Evaluation of the ADREA-HF CFD code against a hydrogen deflagration in a tunnel

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1. Introduction

- Hydrogen
  - very promising alternative fuel
  - significant reductions in greenhouse gas emissions
  - significant improvements in energy efficiency

- Safety issues
  - flammable mixture over a wide range of concentrations
  - slow or fast deflagrations, or even detonations

- CFD: attractive numerical methodology for risk assessment of hydrogen applications
  - high accuracy capabilities
  - can evaluate regulations and standards and provide a new insight

1. Introduction – Aim of the work

- ADREA-HF: a well known CFD code which has been extensively validated against hydrogen dispersion applications

- The **aim of this work** is the evaluation of the recently incorporated in the ADREA-HF combustion model against a near stoichiometric hydrogen-air deflagration experiment in a tunnel

- Generated overpressures
  - The accurate prediction of the overpressure generated by the explosion is a crucial point in assessing hydrogen safety
  - Difficult task as it depends on many factors such as mixture composition, turbulence-chemistry interactions, geometry of the problem and several other physical mechanisms

2. Mathematical Methodology

- Governing equations
  - Navier-Stokes equations
  - Continuity equation
  - Energy equation (conservation equation of static enthalpy)
  - Conservation equations of the mass fraction of the primary species that take part in the combustion process (we assume 1-step reaction)

$$\frac{\partial \bar{\rho}\tilde{q}_k}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j \tilde{q}_k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Sc_t}\frac{\partial \tilde{q}_k}{\partial x_j}\right) + \bar{R}_k, \quad k = 1,\ldots,N_{subs}$$

Reaction rates of species are not independent from each other and can be expressed as a function of the fuel reaction rate as:

$$\bar{R}_k = \frac{\nu_k \cdot MW_k}{\nu_f \cdot MW_f} \cdot \bar{R}_f$$

- Turbulence modelling
  - RNG LES model
  - RNG k-ε model

2. Mathematical Methodology - Combustion model

- The implemented in the ADREA-HF code combustion model was originally developed in the UU [1].
- Gradient method: $\bar{R}_f = \rho_u S_t \left|\nabla q_f\right|$
- The main concern in this type of models is the calculation of the turbulent flame speed.
  - Modified Yakhot's equation

$$S_t = S_t^{SGS} \cdot \exp\left(\frac{u'_{sgs}}{S_t}\right)^2 = \Xi_k \cdot \Xi_{lp} \cdot \Xi_f \cdot S_u \cdot \exp\left(\frac{u'_{sgs}}{S_t}\right)^2$$

Wrinkling factor (**turbulence generated by the flame front itself**): $\Xi_k = 1 + (\psi \, \Xi_k^{\max} - 1) \cdot \left[1 - \exp(-R/R_0)\right]$

Leading point concept[2]: $\Xi_{lp} = \max\left(1 + \frac{(\Xi_{lp}^{\max} - 1) \cdot 2R}{R_0}, \Xi_{lp}^{\max}\right)$

Increase of flame surface due to its **fractal** geometry: $\Xi_f = \left(\frac{R}{R_0} \frac{\varepsilon_{R_0}}{\varepsilon_R}\right)^{D_f - 2}, \quad R \geq R_0$

Laminar burning velocity (**chemistry**): $S_u = S_{u0}\left(\frac{T}{T_{u0}}\right)^{m_0}\left(\frac{P}{P_0}\right)^{n_0} = S_{u0}\left(\frac{P}{P_0}\right)^{\varepsilon}$

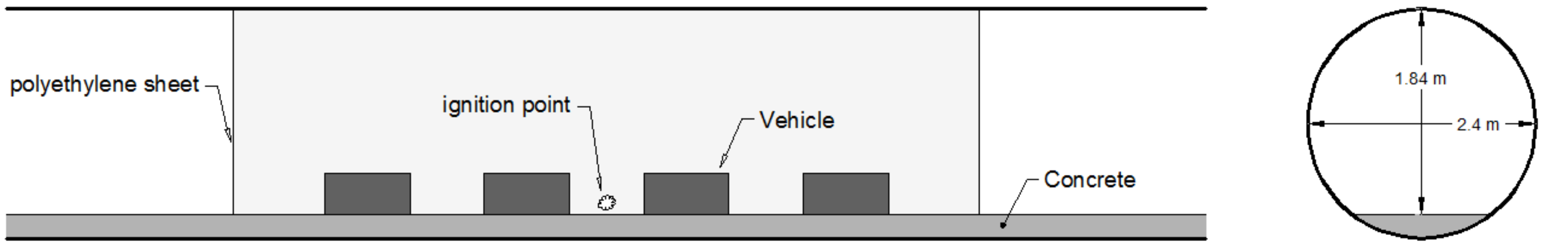
Density of the unburned mixture (ahead of the flame front): $\rho_u = \rho_{u0}\left(\frac{p}{p_0}\right)^{1/\gamma}$

[1]Molkov, V., *Fundamentals of Hydrogen Safety Engineering II, BookBoon, 2012*

[2]Zimont, V.L., Lipatnikov, A.N. (1995). *A numerical model of premixed turbulent combustion of gases. Chemical Physics Reports, 14(7), 993-1025.*

