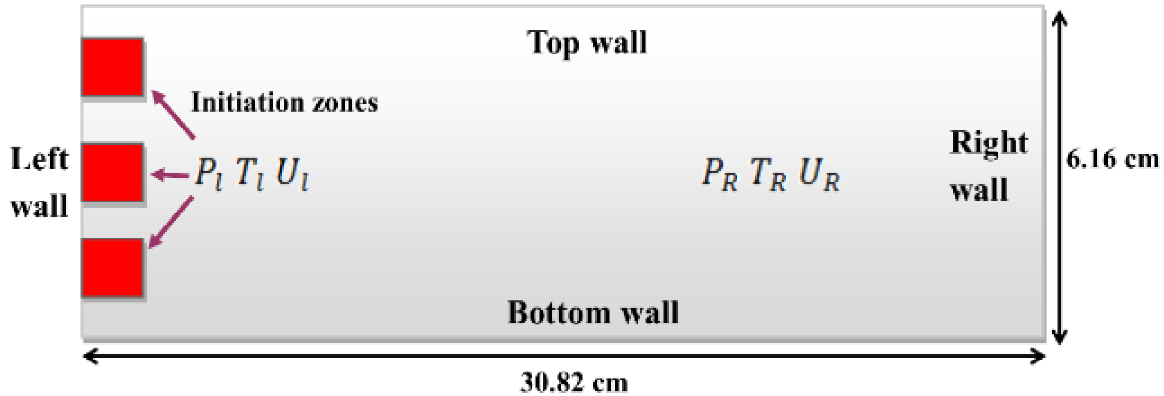




Anderson J., Modern Compressible Flow: With Historical Perspective, McGraw-Hill Series in Aeronautical and Aerospace Engineering, McGraw-Hill, 2004.

Detonation Cellular Structure

$2H_2 : O_2 : 7Ar$

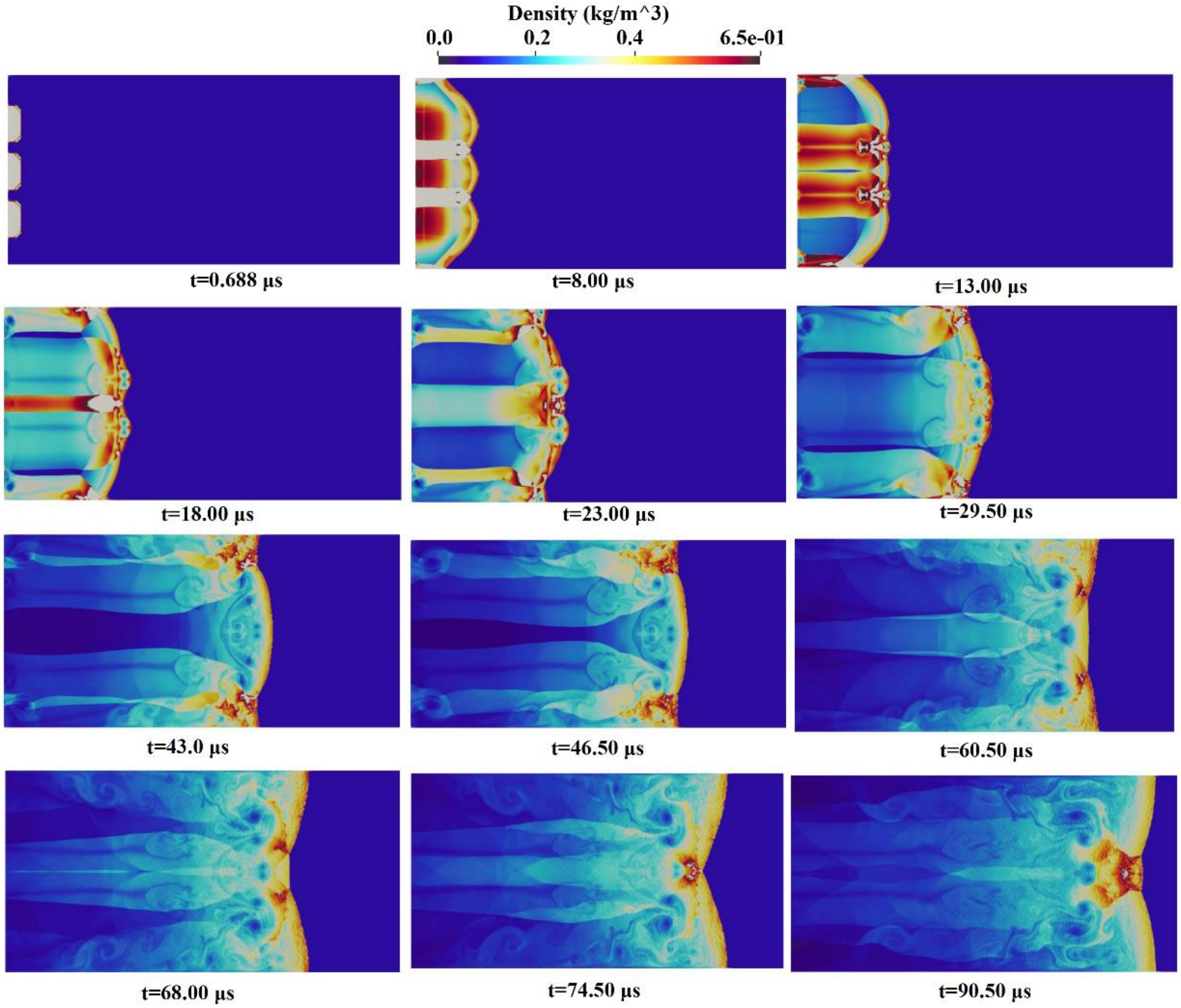


H2/Air mixtures scheme
(Marinov et al. 1996)

