Institute of Particle Science and Engineering
SCHOOL OF PROCESS, ENVIRONMENTAL, AND MATERIALS ENGINEERING

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RANS modelling of confined, vented explosions of methane-hydrogen mixtures for the NATURALHY project

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Overview

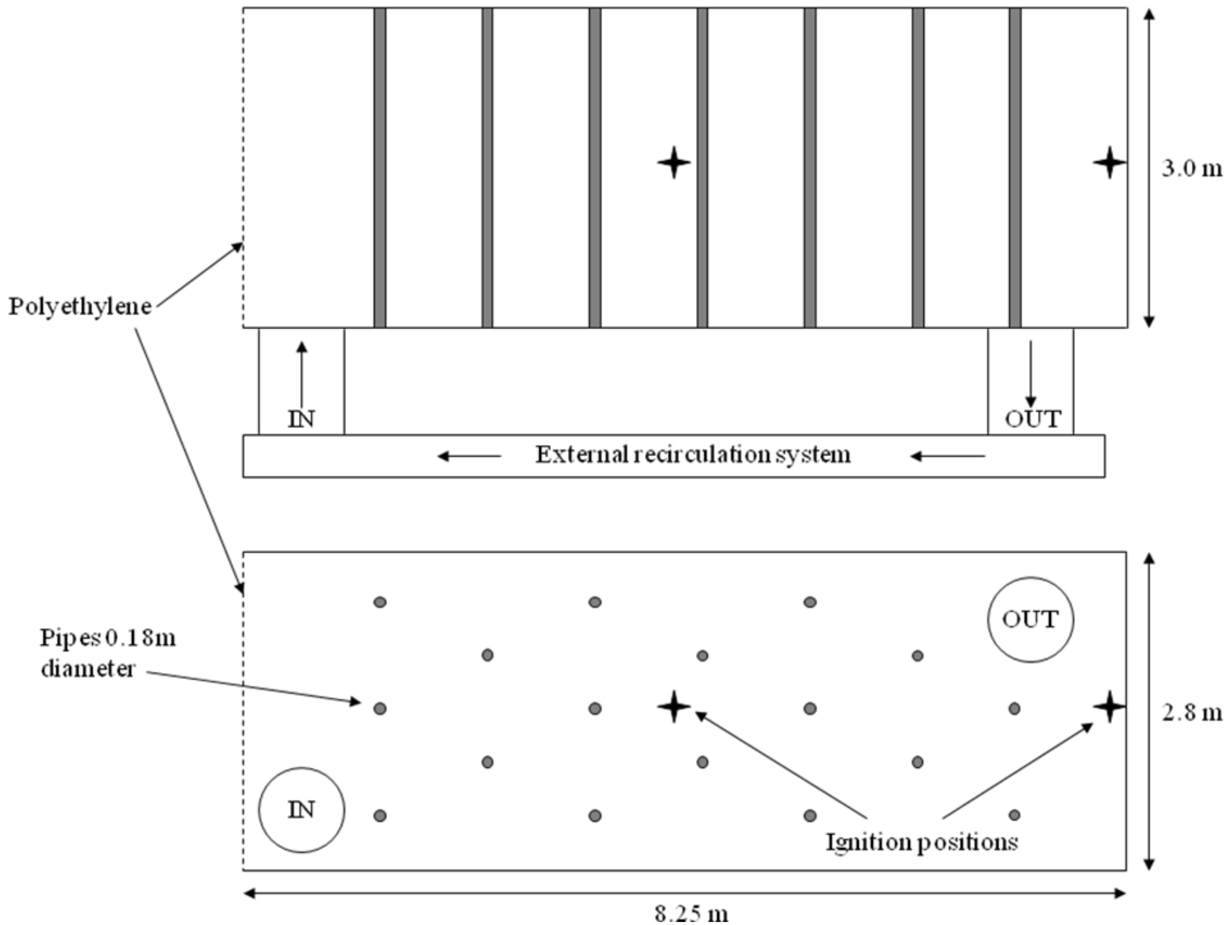
- Introduction.
- Experimental Configuration.
- Mathematical Model and Numerical Solution.
- Results.
- Conclusions.

Introduction

- Increasing interest in use of hydrogen as an energy carrier.
- Work undertaken as part of the NATURALHY project.
- Hydrogen transported in gas network as mixture.
- Essential to investigate the behaviour of such gaseous releases.
- Work concerns confined, venting explosions of 0%, 20%, and 50% H_2 v/v and CH_4 mixtures with and without congestion.