3. Tunnel deflagration experiment overview

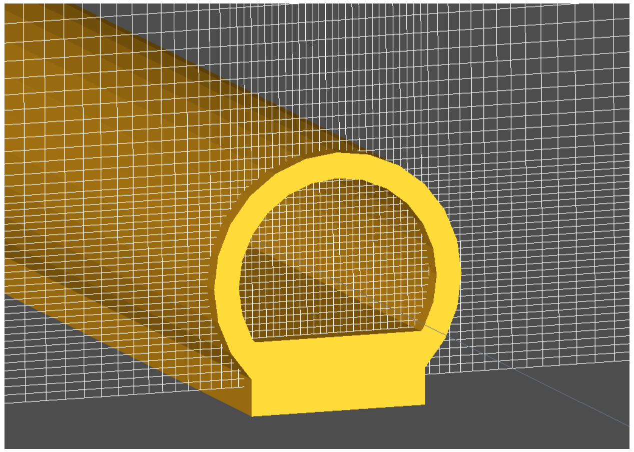
- Hydrogen deflagration in a model of a tunnel
  - Length: 78.5 m
  - Cross-section: part of a 2.4 m diameter circle
  - Homogeneous hydrogen-air mixture of 30% hydrogen volumetric concentration in a 10 m long region in the middle of the tunnel – Ignition at the center
  - Two cases: One with a complete empty tunnel and one with four vehicles positioned inside the mixture
  - Overpressure time history was measured at 1.00, 3.61, 10.61 and 30.40 m from the ignition point

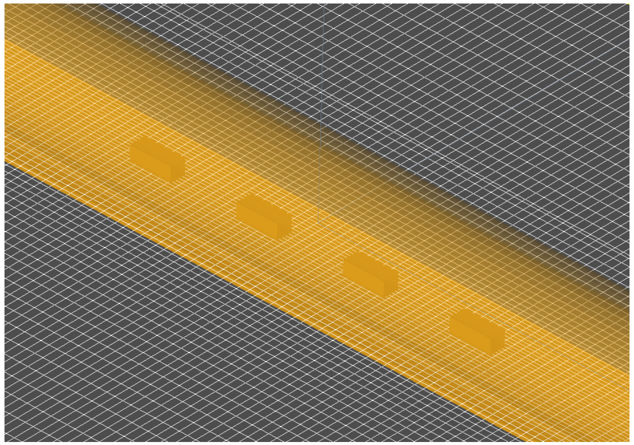


Reference: Groethe, M., et al. "Large-scale hydrogen deflagrations and detonations." *International Journal of Hydrogen Energy,* 32.13 (2007): 2125-2133.

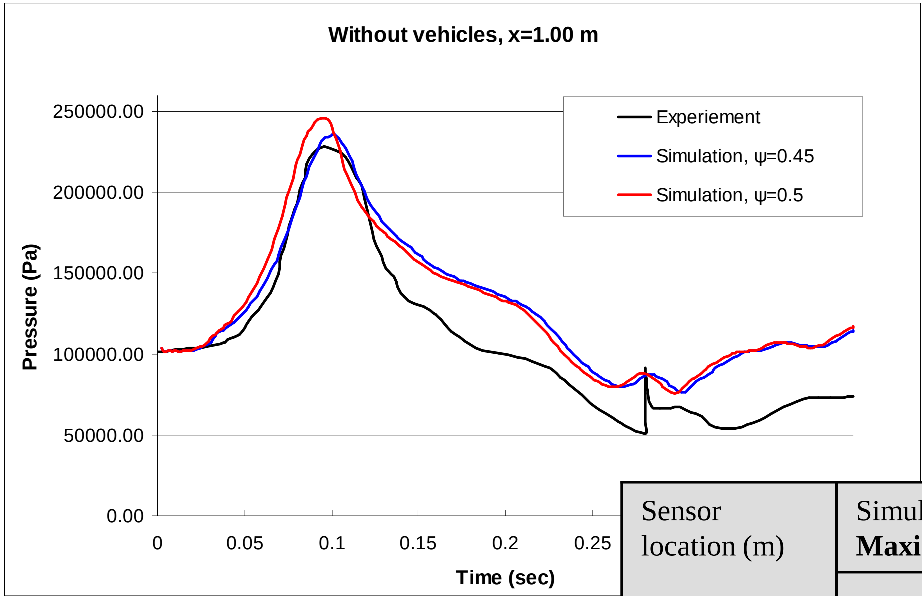
4. Numerical simulation of tunnel deflagration

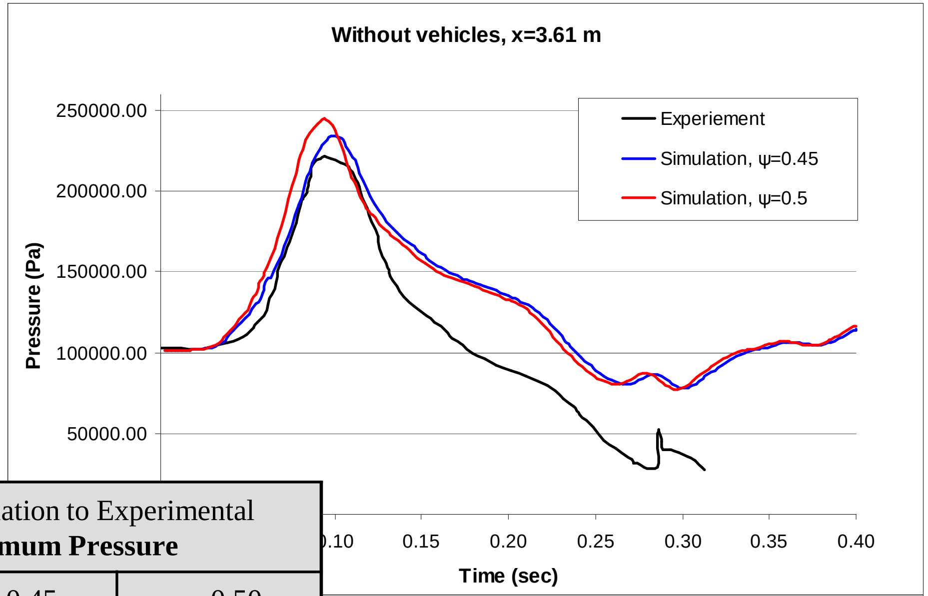
- Computational domain: 200 x 60 x 31 m
- 3D structured grid
  - Basic mesh: 596,692 cells
  - Denser mesh: 941,201 cells
- Convective terms discretization scheme:
  - Momentum equations: 2nd order accurate Bounded Central Differences
  - Species and energy equations: Bounded Linear Upwind
- Temporal discretization scheme: 2nd order accurate Crank-Nicolson
- Non-reflecting boundary conditions for the normal velocities in exit planes