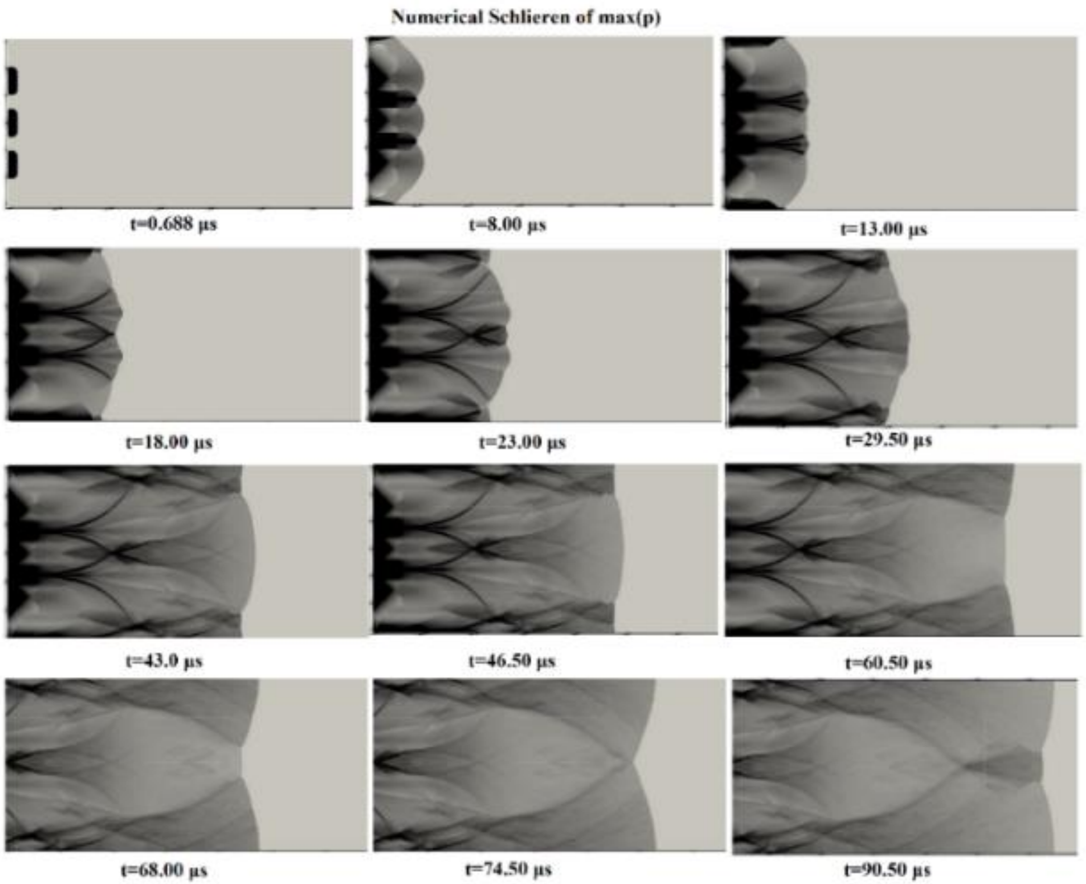
Grid resolution: 0.065 mm,
providing 20 points in the induction length
Courant number < 0.15
High pressure ($1000 \times p_0$ (atm)) and temperature ($25 \times T_0$ (K)) were initiated to trigger the detonation waves in the red regions.
p_0=6670 Pa, T_0=298 K and U_0 =0

Marinov N, Westbrook C, Pitz W, Detailed and global chemical kinetics model for hydrogen-air. Vol. 8 of Int. Symp. on Transport Properties, Lawrence Livermore National Laboratory. p. 118, 1996.

Evolution of triple points illustrated by the predicted density distribution



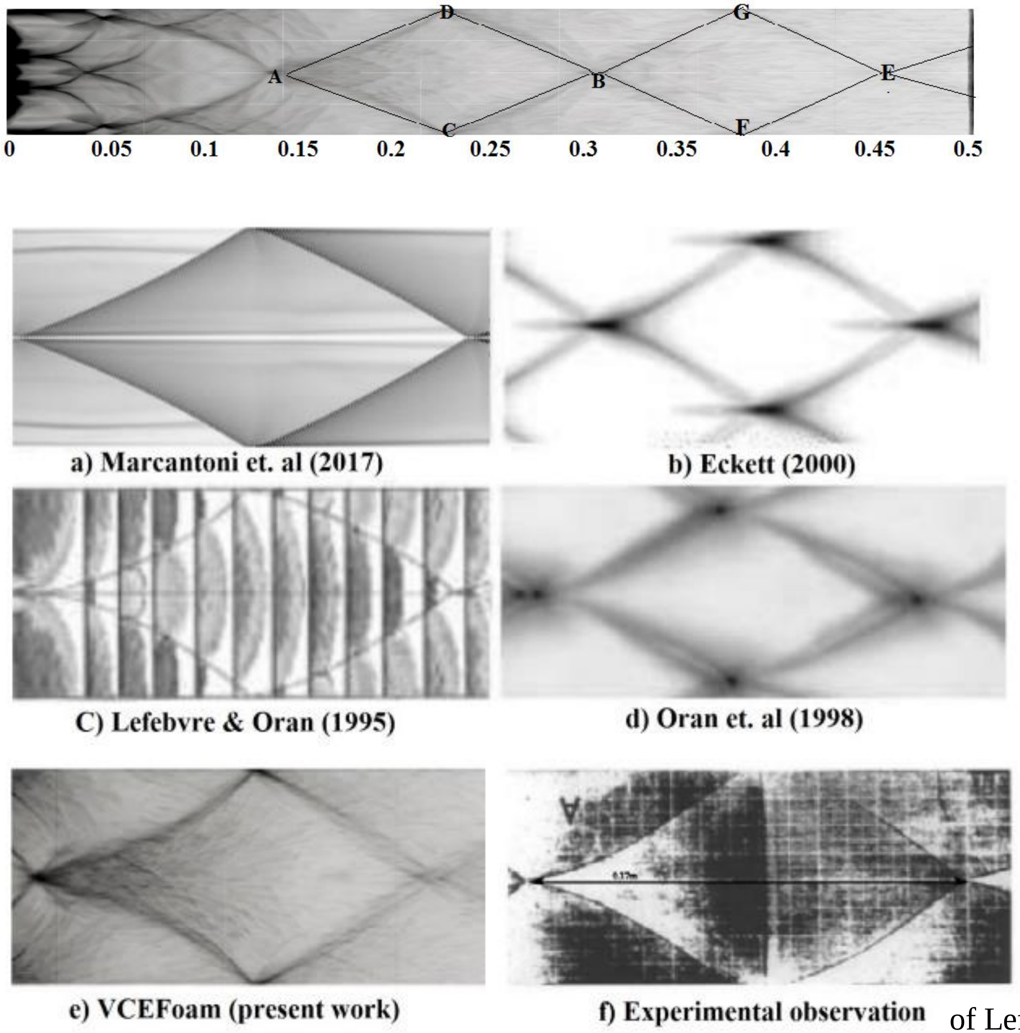
Evolution of triple points illustrated by numerical schlieren of the maximum pressure distribution