Experimental Configuration

Experimental Configuration



Test Number	Fuel / CH_4:H_2	Congestion / pipes	Ignition location
1	100:0	None	Centre
2	80:20	None	Centre
3	50:50	None	Centre
4	80:20	17	Centre
5	50:50	17	Centre
6	100:0	None	Rear
7	80:20	None	Rear
8	50:50	None	Rear
9	80:20	17	Rear
10	50:50	17	Rear

Mathematical Model and Numerical Solution

- Flow fields resolved by solution of time-dependent, density-weighted, partial differential equation conserving mass, momentum, total energy, and a reaction progress variable.
- Godunov's method applied to convective and pressure fluxes. Central differencing used to approximate diffusion and source terms.
- Adaptive grid algorithm enables finer grids to be applied in regions of high spatial and temporal variation.
- Equation set closed with standard k-ε model and Jones and Musonge second-moment model.

Mathematical Model and Numerical Solution

- Premixed combustion represented by conservation of a reaction progress variable, with a source term prescribed using a modified form of an eddy break-up reaction-rate expression.

$$\overline{\rho S(c)} = \overline{\rho R_c} \qquad \overline{\rho S(E)} = \overline{\rho R_c q}$$

$$\overline{\rho R_c} = \bar{\rho} R \tilde{c}^4 (1-\tilde{c}) \left(\frac{\rho_u}{\rho_b} \right)^2 \qquad q = \left(\frac{p_o}{\rho_u} \right) \left(\frac{\rho_u}{\rho_b} - 1 \right) \frac{\gamma}{(\gamma - 1)}$$

- Form of reaction rate expression eliminates the cold-front quenching problem.

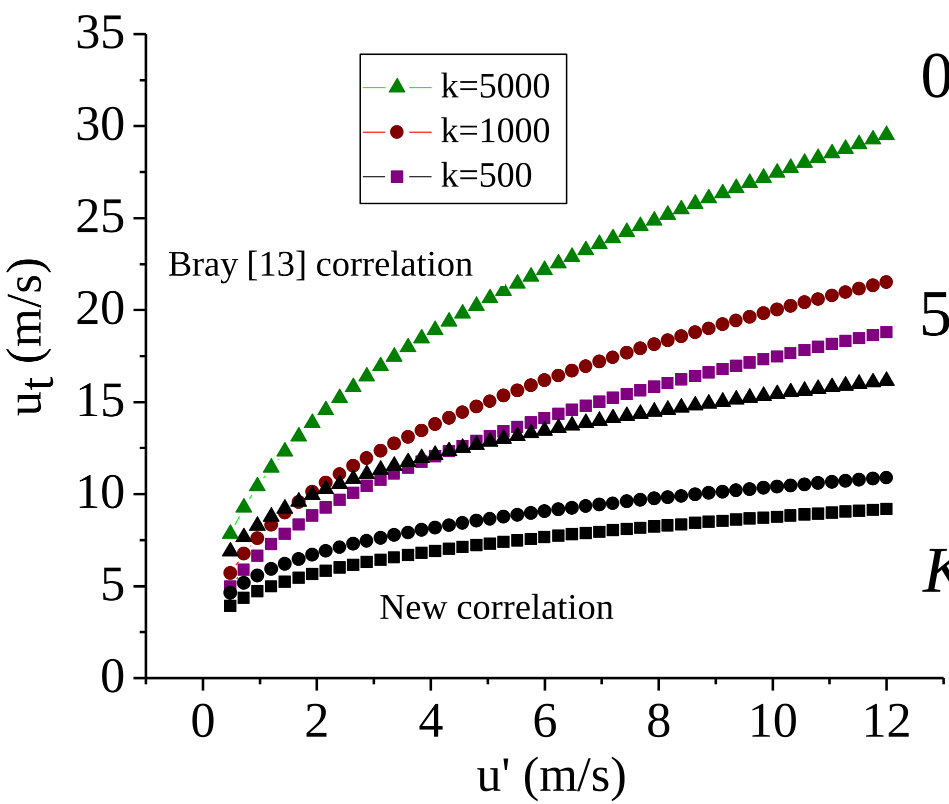
Mathematical Model and Numerical Solution

- Knowledge of turbulent burning velocity and turbulent flame thickness and using the analysis of Catlin and Lindstedt, reaction rate and turbulent diffusion coefficient can be prescribed as:

$$\Gamma = \frac{u_t \delta_t}{\Lambda_1 \Lambda_2} \qquad R = \frac{u_t \Lambda_2}{\delta_t \Lambda_1}$$

- Flame thickness is approximated as a turbulent length scale. Turbulent burning velocity prescribed using latest experimental data from University of Leeds.
- Approach ensures that solutions give rise to a flame which reproduces specified burning velocities.