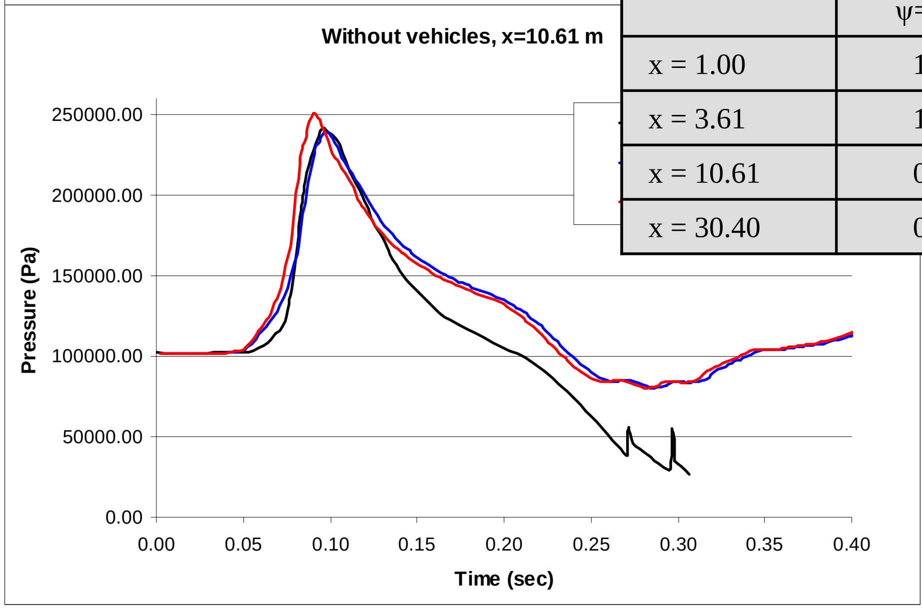


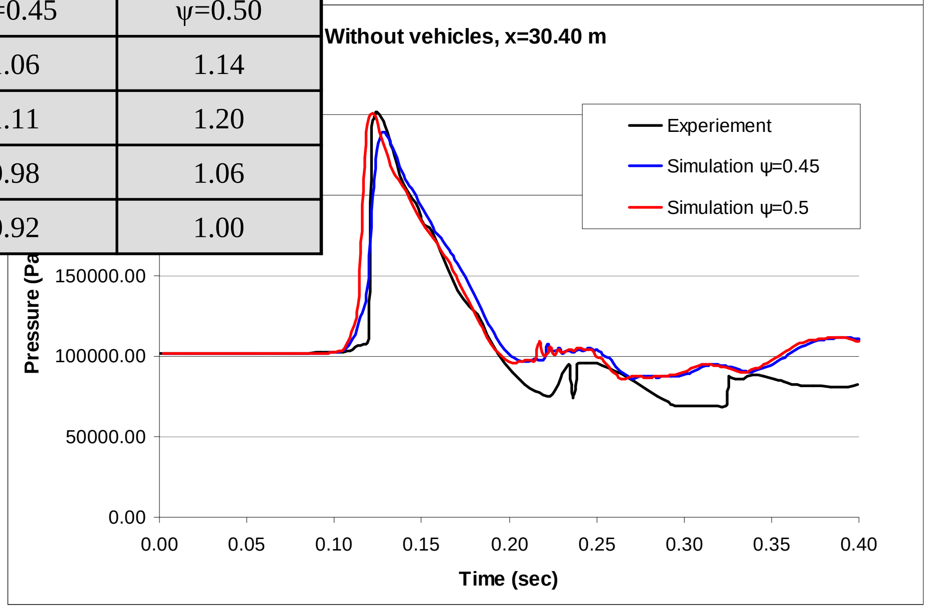


4. Numerical simulation of tunnel deflagration – Empty tunnel case



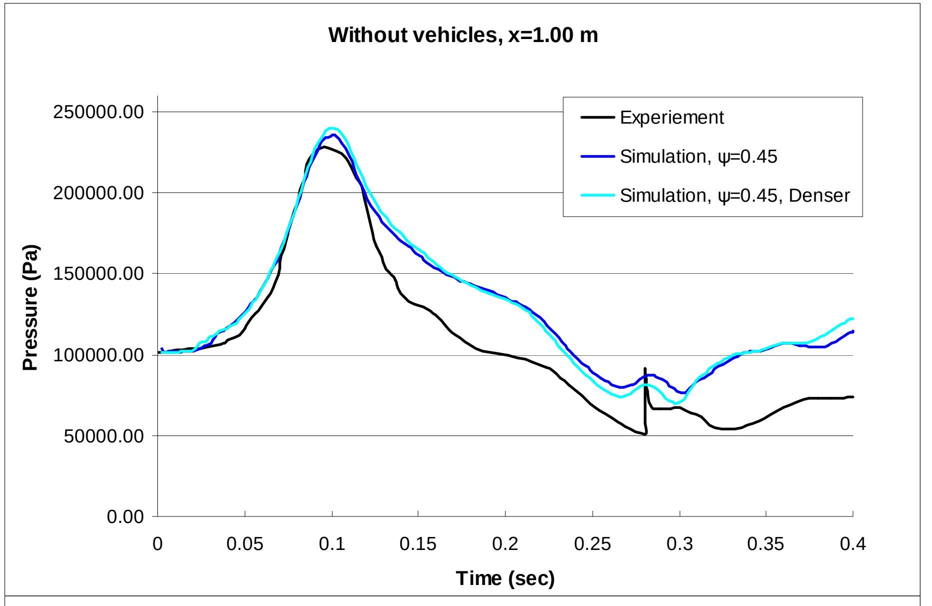


