Analysis of heat flux components on PMMA wall fires and upward flame spread configuration

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WARWICK

NUMERICAL INVESTIGATION OF HYDROGEN-AIR DEFLAGRATIONS IN A REPEATED PIPE CONGESTION

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Outline

- Objective
- CFD Solver description
- Experiments details
- Computational Domain
- Numerical results
- Concluding remarks

Objective

- Study hydrogen turbulent deflagration modelling.
- Numerical solver development and its validation.
- Study overpressure trends with respect congestion.
- Trends of overpressure w.r.t the concentration
- Aid in filling the experimental knowledge gap.

Numerical Solver

- Large Eddy Simulations (LES) method in OpenFOAM.
- The Favre-filtered unsteady compressible Navier-Stokes equations are solved in a segregated manner, wherein each dependent variable equation is solved sequentially.
- The pressure-velocity coupling is handled using Pressure-Implicit Split Operator (PISO) solution method.
- Sub-grid turbulence kinetic energy is solved using the one equation eddy viscosity model.*

* MENON S., YEUNG P. K., and KIM W. W., Effect of Subgrid Models on the Computed Interscale Energy Transfer in Isotropic Turbulence," Computer and Fluids (1996), Vol. 25, No. 2, pp. 165-180

Numerical method

- Large Eddy Simulations (LES) /RANS method in OpenFOAM.
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Combustion model

- The flame wrinkling combustion model of Weller et al. (1998).
- Considering a single step chemistry, **unity Lewis number** and flamelet regime, the thermo chemistry of the reacting flow is described by the unburnt zone volume fraction denoted as regress variable (b), taking values 1 and 0 in unburnt and fully burnt region. The transport equation for the regress variable:

$$\frac{\partial \overline{\rho}\tilde{b}}{\partial t} + \nabla.\left(\overline{\rho}\tilde{U}\tilde{b}\right) - \nabla.\left(\overline{\rho}D\nabla\tilde{b}\right) = -\overline{\rho_u}S_u\Xi\left|\nabla\tilde{b}\right|$$

where, Ξ is sub grid flame wrinkling, S_u is laminar flame speed

- Mixture fraction equation is also solved – inhomogeneous mixtures

WELLER, H. G., TABOR, G., GOSMAN, A. D. & FUREBY, C. (1988) Application of a flame-wrinkling les combustion model to a turbulent mixing layer. Symp. (Int.) on Combustion, 27**,** 899-907.

Flame wrinkling due to turbulence

The surface wrinkling factor due to turbulence (Ξ) is modelled as transport equation *

$$\frac{\partial \overline{\rho}\Xi}{\partial t} + \widehat{U}_s.\nabla\Xi = \overline{\rho}G\Xi - \overline{\rho}R(\Xi - 1) + \overline{\rho}\max\left[(\sigma_s - \sigma_t), 0\right]\Xi$$

The modelling for the respective terms in above equation are given as,

$$\sigma_t = \frac{1}{2}\left\|\nabla\widehat{U}_t + \widehat{U}_t^{\,T}\right\| \qquad \text{and} \qquad \sigma_s = \frac{1}{2}\left\|\nabla\widehat{U}_s + \widehat{U}_s^{\,T}\right\|$$

resolved strain rates,

$$\mathrm{G} = \mathrm{R}\,\frac{\mathrm{E}_{eq} - 1}{\mathrm{E}_{eq}} \qquad \text{and} \qquad \mathrm{R} = \frac{0.28}{\tau_{\mathrm{n}}}\,\frac{\mathrm{E}_{eq}^{\;*}}{\mathrm{E}_{eq}^{\;*} - 1}$$

are subgrid turbulence generation and removal rates with

$$\mathrm{E}_{eq} = 1 + 2(1-b)(\mathrm{E}_{eq}^{\;*} - 1), \qquad \mathrm{E}_{eq}^{*} = 1 + 0.62\sqrt{\frac{\hat{u}}{S_{L\ \eta}}}\,R_{\eta}$$

* WELLER, H. G., TABOR, G., GOSMAN, A. D. & FUREBY, C. (1988) Application of a flame-wrinkling les combustion model to a turbulent mixing layer. Symp. (Int.) on Combustion, 27, 899-907.