Burning Velocities



$0-20\%$ $$\frac{u_t}{u_l} = 0.37K^{(-0.49)}\frac{u'}{u_l}$$

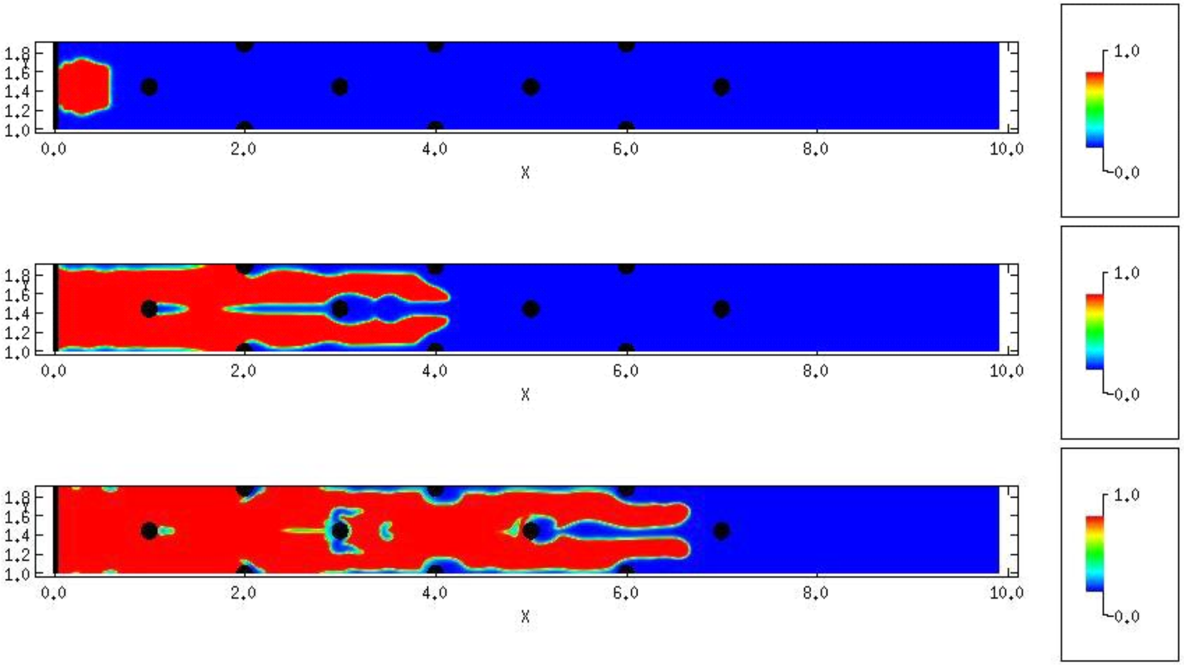
50% $$\frac{u_t}{u_l} = 0.54K^{(-0.47)}\frac{u'}{u_l}$$

$$K = 0.157\left(\frac{u'}{u_l}\right)^2 \frac{1}{\sqrt{R_l}}$$

$$R_l = \bar{\rho}u'\frac{\delta_t}{\mu_l}$$

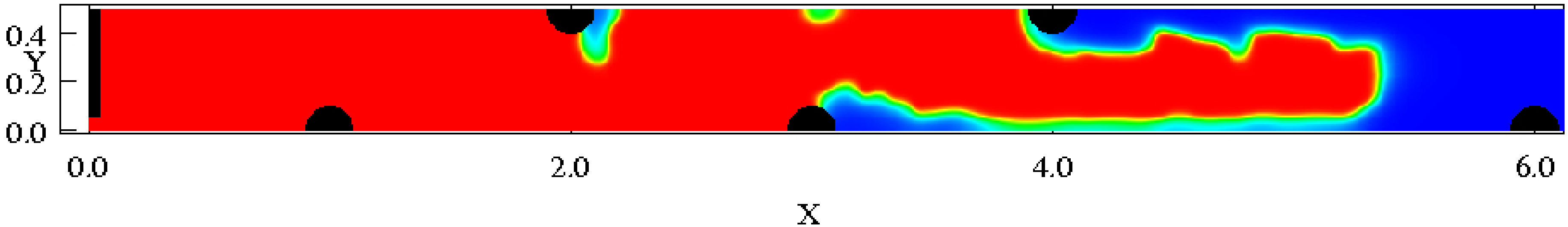
Mathematical Model and Numerical Solution

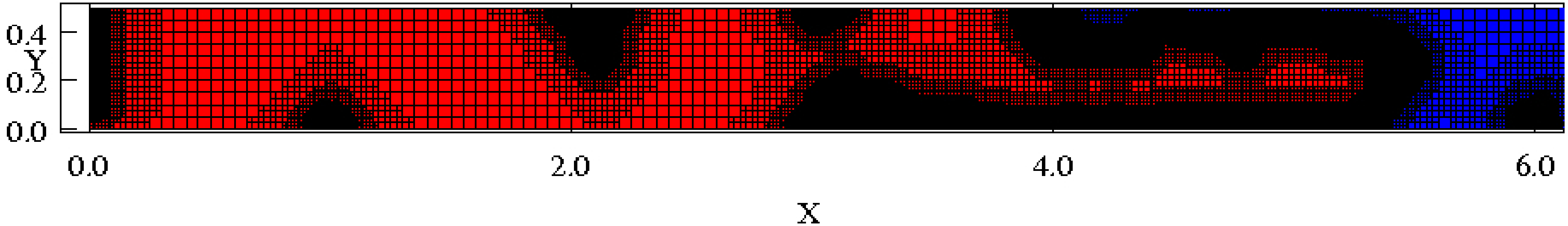
- Geometry modelled using three approaches.
  - 2-d symmetry approach