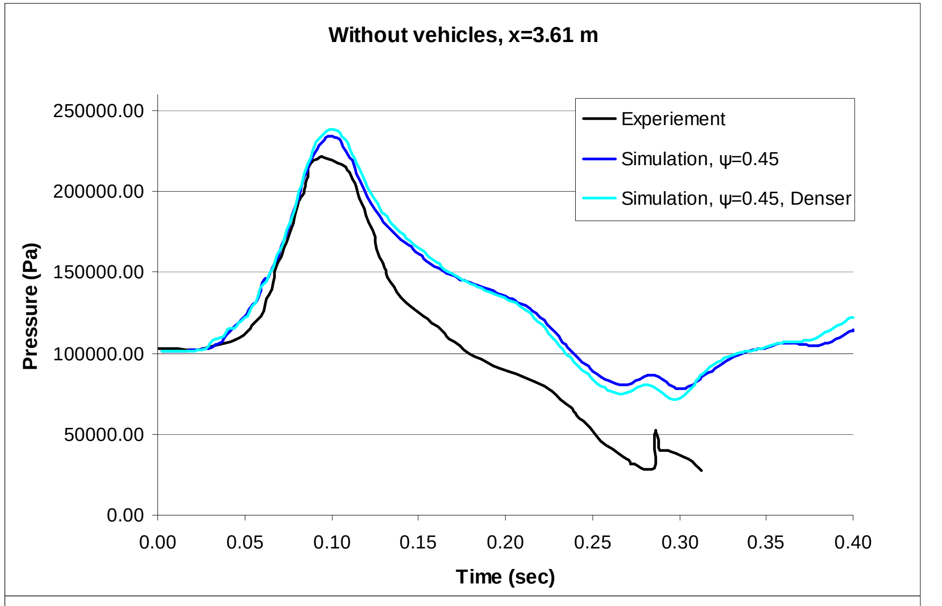


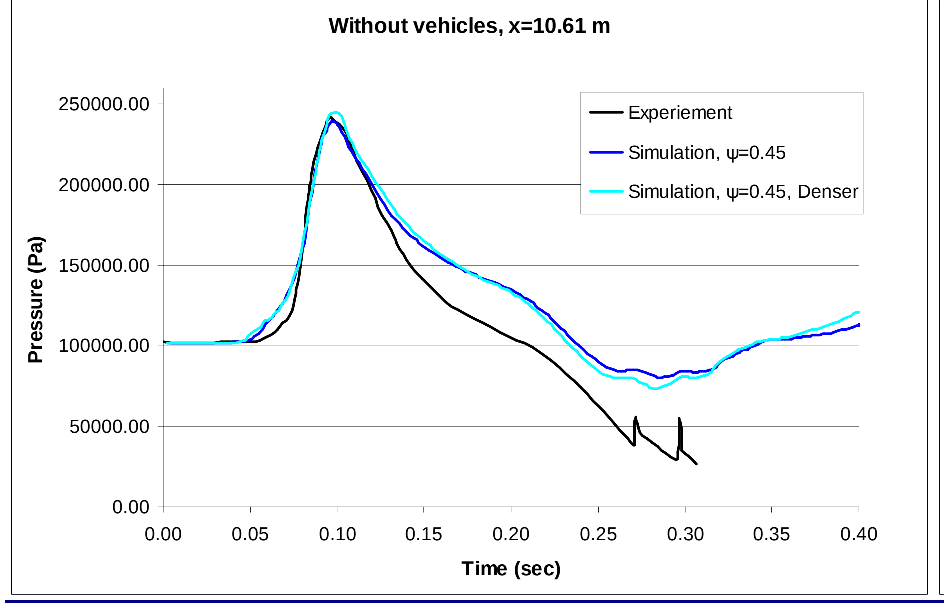


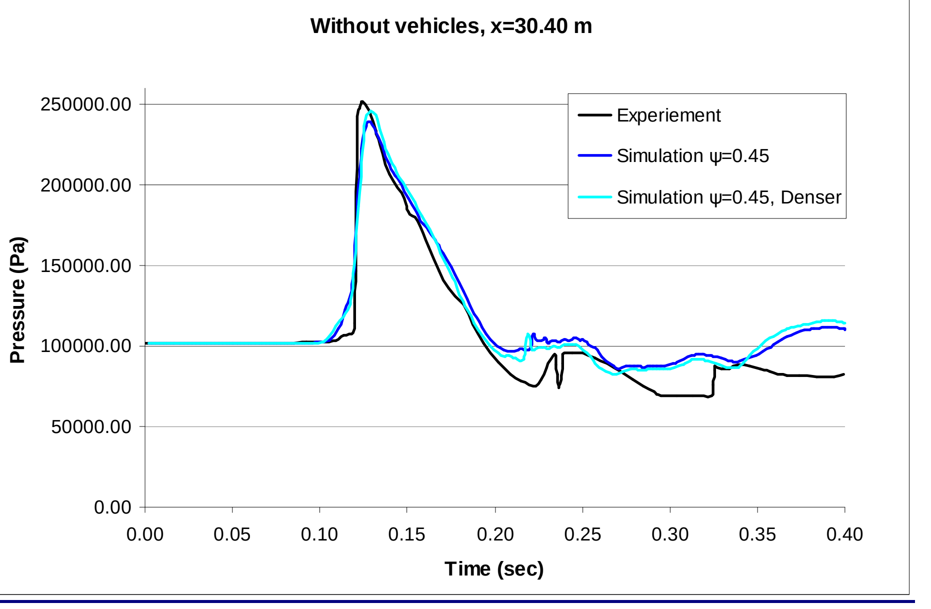
Sensor location (m)	Simulation to Experimental **Maximum Pressure**	
	ψ=0.45	ψ=0.50
x = 1.00	1.06	1.14
x = 3.61	1.11	1.20