Comparison of cellular structure cell size for $2H_2: O_2: 7Ar$ mixtures

Reference	α **(Cell length)**	λ **(Cell height)**	c^{ar} **(aspect atio** λ/α**)**	**Reaction kinetic**
Marcantoni et. al [14]	0.074	0.032	0.43	Marinov [13]
Kirillov et. al [15]	0.078	0.033	0.42	Marinov [13]
Eckett [16]	0.054	0.03	0.55	8species/24reactions [20]
Oran et. al [17]	0.055	0.03	0.54	8species/24reactions [20]
Lefebvre & Oran [18]	0.077	0.03	0.42	Two steps model [18]
Lefebvre et al. [19]	0.17	0.09	0.52	smoke foil
Present predictions	0.0785	0.033	0.0420	Marinov [13]

Cellular Structure in the Extended Channel



of Lefebvre and oran (1995)

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- **FA and DDT in mixtures with and without concentration gradients**
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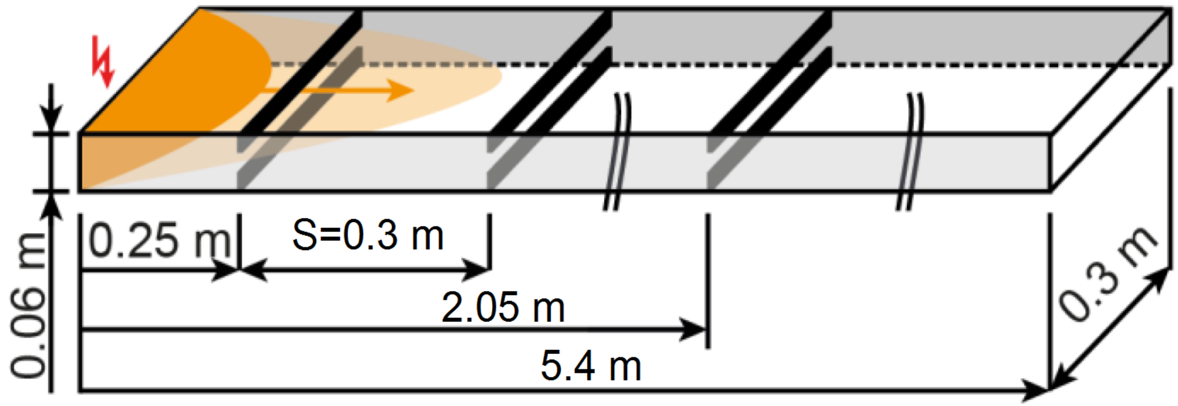
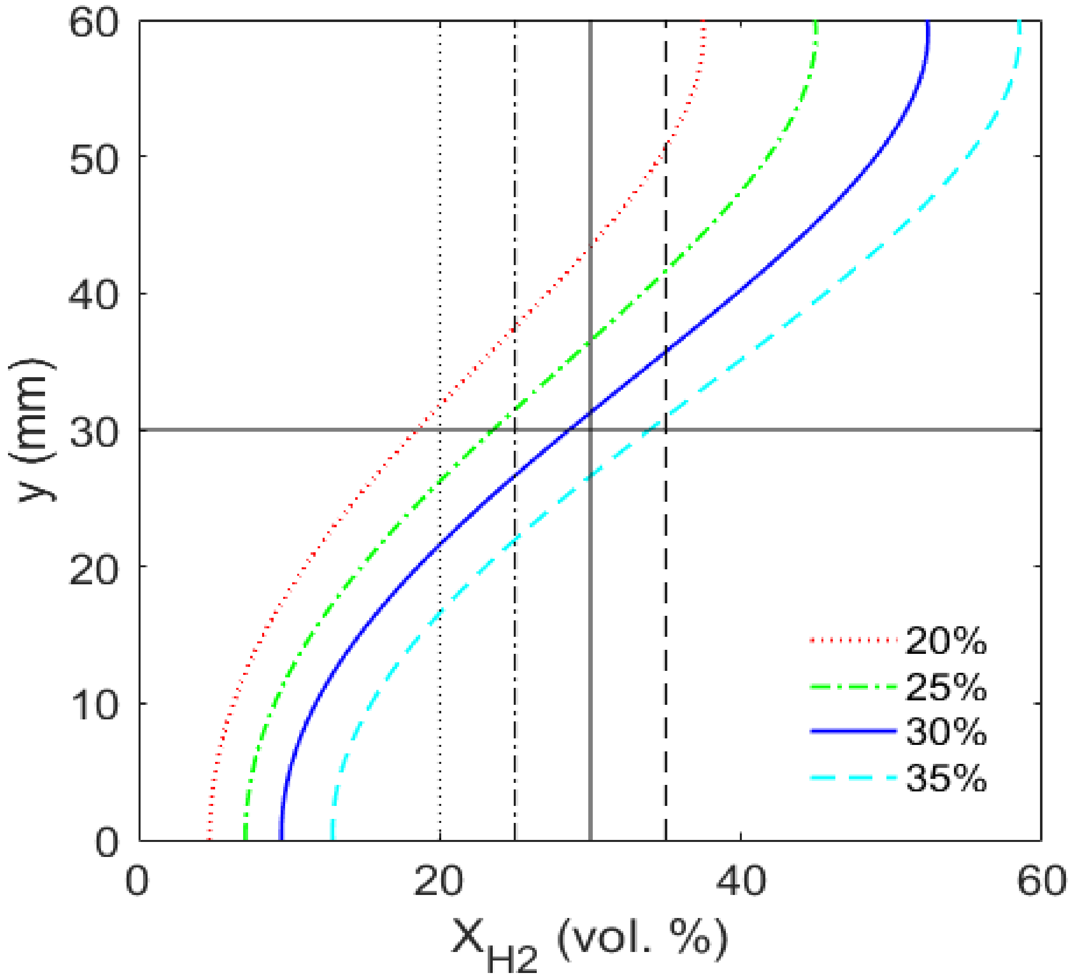
The Experiments Considered



Boeck LR, Katzy P, Hasslberger J, Kink A & Sattelmayer T. (online 03/2016). The "GraVent DDT Database". Shock Waves

The Computational Model



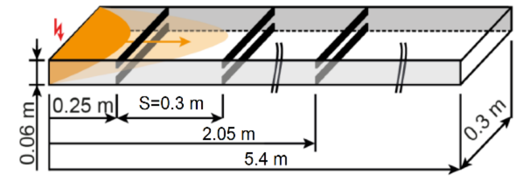
Ignition: Patch cells within a radius of 10 mm around the point of ignition to the burnt state (adiabatic burnt mixture, and products).