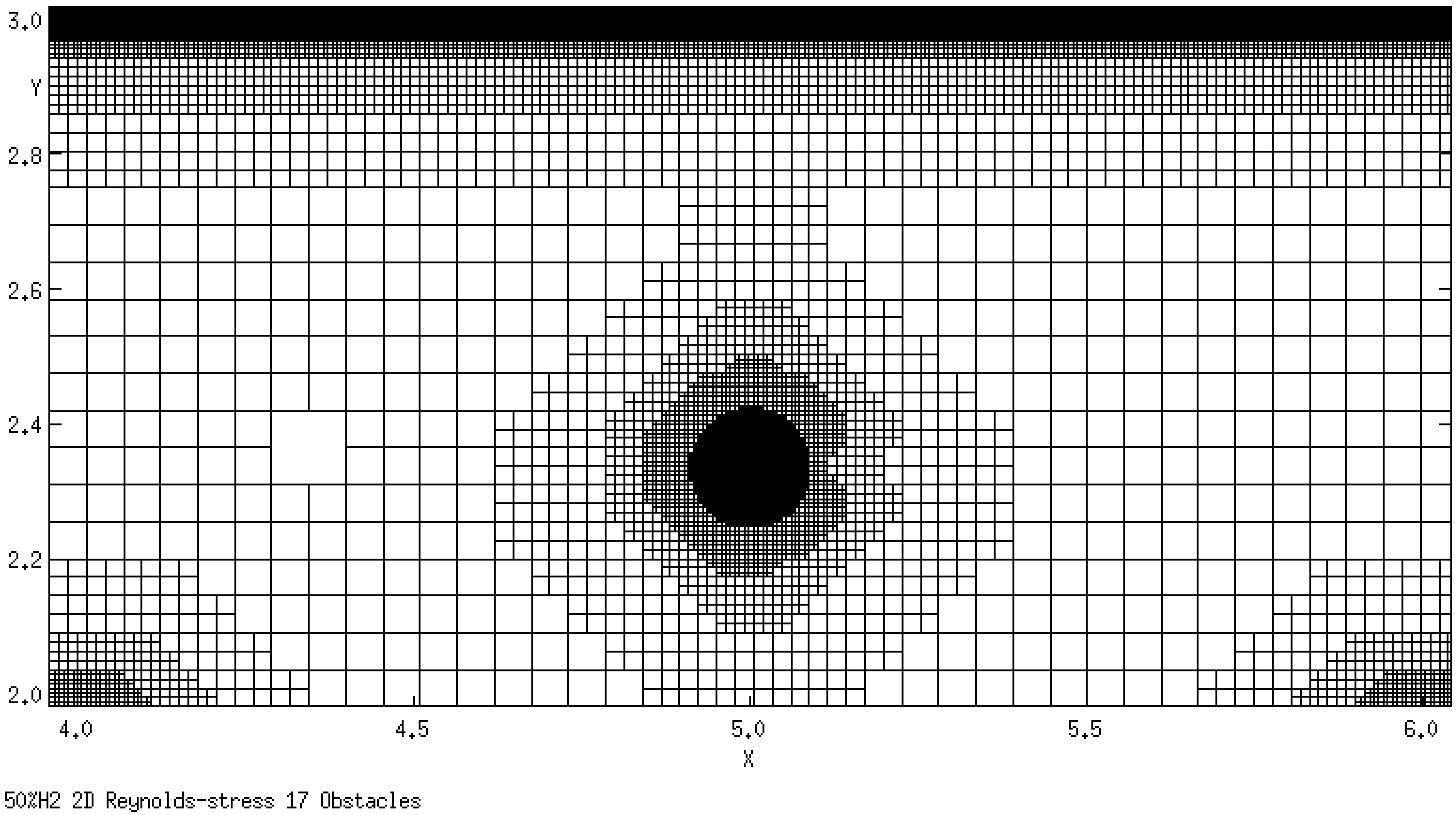
Mathematical Model and Numerical Solution