x = 10.61	0.98	1.06
x = 30.40	0.92	1.00

4. Numerical simulation of tunnel deflagration – Empty tunnel case









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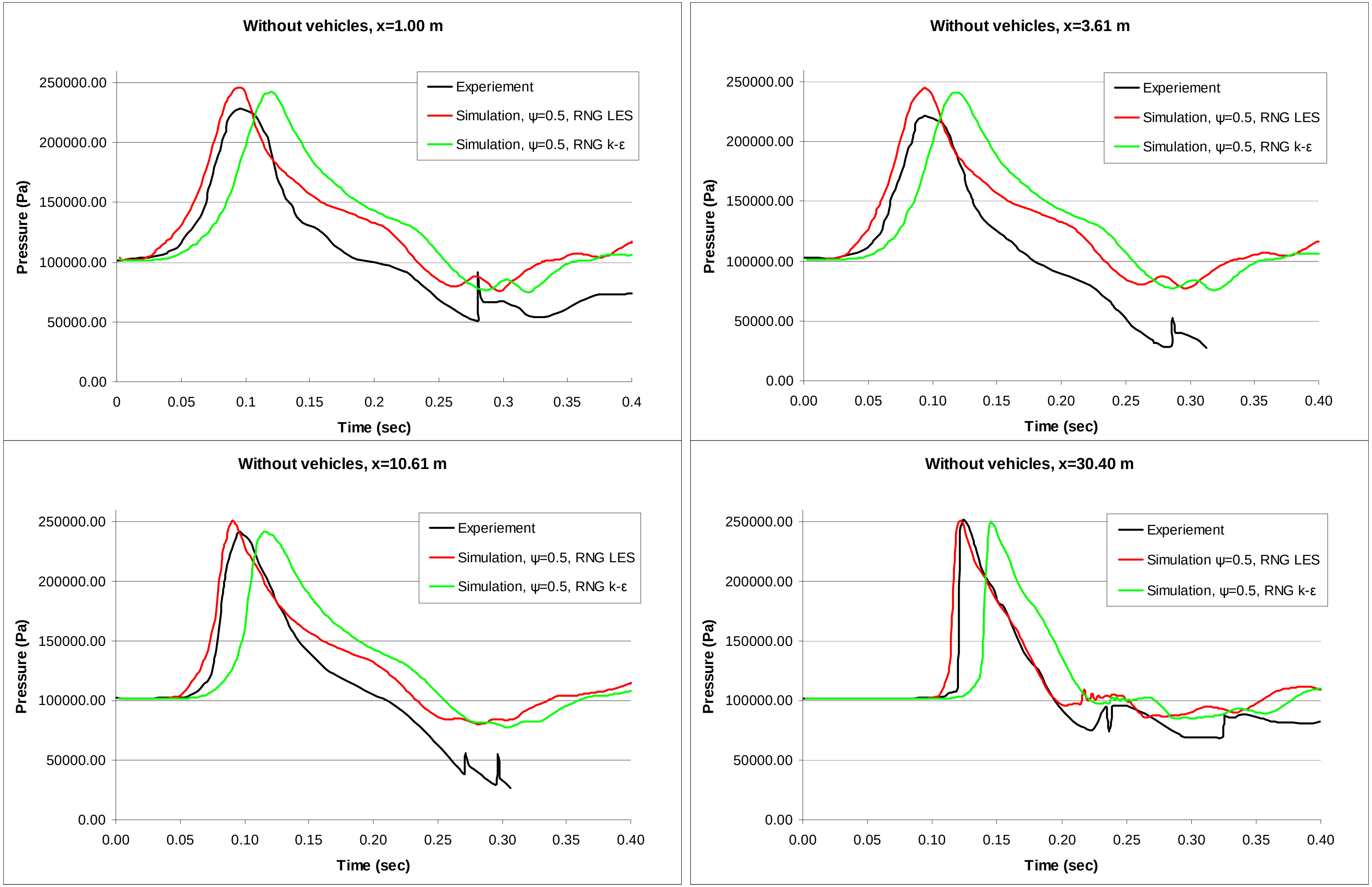