Boeck LR, Katzy P, Hasslberger J, Kink A & Sattelmayer T. (online 03/2016). The "GraVent DDT Database". Shock Waves

Test conditions numerically simulated

Hydrogen concentration (%)	Homogeneous			Inhomogeneous		
	Unobstructed	BR60	BR300	Unobstructed	BR60	BR300
20		✓			✓	✓
25	✓			✓		
30	✓	✓	✓	✓	✓	✓
35	✓			✓		✓
40				✓	✓	✓

60 % Blockage ratio



30 % H2

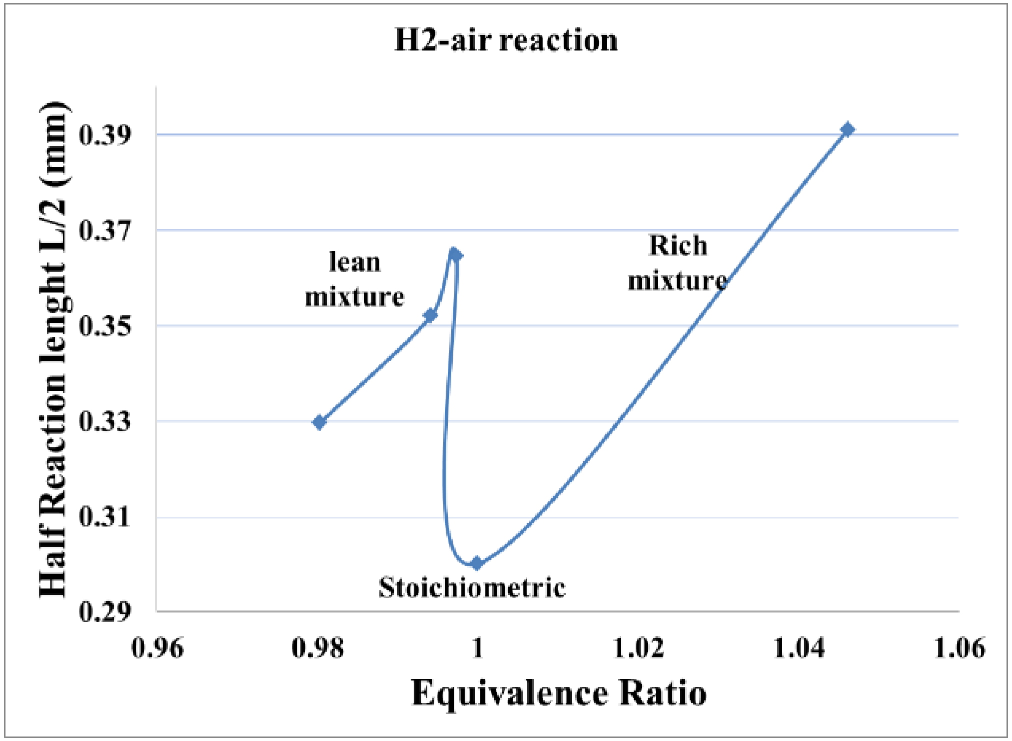
- Homogenous
- Inhomogeneous

20 % H2

- Homogenous
- Inhomogeneous

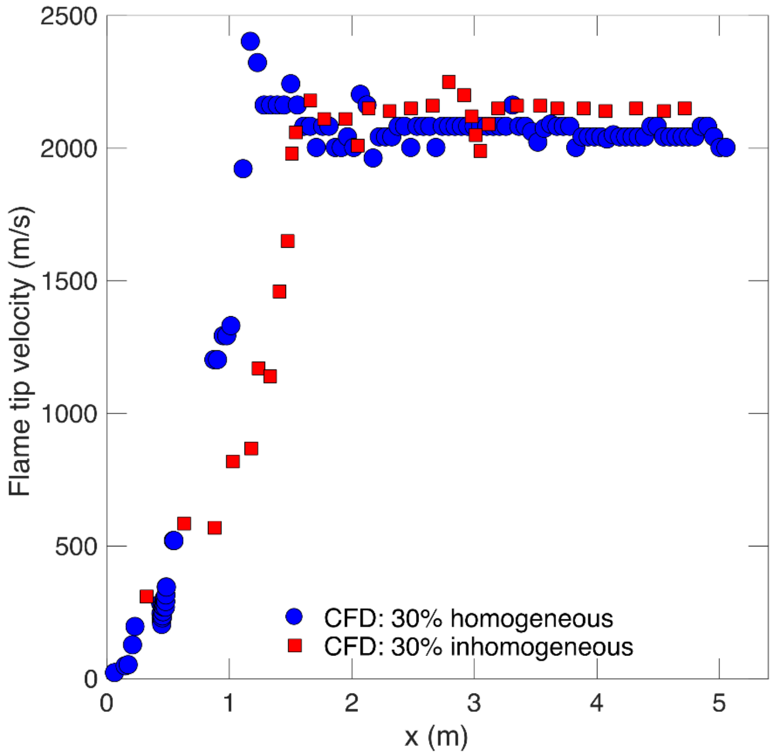
Numerical setup

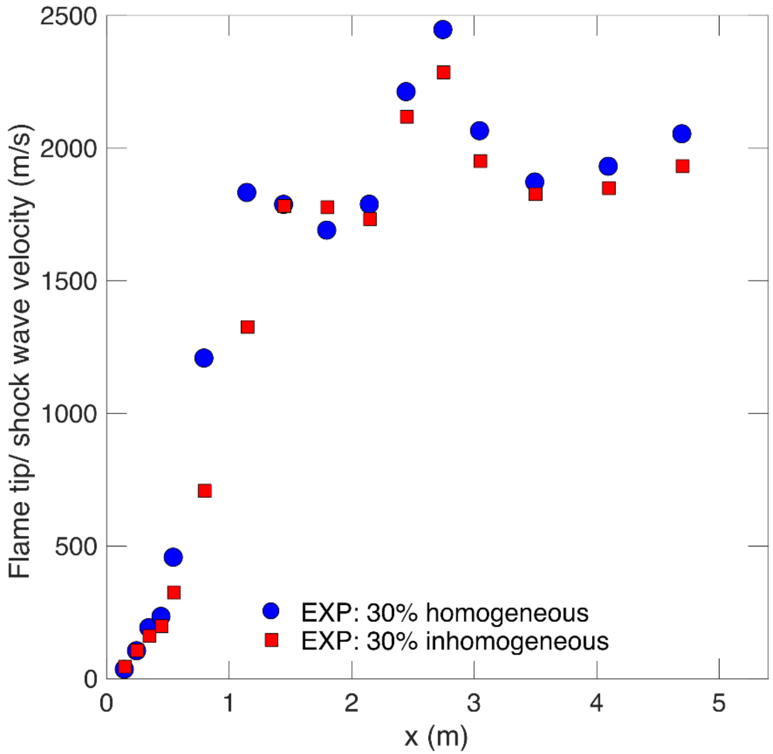
- Reaction mechanism: *hydrogen-air which contains 9 species and 21 detailed reactions (Ó Conaire et al., 2004)*
- Max Courant number: 0.3
- Time step = 3.28084E-08
- Minimum cell size 10 µm (30 grid points per HRL)
- Running duration: 60 days, with using 128 cores in cluster