- Grid adaption at obstacles and flame front



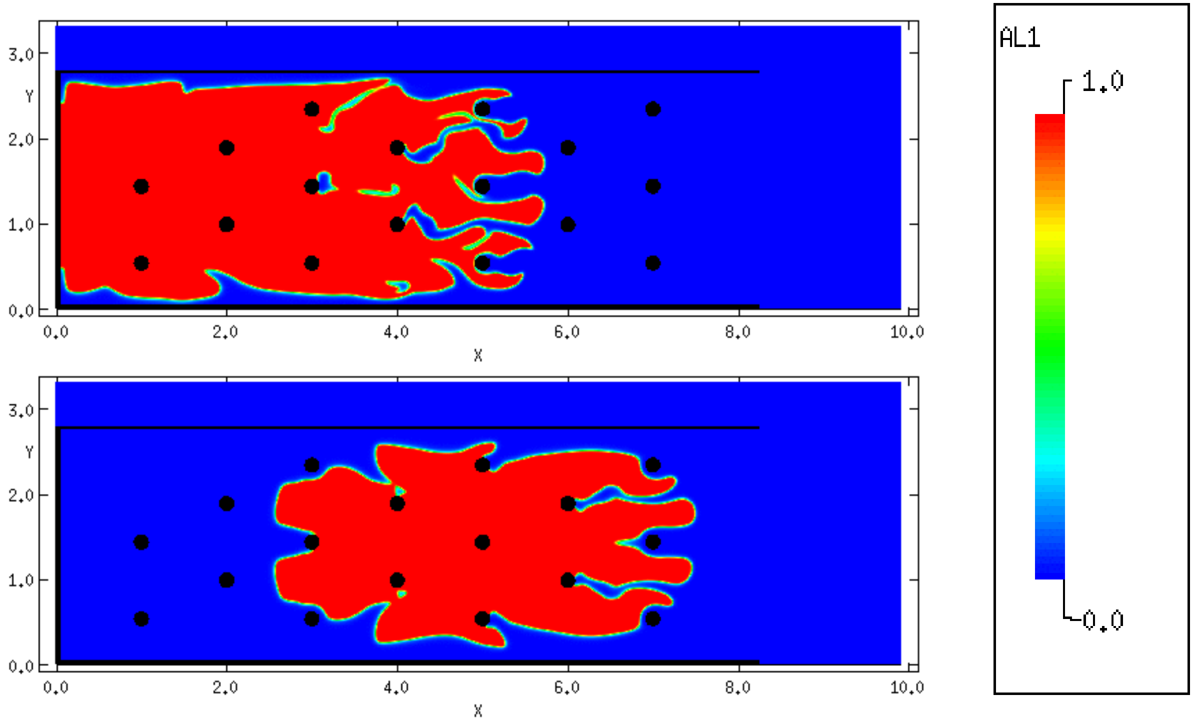


Mathematical Model and Numerical Solution



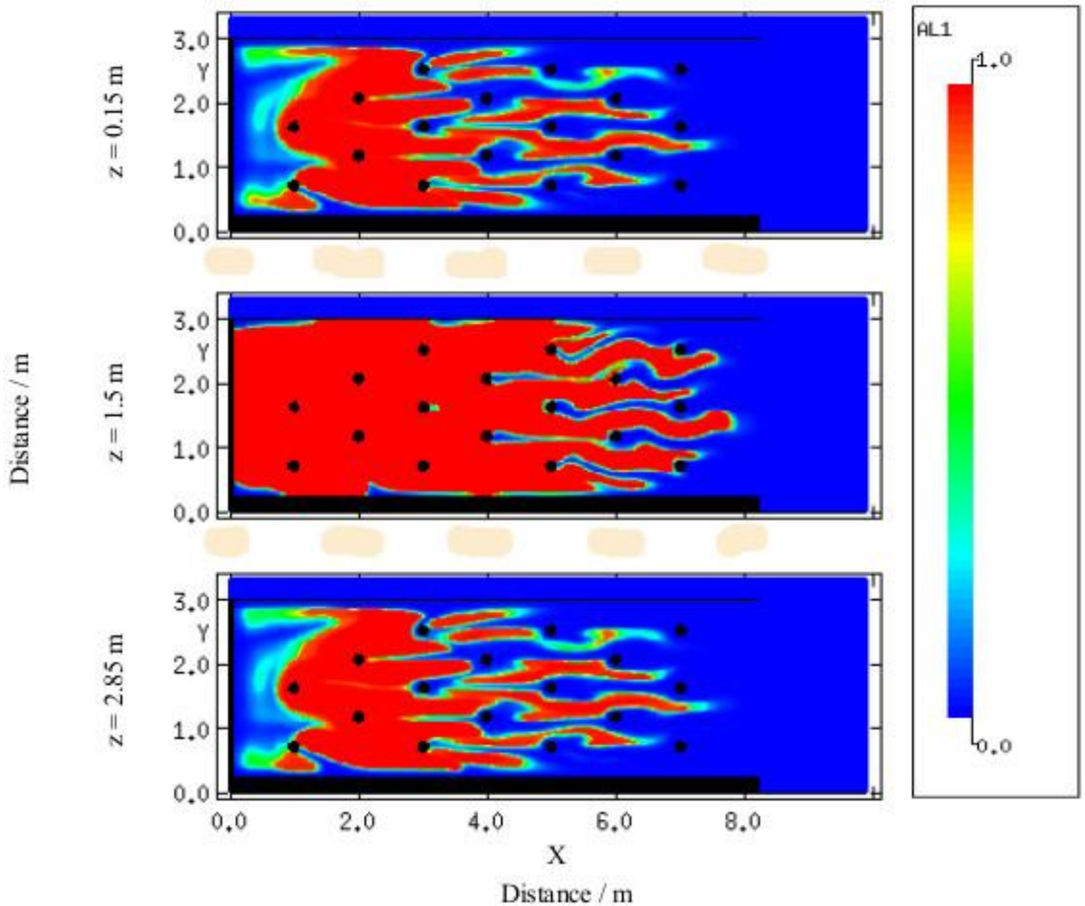
Mathematical Model and Numerical Solution