Laminar flame speed for hydrogen-air mixtures

- Power law function of elevated temperature and pressure*

$$S_L(\tilde{T},\overline{P}) = S_{L,0}\left(\frac{\tilde{T}}{T_0}\right)^{\alpha}\left(\frac{\overline{P}}{P_0}\right)^{\beta}$$

$$S_{L,0} = 2.1087\phi^5 - 8.6278\phi^4 + 10.455\phi^3 - 2.8908\phi^2 + 1.3031\phi - 0.1075 \text{ for } \phi > 1.7$$
$$S_{L,0} = 0.0027\phi^5 - 0.067\phi^4 + 0.645\phi^3 - 2.8799\phi^2 + 5.1941\phi - 0.1446 \text{ for } \phi > 1.7$$

$$\alpha = 1.4 \text{ and } \beta = 0.194$$

S_L in m/s , P is pressure in bar and unburnt gas temperature in K.

* Ravi, S., Petersen, E. L., Laminar flame speed correlations for pure-hydrogen and high-hydrogen content syngas blends with various diluents, International Journal of Hydrogen Energy 37 (24), 19177-19189

Experiments

The premixed hydrogen-air experiments were performed at the HSL (UK) experimental site.

(a) 4-gate congestions

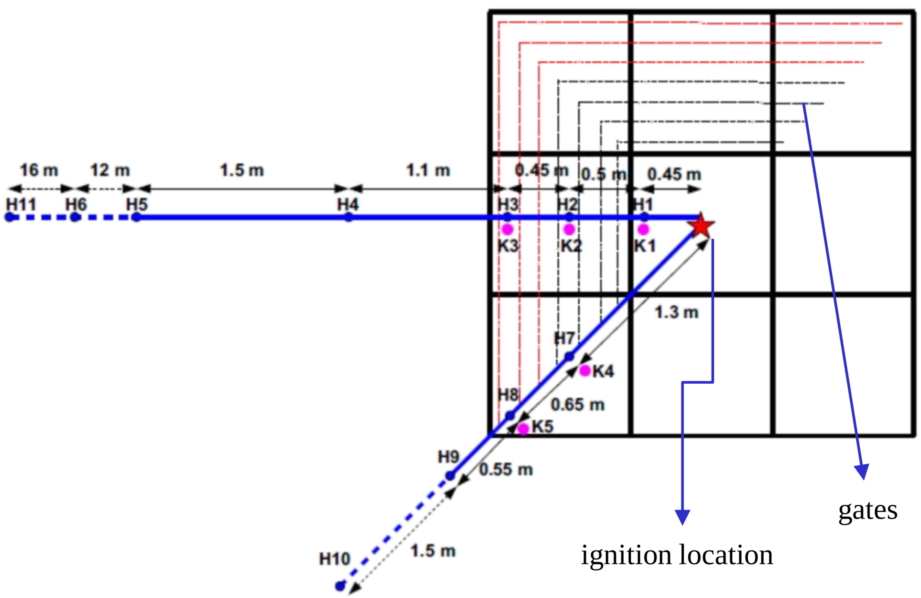
(b) 7-gate congestions

Experiment details

- The pipe rig comprises of a 3 m (width) x 3 m (depth) x 2 m (height) metal frame structure.
- 9 cubes in bottom layer and 9 in top layer, total eighteen 1 m^3 cubic units.
- Each gate grid comprised of several 26 mm diameter bars spaced at 125 mm apart.
- The gates are inserted vertically into the lower layer of cubes and horizontally into the upper layer of cubes.
- Gates are arranged within the rig to form concentric squares around the centre cube, concentric squares of 4 or 7 grids the around the central cube

Shirvill, L. C., Roberts, T. A., Royle, M., Willoughby, D. B., Sathiah, P., Experimental study of hydrogen explosion in repeated pipe congestion – Part 1: Effects of increase in congestion, International Journal of Hydrogen Energy, 2018. 1-18