Reproduced from Stamps et al. (1991)

Comparison between Predictions and Measurements





Homogenous mixture DDT happened at x=1.09

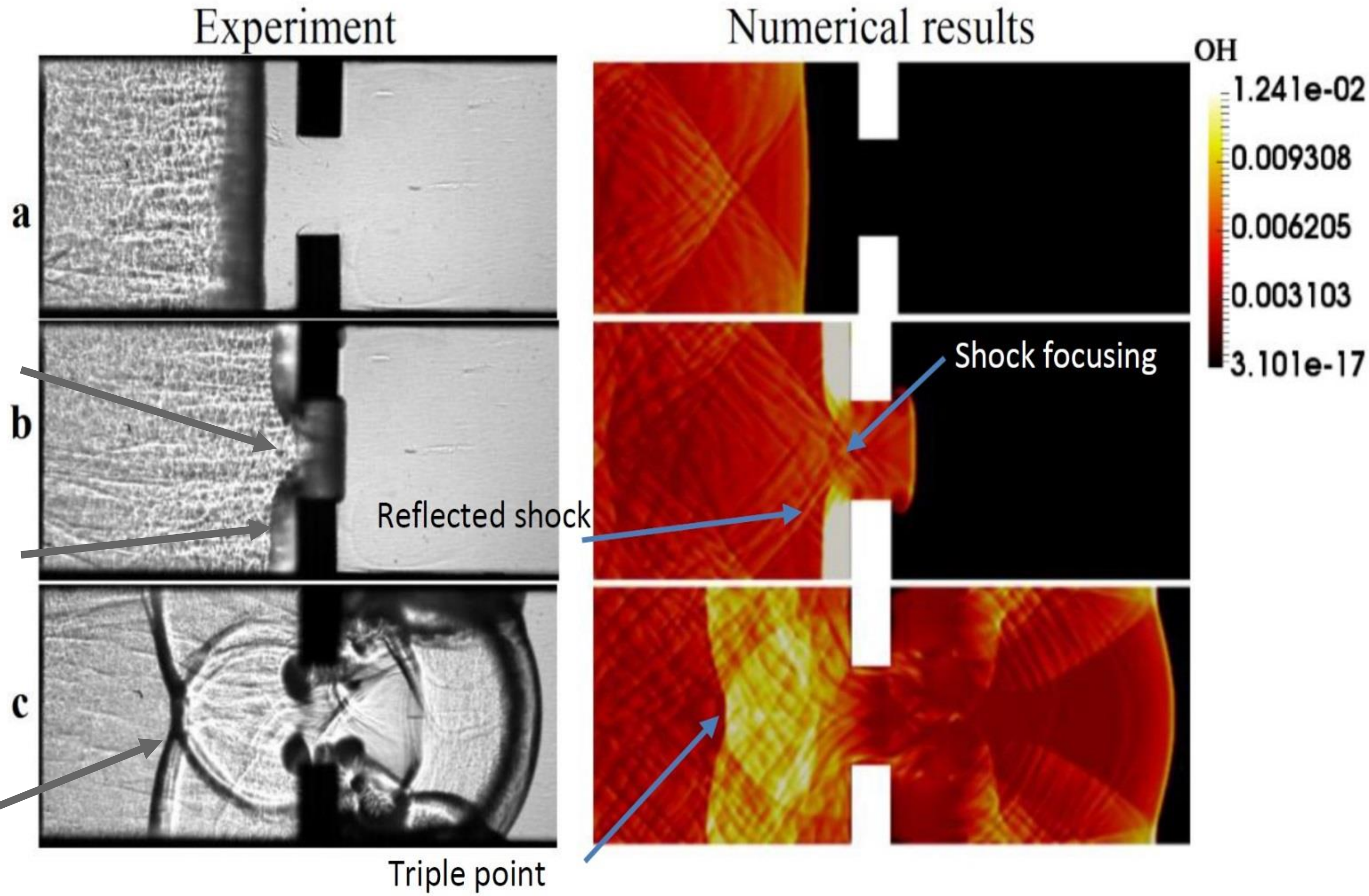
Inhomogeneous mixture DDT happened at x=1.45 m