- 2-d



Mathematical Model and Numerical Solution

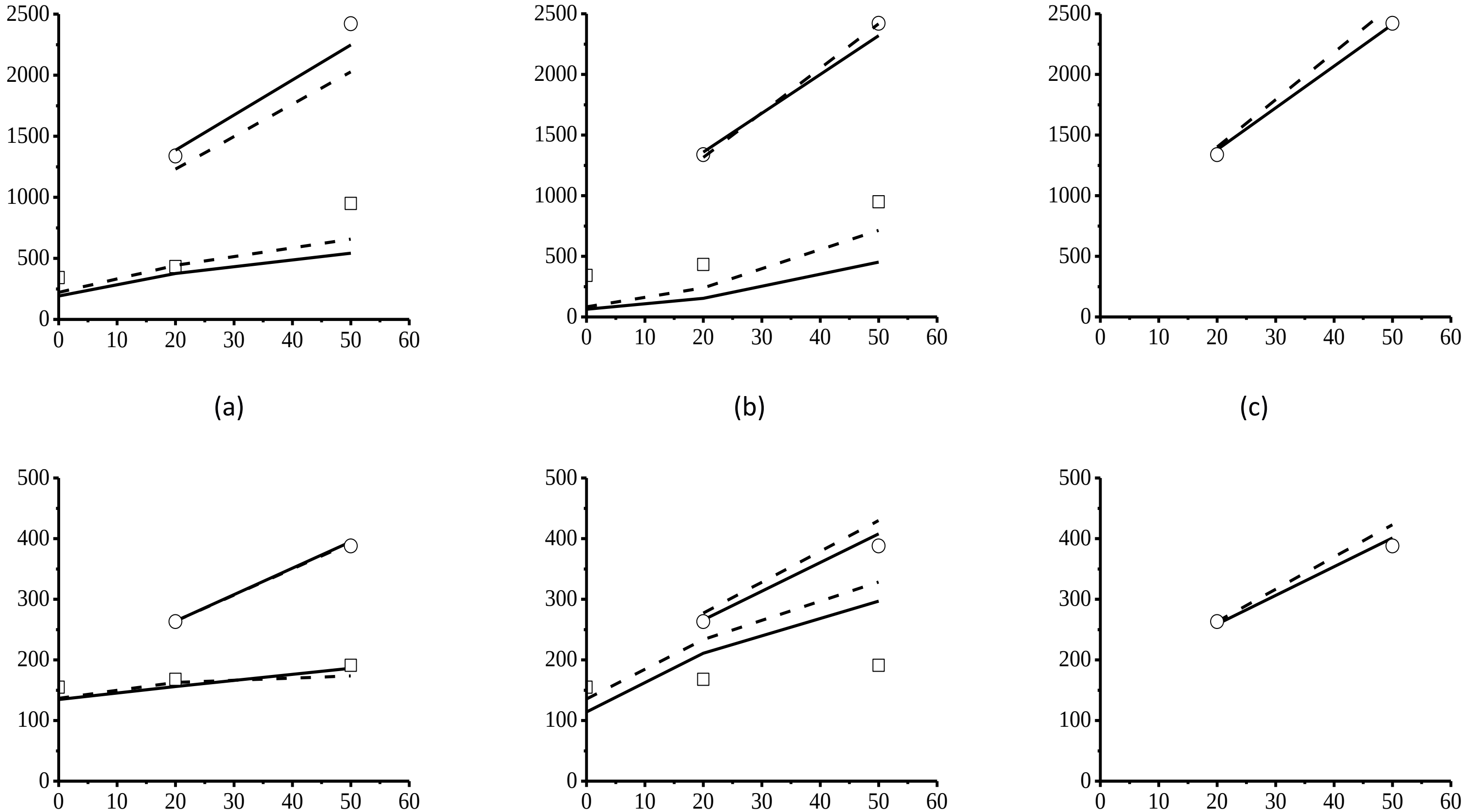
- 3-d



Results