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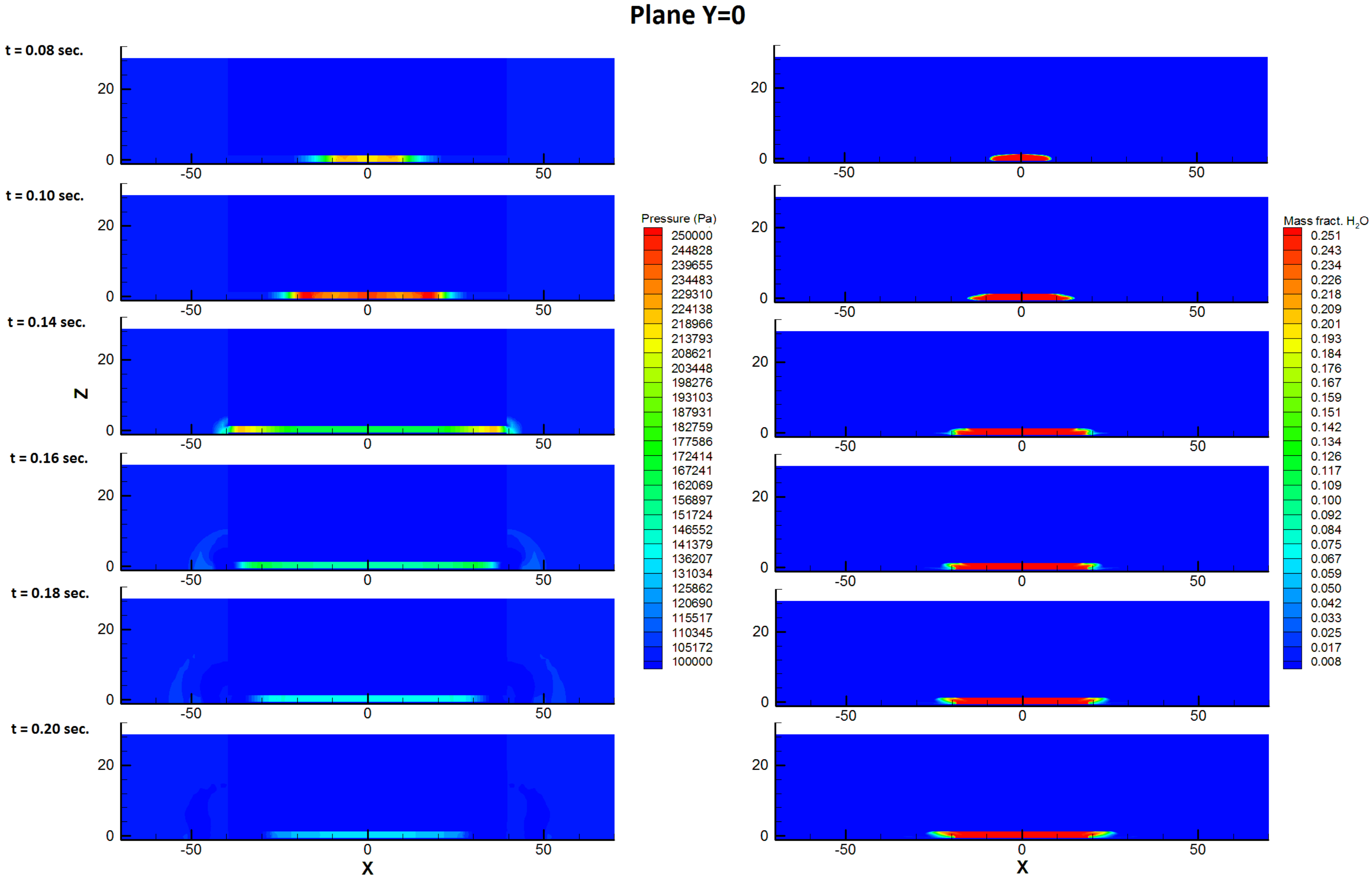
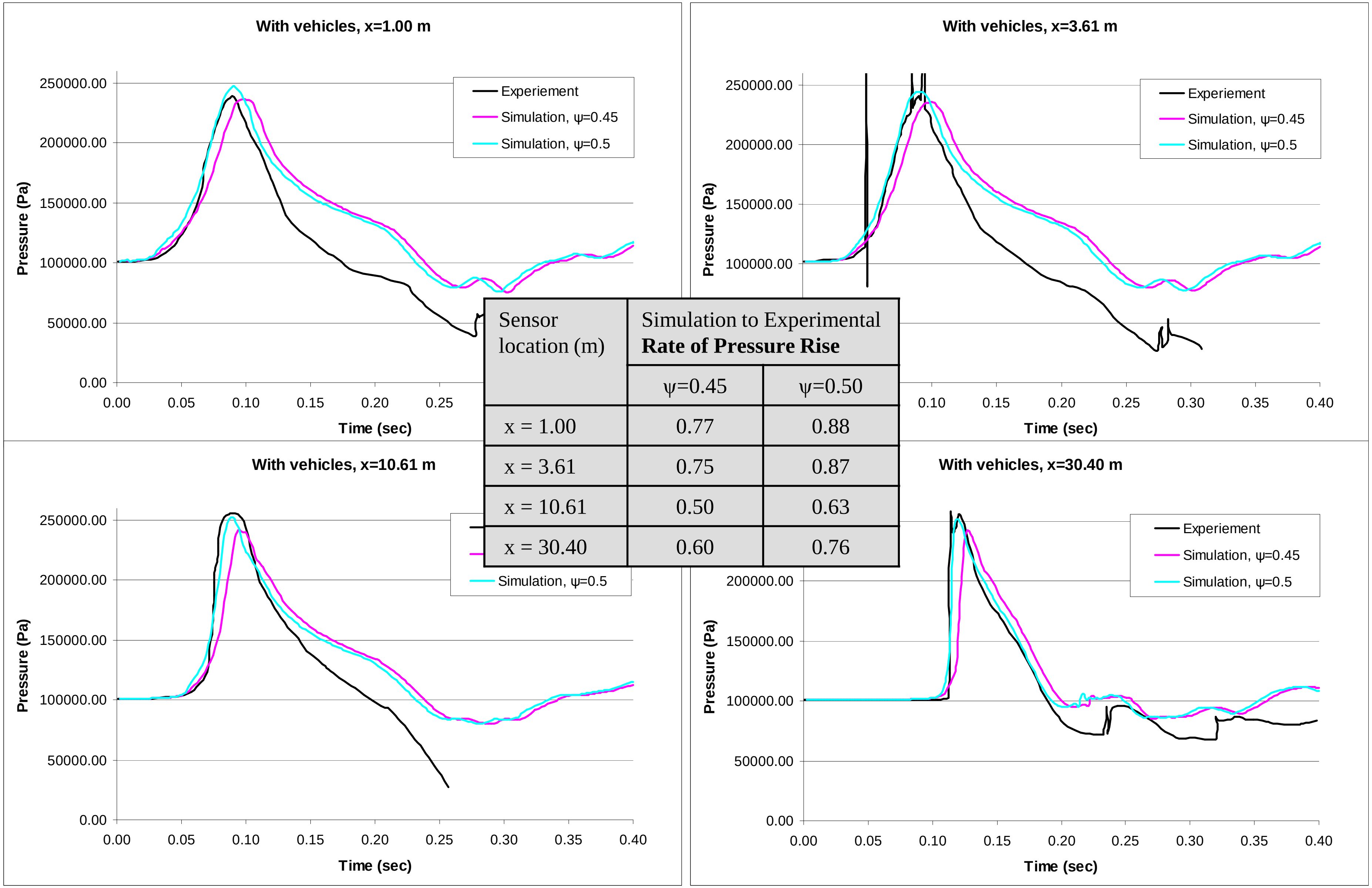
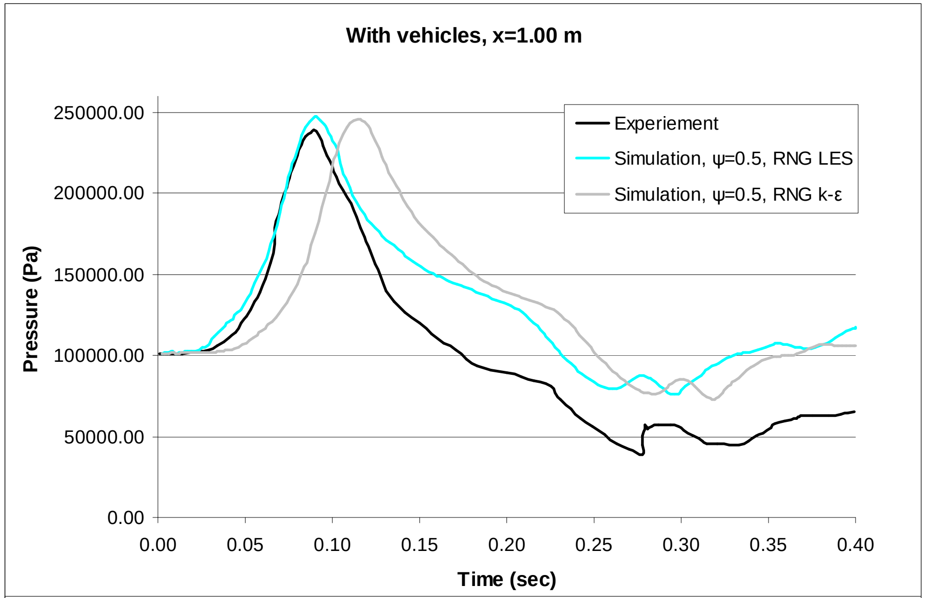