Comparison Between Predictions and Experimental Observations

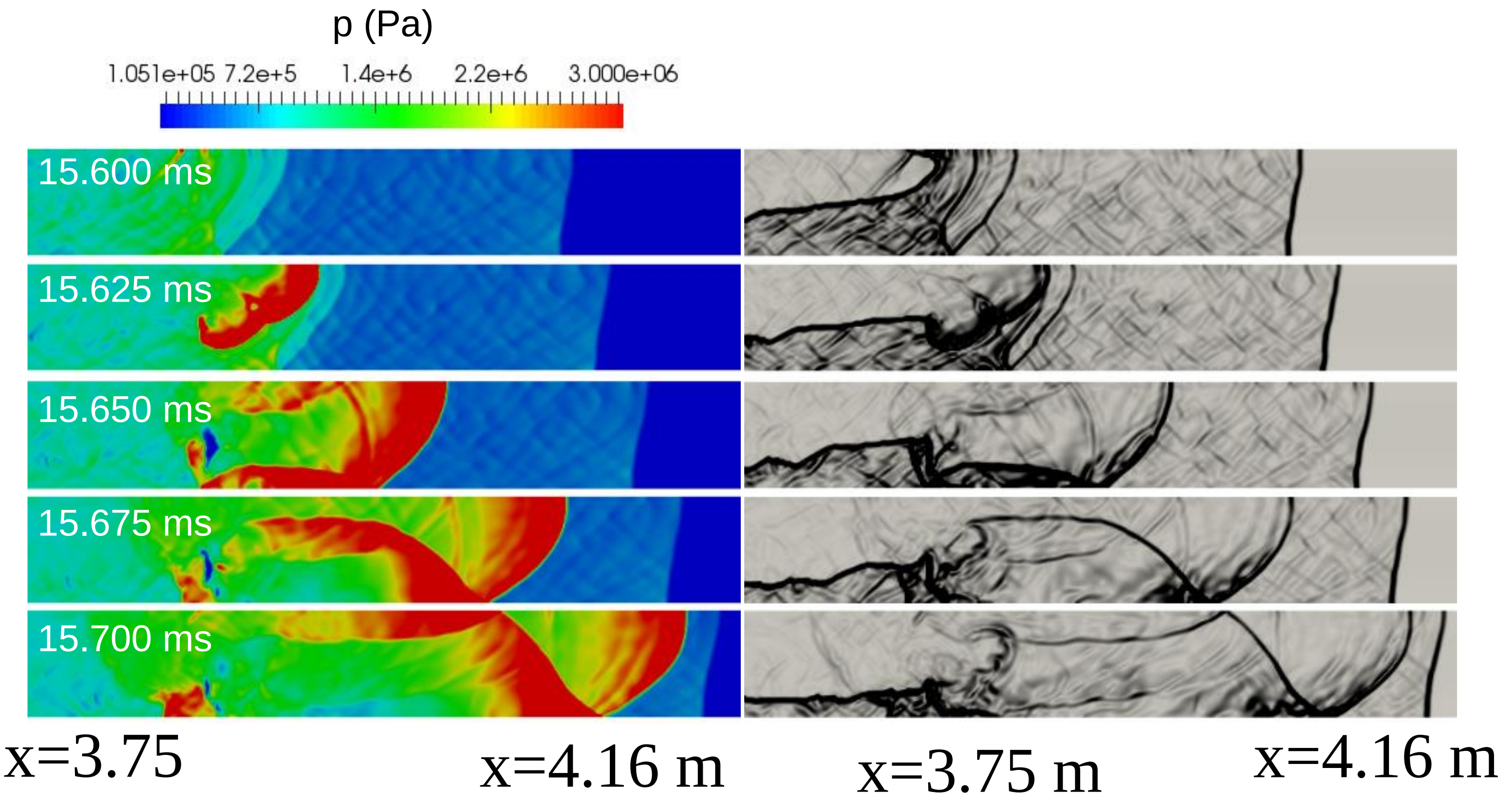
Shock focusing

Reflected shock

Triple point



20% H_2/Air mixture with concentration gradients BR60



Homogenous mixture	DDT did not happen
Inhomogeneous mixture	DDT happened at x=3.95 m

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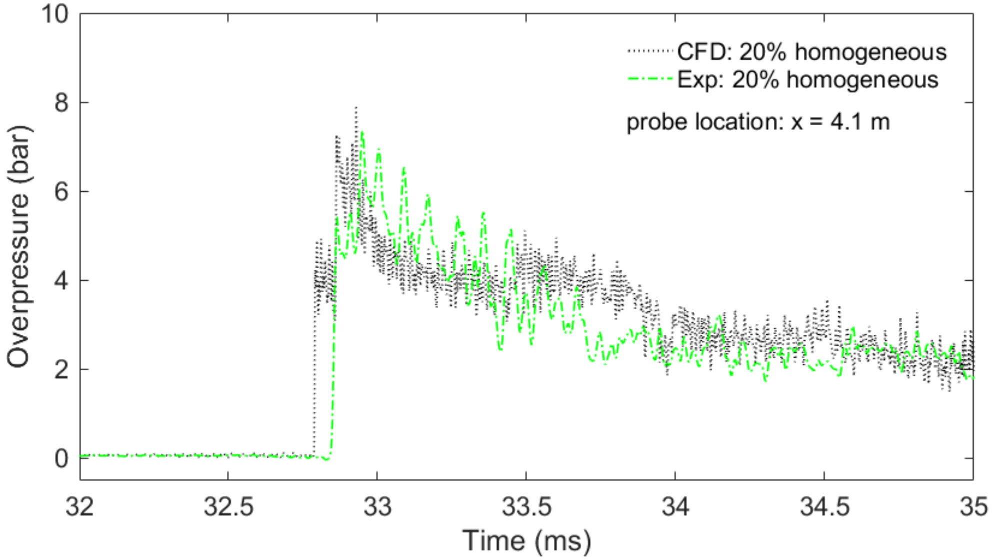
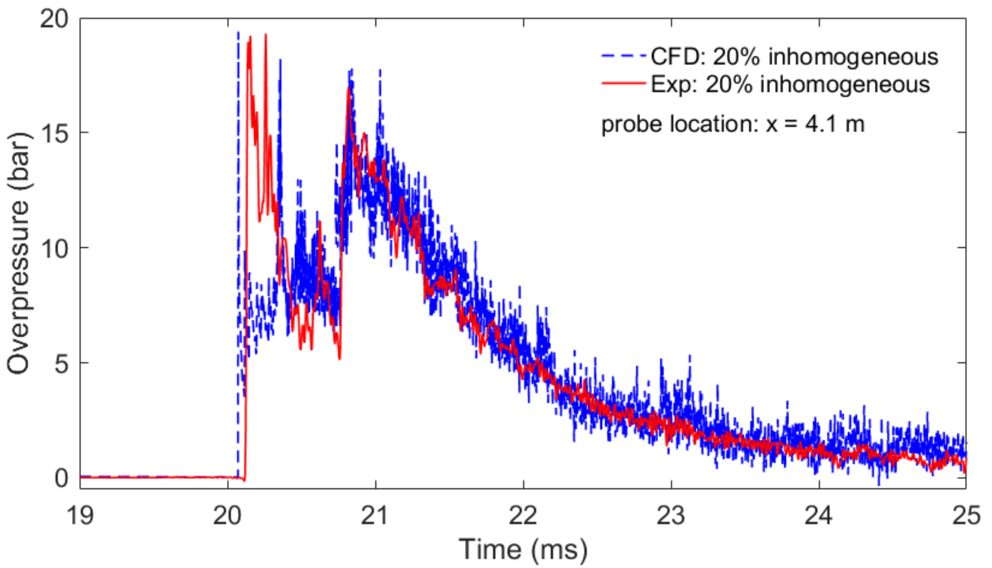
20% H_2/Air mixture with concentration gradients BR60