Maximum overpressure / mbar

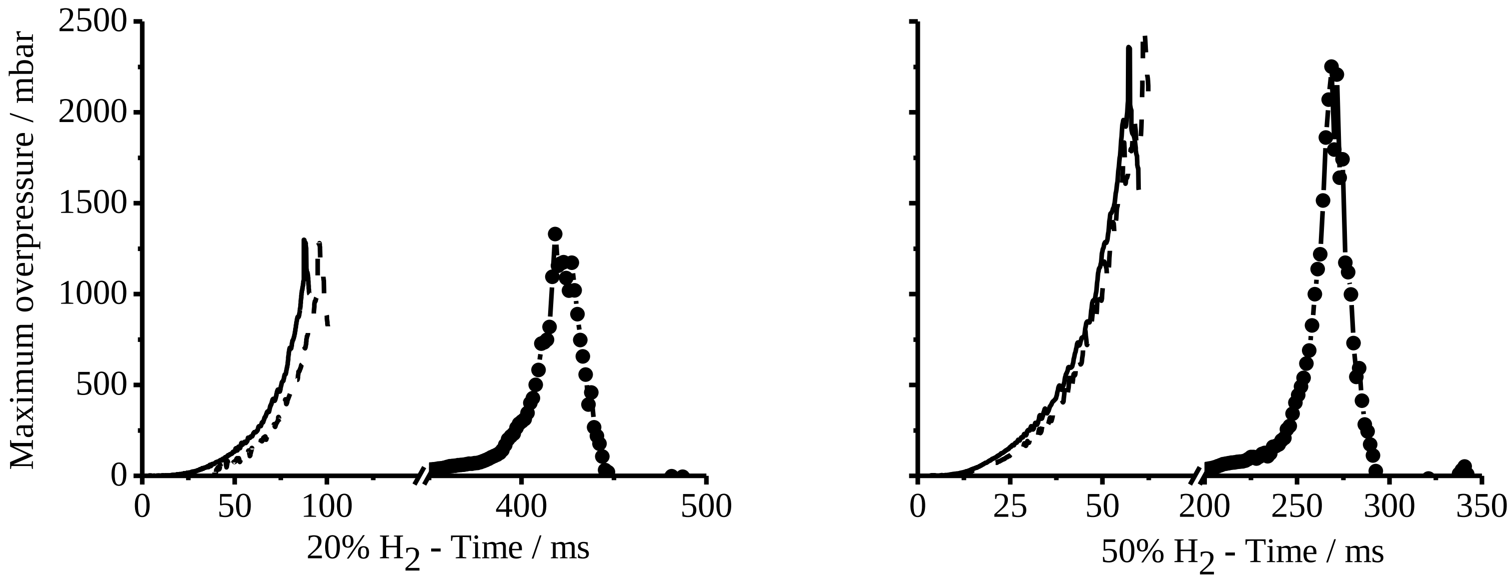
Flame speed at exit / m s^{-1}



(a) (b) (c)