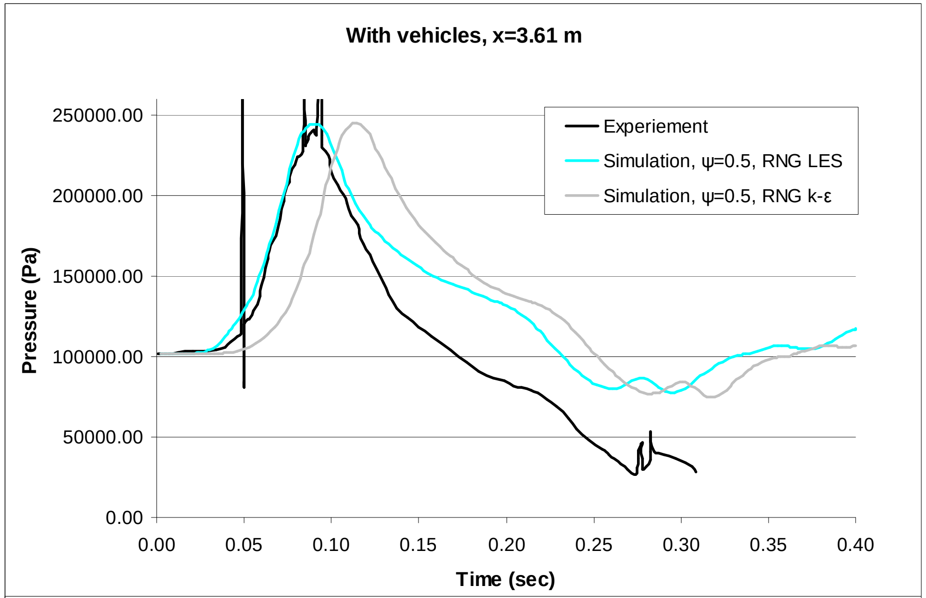
4. Numerical simulation of tunnel deflagration – Non-Empty tunnel case