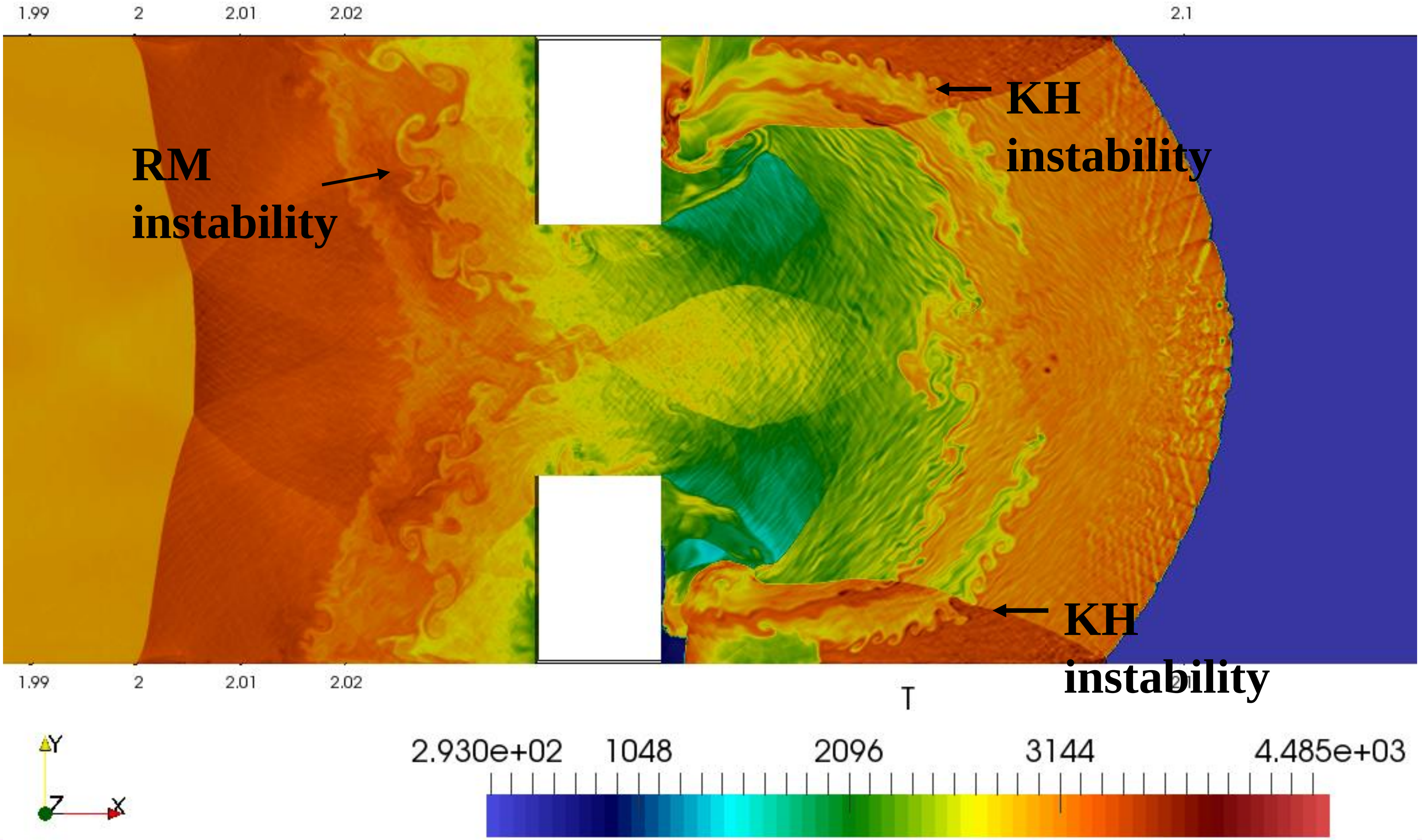




Higher resolution results

- Max Courant number: 0.3
- Time step = 3.28084e-08
- Minimum cell size 6 µm (50 grid points per HRL)
- Running duration: 75 days, with using 128 cores in cluster

Homogeneous 30% H_2/Air mixture BR60



DDT in Industrial Scale RUT facility

Dorofeev et al., 1996; Efimenko and Gavrikov, 2007)

Summary of the Cases

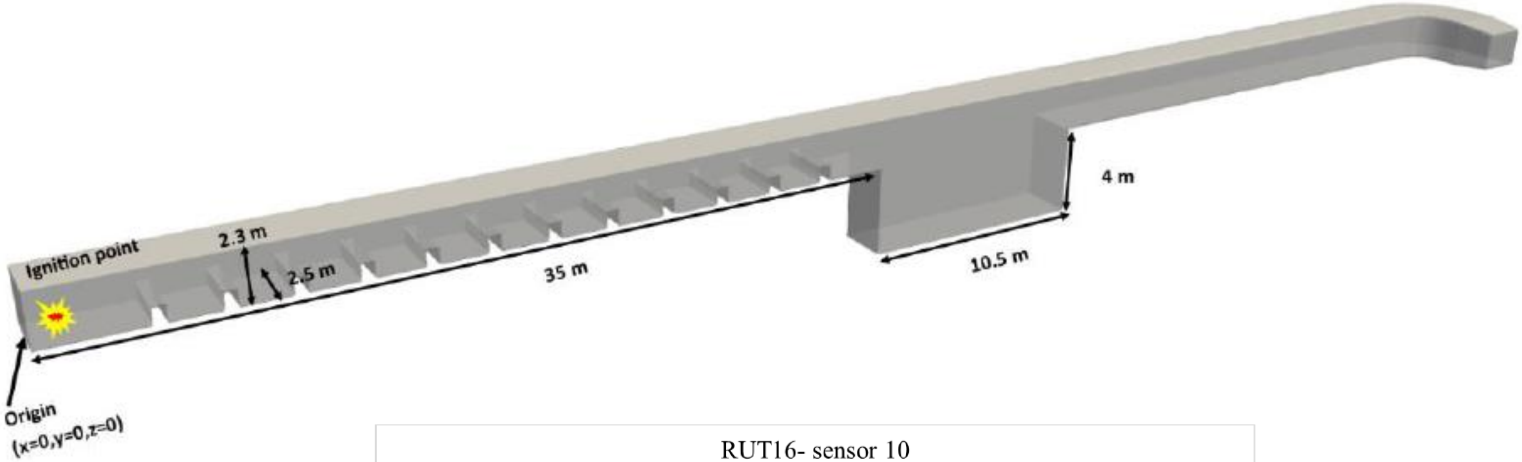
	RUT16	RUT22	RUT09
Hydrogen fuel concentration	12.5 %	14 %	25.5 %
Blockage ratio	30 %	60 %	0 (smooth channel)
Number of obstacles	12 (with 2.5 m spacing)	6 (with 5 m spacing)	0 (smooth channel)
Inner volume (without obstruction)	423.9 $[m^3]$	423.7 $[m^3]$	242.5 $[m^3]$
Ignition source	spark	spark	200 g TNT
Main feature	DDT	DDT	Direct detonation initiation

The Modelling Approach for Large Scale FA and DDT

Modified combustion treatment in the density-based solver VCEFoam

- Different source terms for deflagration and detonation.
- For the deflagrative source term, the effect of flame instabilities such as Darrieus-Landau (DL) and Ryleigh Taylor (RT) instabilities in flame surface wrinkling factor has been taken into account.
- The thermal diffusive instabilities in large-scale models is accounted for using a published model
- Unsteady RANS turbulence model