Overpressure Monitoring points



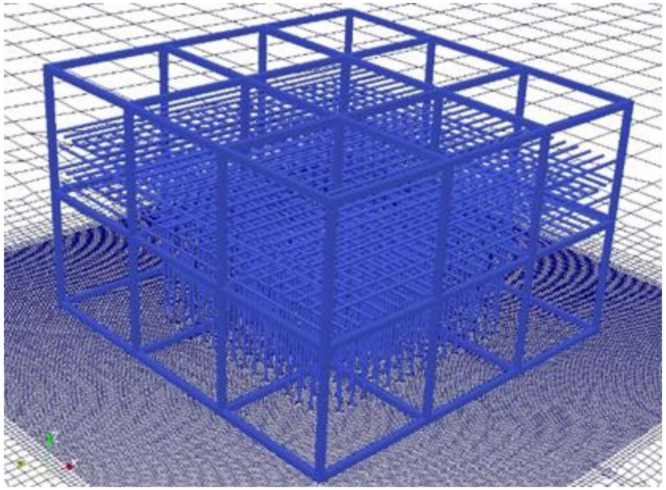
S.no	Sensor	Angle	Horizontal distance from spark (m)	Height above ground (m)
1	H1	180	0.45	0.5
2	K1	180	0.45	0.5
3	H2	180	0.95	0.5
4	K2	180	0.95	0.5
5	H3	180	1.4	0.5
6	K3	180	1.4	0.5
7	H4	180	2.5	0.5
8	H5	180	4	0.5
9	H6	180	16	1.2
10	H11	180	32	0.5
11	H7	135	1.3	0.5
12	K4	135	1.3	0.5
13	H8	135	1.95	0.5
14	K5	135	1.95	0.5
15	H9	135	2.5	0.5

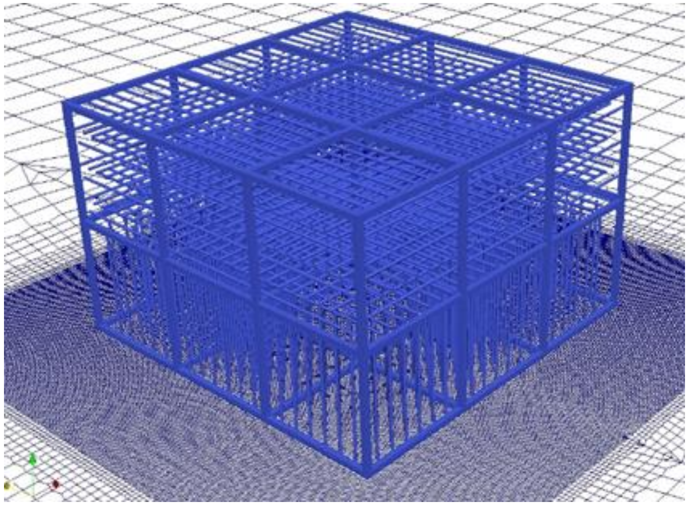
Experimental plan view and pressure sensor locations

Experimental and Numerical Case-studies

S.no	Parameters	Numerical Hydrogen04	Numerical Hydrogen05	Numerical Hydrogen06	Numerical Hydrogen07	Numerical Hydrogen15	Numerical Hydrogen16
1	Number of gates	4	7	4	7	4	7
2	Gas mixture temperature	35.2	35.2	35.2	39.3	15.6	23.9
3	Stoichiometric ratio of mixture	0.5	0.5	0.969	0.967	1.253	1.167
4	Mass of hydrogen ignited (kg)	0.31	0.31	0.422	0.417	0.524	0.481