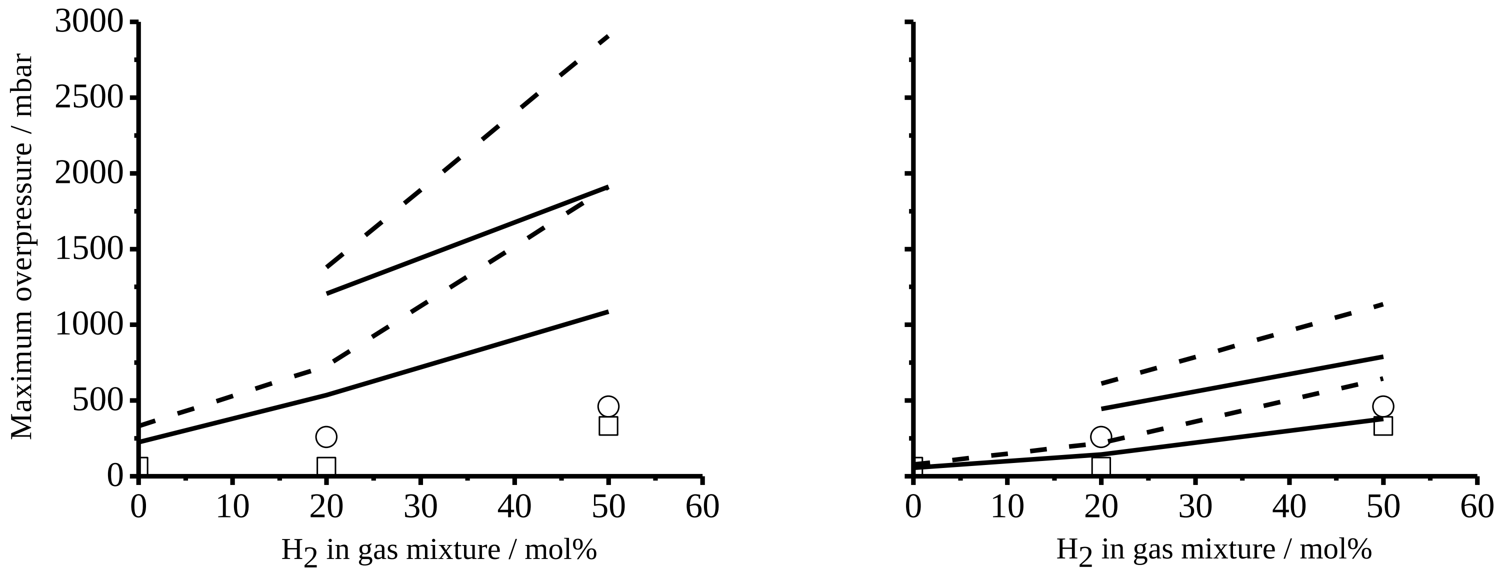
H_2 in gas mixture / mol%

Results



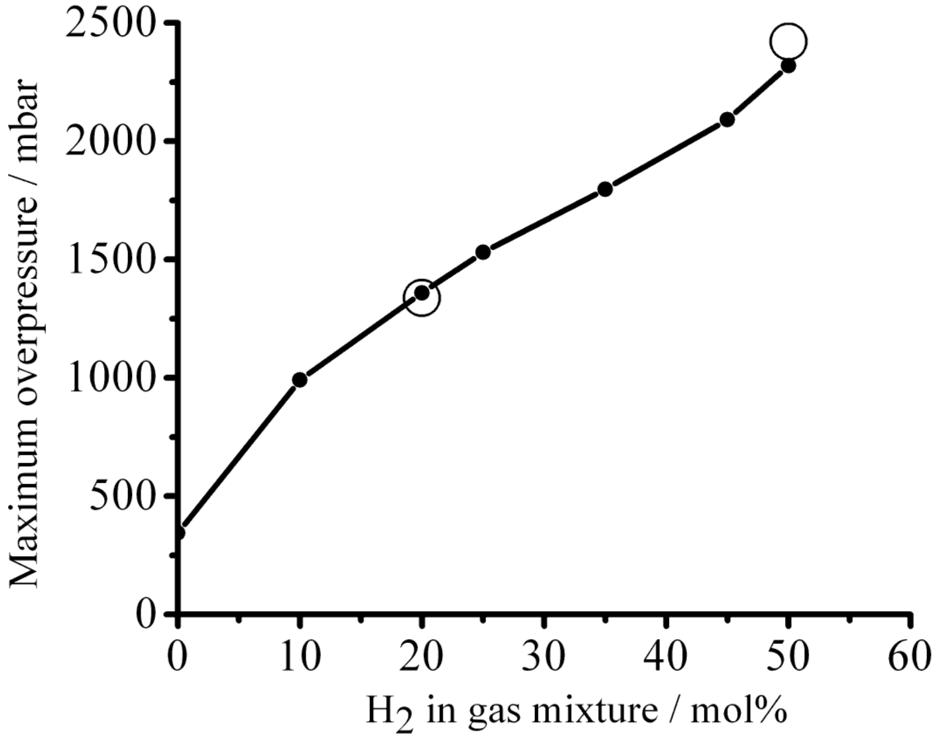
Pressure traces of observed peaks for 17 obstacle geometry with 20% and 50% hydrogen concentrations (symbols – experiment, solid line – Reynolds stress, dashed line – k-ε) calculated using the 3-D approach for the rear ignited cases.

Results



Maximum overpressures observed for 0 and 17 obstacle geometries and 0%, 20% and 50% hydrogen concentrations (symbols – experiment; o 21-objects, □ 0-objects; solid line – Reynolds stress; dashed line – k-ε) calculated using the symmetry approach (left) and 2-D approach (right) for the centrally ignited case.

Results



Maximum overpressure versus H_2 content of mixture for 17 obstacle rear-ignited case (symbols – data, solid line – Reynolds stress).

Conclusions

- Reynolds-stress turbulence model applied to prediction of large-scale vented explosions, coupled to turbulent premixed combustion model, for first time.
- Reynolds-stress model is generally at variance with isotropic approach, although differences in predicted overpressures and flame-front velocities often small.
- Combustion model, incorporated with the most recently available experimental data, can predict to a high degree of accuracy.
- 45% level of H_2 concentration could be a barrier in the consideration of mixture usage.
- 2-dimensional calculations viable for future studies.

Future work

- Code is now parallel. Further 3-dimensional work can be undertaken to validate the models.

- Consideration of laminar to turbulent transition.

- Moving towards LES with greater processor availability.

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