Numerical Simulation of Gaseous Detonation in Unconfined and Confined Spaces.

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Highlights

- CFD modeling approach to simulation of gaseous detonations is presented in this work
- The model is applicable to industrial scale gas explosion accidents
- Simulation of H_2-air detonations are demonstrated for unconfined and confined spaces
- The predicted overpressure and velocity of the blast wave agrees with the measurements

1. Introduction

Gas explosions are identified as the most destructive accident scenarios and consequence of uncontrolled release of flammable gas or vapour resulting in formation of explosive mixture with air. The most frequent mode of flammable gas explosions is deflagration when combustion front propagates at a velocity lower that of sound in the unburned mixture. Deflagration can convert into much more destructive detonation due to flame acceleration in a very reactive gas mixture, especially in presence of turbulence promotors. In such a case combustion wave is coupled with the leading shock wave, which propagates at supersonic velocity (order of 2000 m/s) with peak overpressures reaching 20 bars.

Numerical simulation can be a valuable tool for estimation of consequences of gas explosions (e.g. blast loads on surrounding buildings, estimation of safety distances) allowing to avoid very costly industrial scale tests.

2. Methods

A simplified model based on Computational Fluid Dynamics (CFD) methodology was utilized for simulation of industrial scale hydrogen detonation accident scenarios in this work.

The CFD model based on reactive Euler equation set and simplified chemical reaction kinetics equipped with tuned parameters allowed for satisfactory agreement of calculated overpressure field and detonation front velocity with the published measurement results of unconfined and partially confined detonation of hydrogen-air mixtures at moderate computational cost.

An additional experimental program is scheduled in order to validate the model against own data obtained during unconfined detonations of hydrogen and hydrocarbon - air mixtures.

3. Results and discussion

The results of CFD simulation of stoichiometric hydrogen-air mixture detonation tests performed in unconfined space conditions (300 m^3 hemisphere) [1] and confined space (263 m^3 tunnel, Kurchatov Institute, RUT, Russia) [2] were in agreement with the published measurement results in regard to overpressure of detonation wave and subsequent blast wave (see figs 1 and 2). The predicted velocity of the detonation wave was also in agreement with the measurements. It was observed that detonation wave velocity in the tunnel was significantly higher than detonation front velocity measured in unconfined space conditions, which was also in agreement with the theoretical value of Chapman-Jouguet detonation velocity. Similar conclusion can be drawn in regard to the overpressure for the two tested cases.

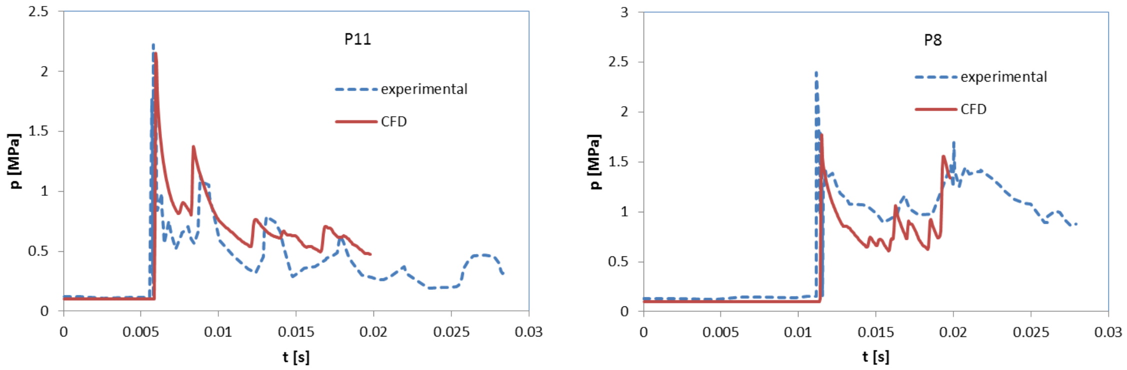

Figure 1. Overpressure at two different locations during detonation of H_2 – air mixture in a confined geometry (RUT tunnel). Experimental data from [2]

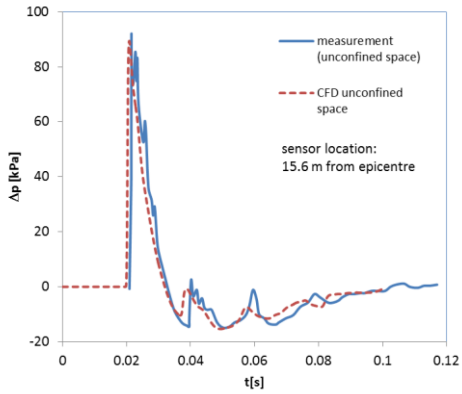

Figure 2. Blast wave overpressure at 15.6 m from the center of unconfined detonation (300 m^3 hemispherical tent filled with H_2 – air mixture). Experimental data from [1]

4. Conclusions

The simplified reaction kinetics and the CFD model allows its application to industrial scale gas explosion accidents. The predicted overpressure of the detonation wave and the blast wave caused by hydrogen-air mixture detonation compares favorably with the results of measurements.

The results of simulations performed in this work were also compared with the predictions of simplified models based on scaling laws and TNT equivalence used routinely to predict maximum overpressure and impulse of the blast wave caused by an explosion. The obtained results demonstrate greater universality and accuracy of the CFD approach especially in the case of geometries of various degree of congestion

References

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[2] A.Heidari, S.Ferraris , J.X. Wen, V.H.Y.Tam, Int. J. Hydrogen Energy, 36 (2011) 2538 – 2544

Keywords

accident scenario, CFD, detonation, hydrogen safety.

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