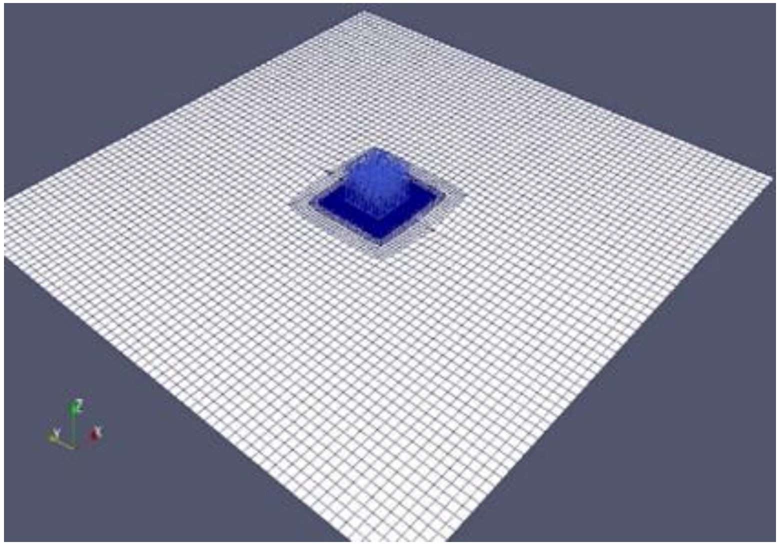
Computation Domain

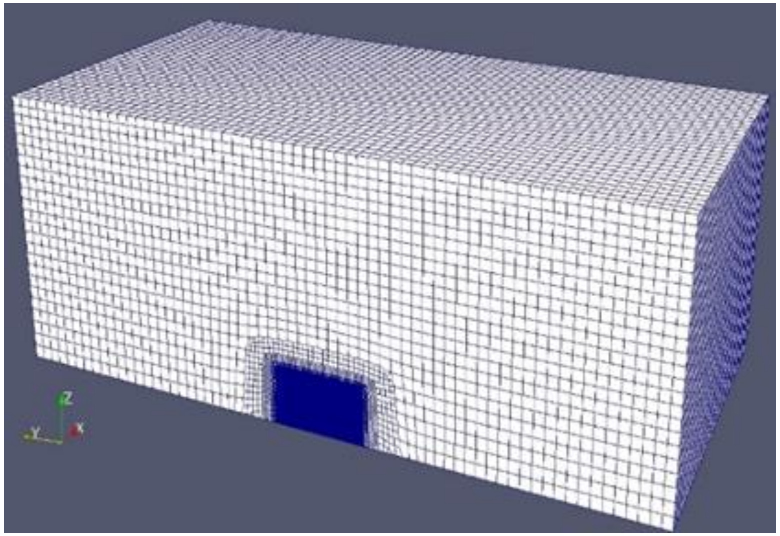




Computational geometry for the 4 & 7-gate pipe rig configuration

Computational domain





Mesh distribution in the vertical and horizontal plan.

- The computational domain dimensions are 40 m x 40 m x 15 m to also enable the pressure sensor measurements at 16 m from the pipe rig.
- Cell size varied from 5 mm at the ignition location to 0.5 m at the

Numerical Setup

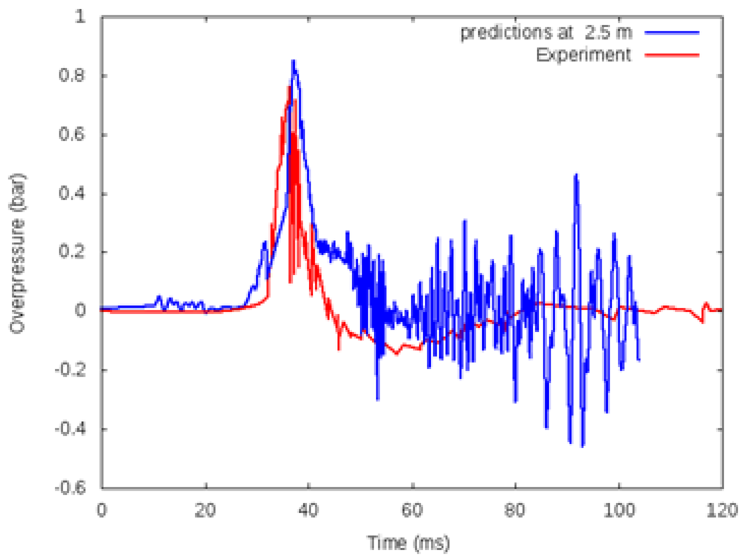
- Boundary conditions

Variable	boundary	condition
velocity	Opening	ZeroGradient
	Wall	No-Slip
Pressure	Opening	WaveTransmissive
	Wall	Zero Gradient
Temperature	Opening	inletOutlet
	Wall	FixedValue