RUT16 – Mesh Sensitivity Study



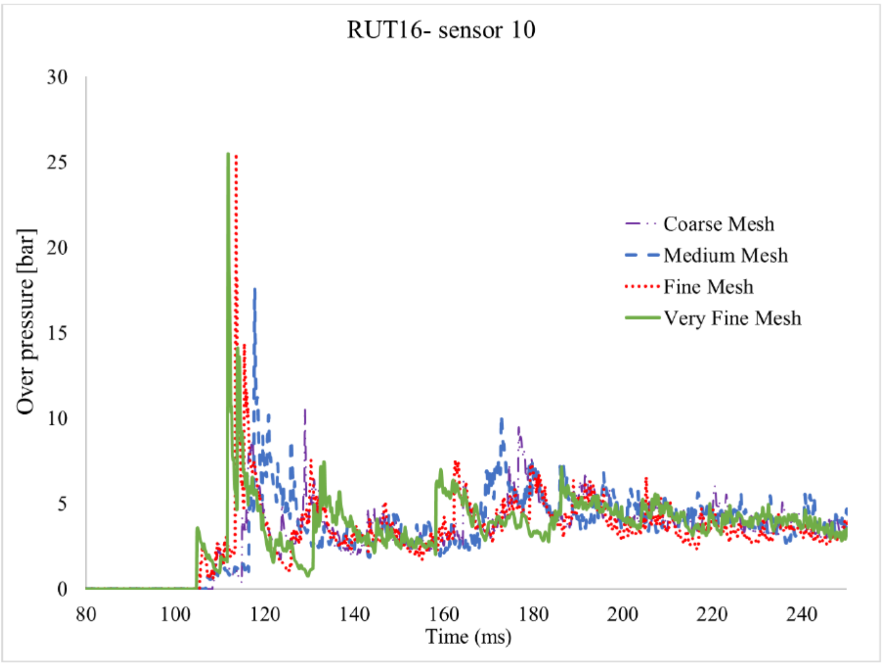
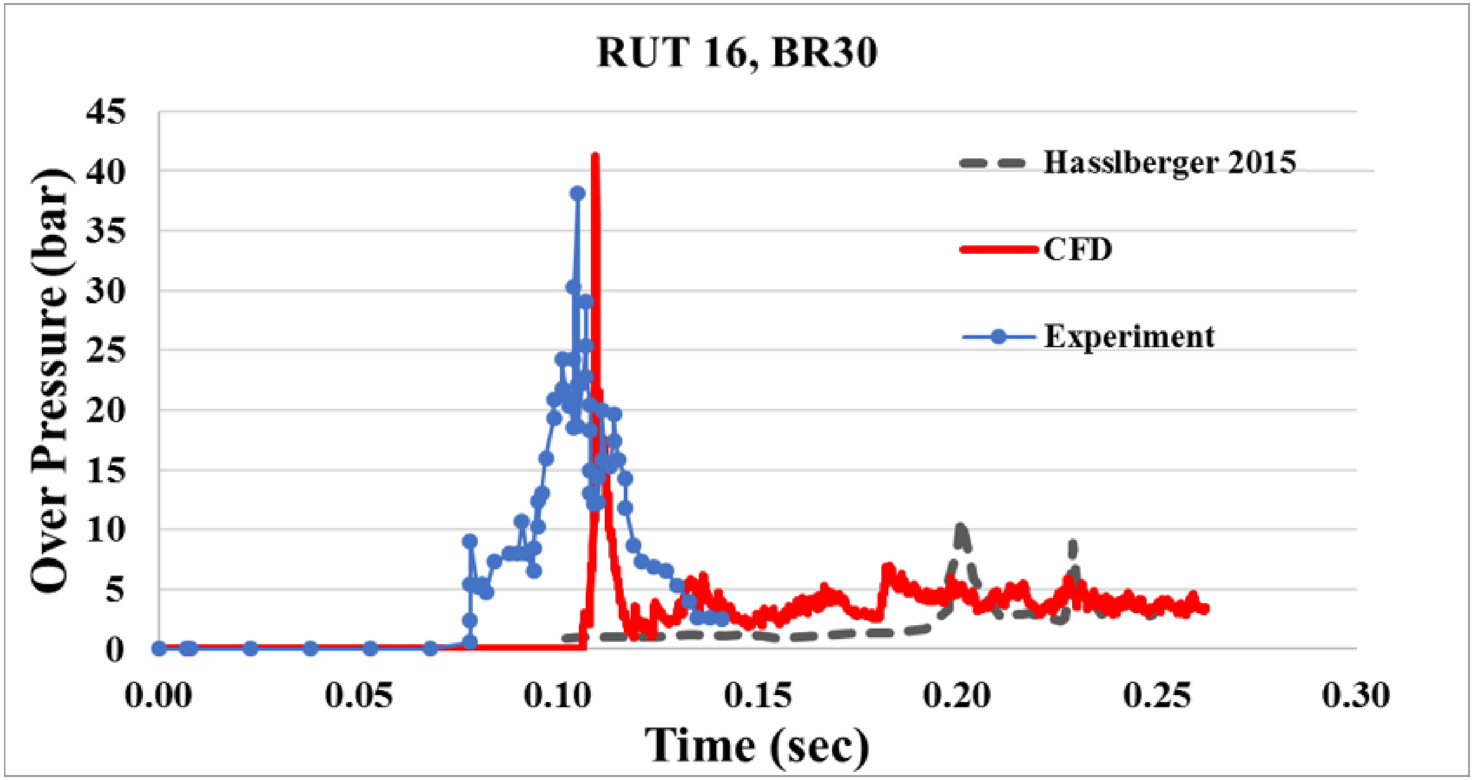


Figure 7-7: Grid independency study: overpressure vs time for the RUT 16 case; probe location at sensor 10.

Validation with RUT 16



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Concluding Remarks

- VCEFoam, a density-based solver has been developed within OpenFOAM for simulating flame acceleration (FA) and deflagration to detonation transition (DDT).
- Predictions have been conducted for FA and DDT in a horizontal obstructed channel. Both homogeneous H_2/air mixtures and mixtures with vertical concentration gradients have been considered.
- The predictions are generally in reasonably good agreement with the experimental measurements and observations.
- For 30% H_2/air mixtures considered here, onset of detonation occurs within the obstructed channel section. The homogeneous mixture shows slightly faster FA and earlier DDT.
- For 20% H_2/air mixtures, DDT was predicted only for the inhomogeneous mixture, where the concentration gradient enables stronger FA, especially in the unobstructed section.

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.

The work reported here were conducted by PhD graduate Reza Khodadadi.