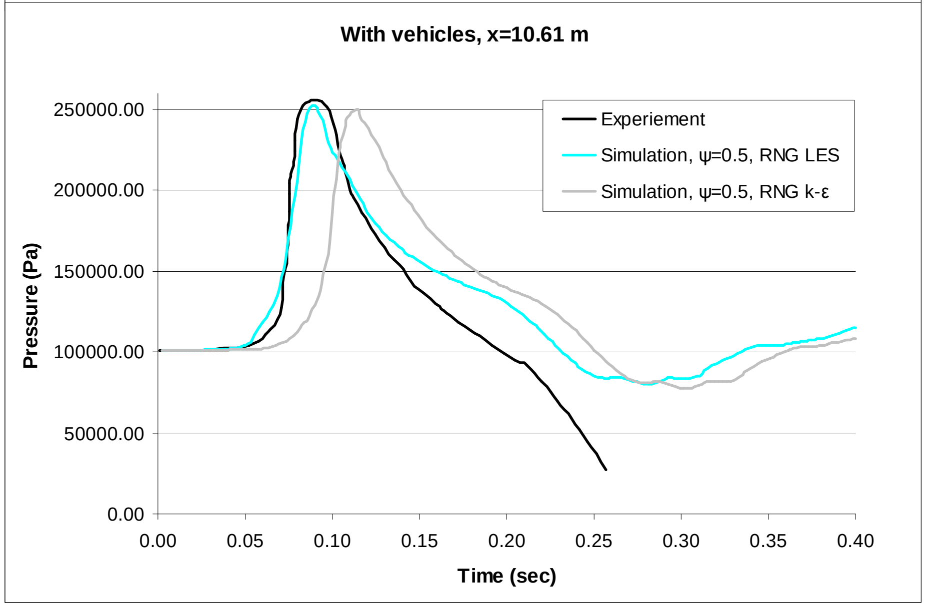


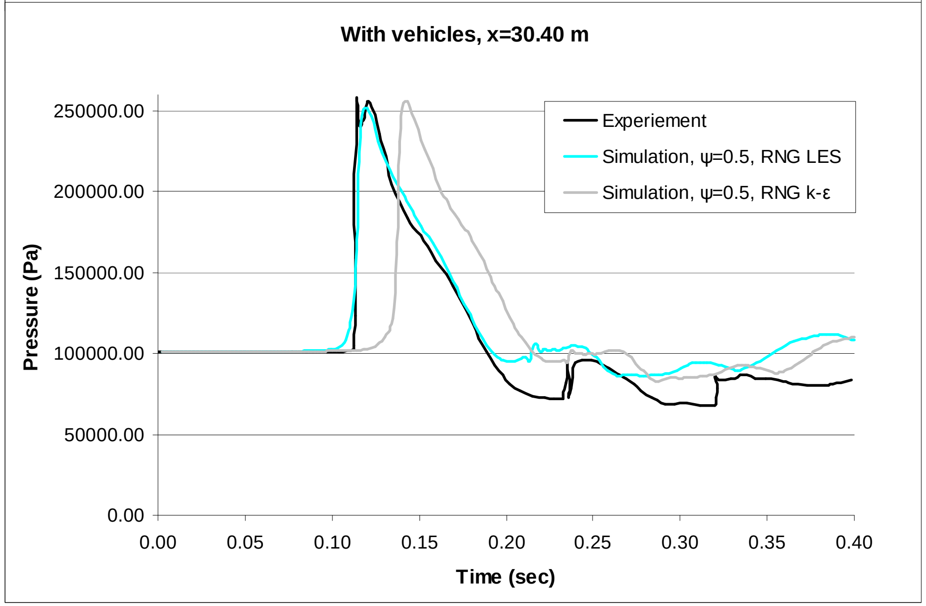
Sensor location (m)	Simulation to Experimental **Rate of Pressure Rise**	
	ψ=0.45	ψ=0.50
x = 1.00	0.77	0.88
x = 3.61	0.75	0.87
x = 10.61	0.50	0.63
x = 30.40	0.60	0.76

4. Numerical simulation of tunnel deflagration – Non-Empty tunnel case









5. Summary / Conclusions

- The ADREA-HF CFD code was evaluated against a hydrogen deflagration in a 78.5 m model of a tunnel.
- The incorporated combustion model was based on the turbulent flame speed concept. A modified Yakhot's equation was used in order to take into account the various phenomena.
- Two cases were examined: one of a complete empty tunnel and one with four vehicles located near the ignition point.
- The code was found capable of simulating the combustion process and predicting the generated overpressures. Concerning the value of the maximum pressure and the time it appears, the agreement between experimental and computational results was satisfactory in both empty and non empty cases.
- The case with ψ=0.50 led to a better prediction of the rate of the pressure rise.
- The sensitivity analysis for the mesh resolution showed that the results with the dense grid had no significant differences compared to the coarse grid.
- The use of a RANS turbulent model (RNG k-ε) gives, with a delay in time, similar to the LES model overpressure curves. This time delay is because of the smaller values of u' that the k-ε predicts comparing to the LES.

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Thank you for your attention

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