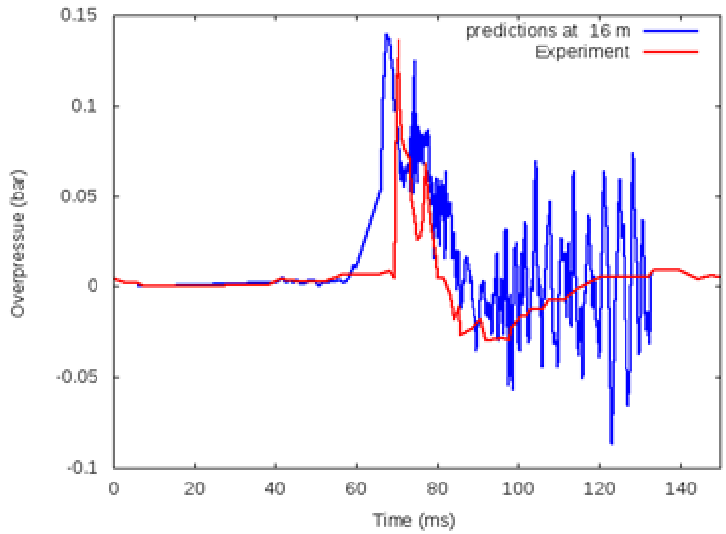
- The flow field is initialized with zero mean and u' = 0.1 m/s rms velocity.
- The mixture faction value of 0.0356 was initialized for the near stoichiometric mixtures in region of premixed vapor cloud.

Numerical predictions Vs Experiments

Hydrogen15 : 4 - gate



(a) 2.5 m

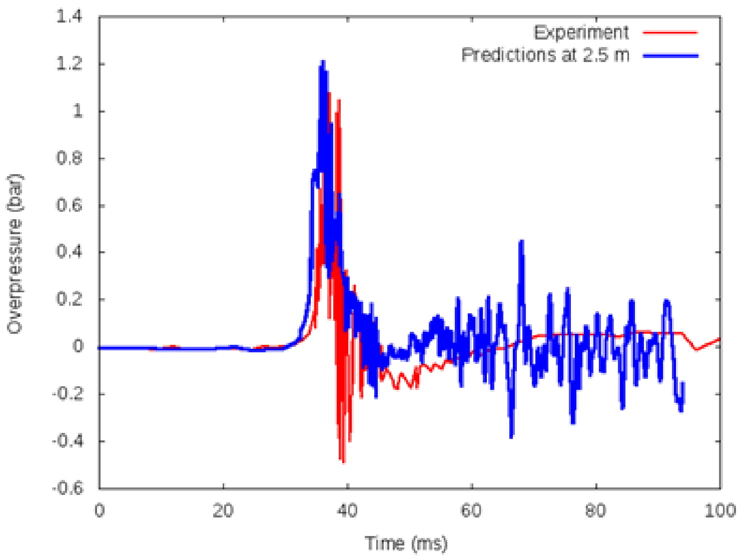


(b) 16 m

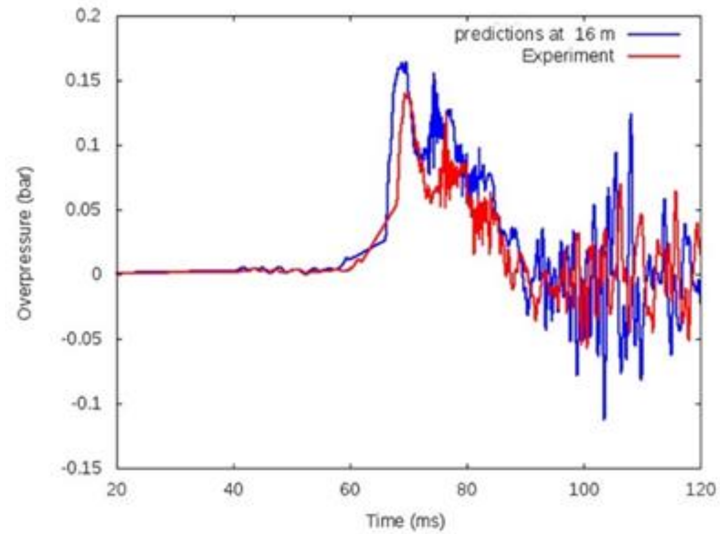
Overpressure trace curve at the probe location

Numerical predictions Vs Experiments

Hydrogen16 : 7- gate
nt



(a) 2.5 m



(b) 16 m

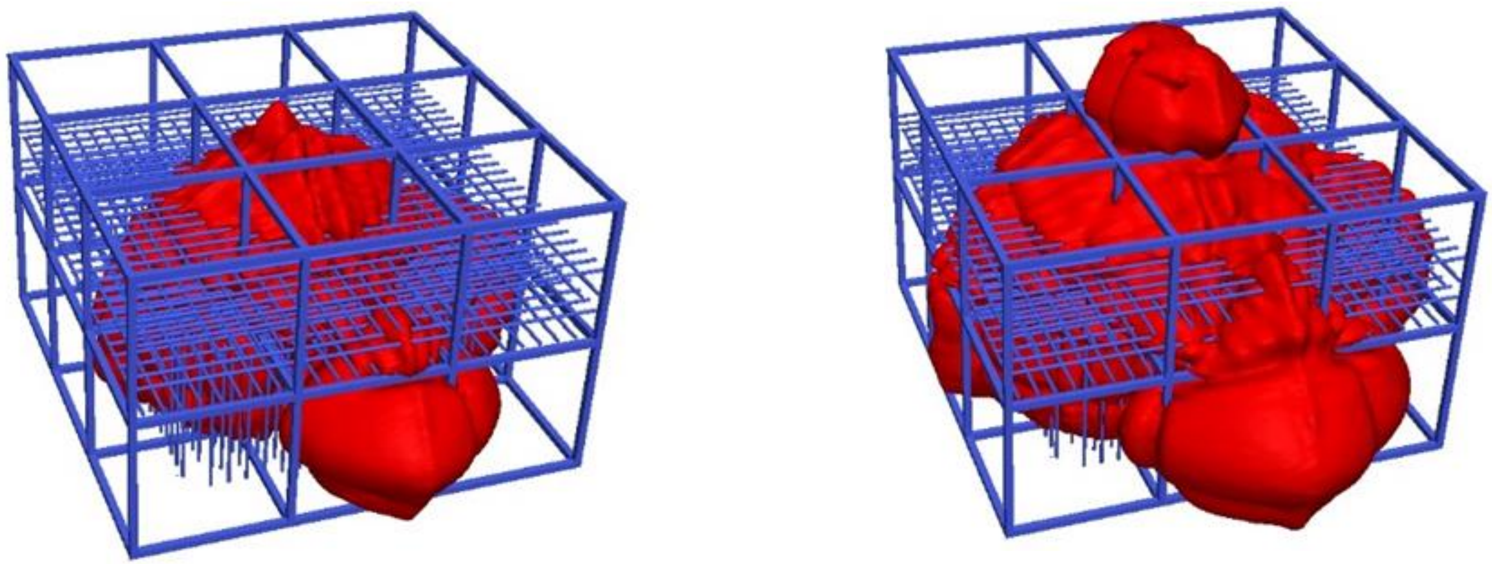
Overpressure trace curve at the probe location

Overall Overpressure trends

S.0	Test	No. of gates	laminar flame speed (m/s)	Equivalence ratio	Experiments overpressure (bar)		Predicted overpressure (bar)	
					at 2.5 m	at 16 m	at 2.5 m	at 16 m
1	Hydrogen16	7	2.38	1.167	1.17	0.148	1.21	0.172
2	Hydrogen15	4	2.52	1.253	0.72	0.145	0.822	0.148
3	hydrogen07	7	1.89	0.967	-	-	0.931	0.233
4	Hydrogen06	4	1.89	0.969	0.48	0.152	0.61	0.186
5	Hydrogen05	7	0.45	0.5	-	-	0.356	0.083
6	Hydrogen04	4	0.45	0.5	-	-	0.282	0.052

Summary of the peak overpressure magnitudes

Flame dynamics



(a) (b)

Flame front contour at some instant of time propagation

Conclusion Remarks

- Solver for hydrogen deflagration modelling in LES method.
- Flame area wrinkling model is used for modelling turbulent deflagrations.
- Exact experiments geometry details are included in modelling.
- Two gates congestions and three hydrogen-Air mixtures are numerically simulated and the predictions are compared with available experimental results.
- Discussed overpressure trends for change in congestion and concentrations of H_2 .
- Parametric study to aid in filling the experimental knowledge gaps.

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