Piotr MACHNIEWSKI, Eugeniusz MOLGA

e-mail: piotr.machniewski@pw.edu.pl

Wydział Inżynierii Chemicznej i Procesowej, Politechnika Warszawska, Warszawa

Simulation of large scale hydrogen-air detonation with the aid of CFD

Introduction

Hydrogen is an important reagent in chemical industry. It is also regarded as potential energy carrier and means for storage of energy from renewable sources (e.g. solar energy), which can conveniently be converted into electric power in a fuel cell thus minimizing pollution connected with exploitation of fossil fuels. However common use of hydrogen rises safety issues connected with the possibility of leaks and danger of explosion. Hydrogen–air flammability limits and explosion (detonability) concertation ranges are very wide due to high reactivity of hydrogen [*Bjerketvedt et al., 1997*]. It is thus necessary to estimate risk and consequences of explosion when considering localization of hydrogen storage and handling facilities.

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. Due to flame acceleration in a very reactive gas mixture, especially in presence of obstacles acting as turbulence promotors, deflagration can convert into much more destructive detonation. In such a case combustion wave is coupled with the leading shock wave, which propagates at supersonic velocity (in reference to the unburned mixture). The peak overpressure caused by open-space detonation of hydrogen-air mixture can reach 15-18 bar and shock wave propagation velocity of 2000 m/s [cf. *Bjerketvedt et al., 1997*]. Detonation of gaseous mixture can be also initiated by a small amount of high energy explosive or strong external shock wave. Numerical simulation based on CFD methodology can be a valuable tool for estimation of consequences of gas explosions allowing to avoid very costly industrial scale tests.

CFD Modelling

Although simulations of gaseous detonations in small geometries (few centimeters) are numerously reported in the literature, large scale detonation (geometry size of 10-100 meter) reports are quite scarce. Complete resolution of detonation wave structure (of mm size) based on detailed reaction mechanism and μm cell size grid is not possible in the case of large scale simulations, when number of mesh nodes has to be reduced to fit present computing hardware capabilities.

A simplified model based on mass, momentum and energy balance in the form of reactive *Euler* equations assuming inviscid ideal gas medium, neglecting mass diffusion and heat conduction, was applied in this work. The following coupled equations supplemented with species mass balance:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{1}$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) + \nabla p = 0 \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)\vec{u}) = q_r R \tag{3}$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho Y_i \vec{u}) - R_i = 0 \tag{4}$$

where:
E　– total energy per unit volume,
$q_r R$　– energy source due to chemical reaction,
Y_i　– mass fraction of component I,

with suitable source term due to chemical reaction were numerically integrated using finite volume method with the aid of *ANSYS Fluent* CFD software package.

A one-step (hydrogen oxidation) reaction was assumed in this work, described by *Arrhenius* type kinetic equation

$$R = A\exp\left(-\frac{E}{RT}\right)c_{H2}c_{O2} \tag{5}$$

with parameters adjusted to reproduce detonation velocity and pressure observed in experiments.

Similar approach was also taken by *Heidari et al.* [*2011*] for simulation of large scale hydrogen detonation in the 263 m³ RUT tunnel facility. The confined volume detonation tests performed in this facility were also used for validation of different CFD codes by *Yanaz et al.* [*2011*].

The adjusted values of parameters in eq. (5): A = 2·10⁸ m³/mol and E = 191 kJ/mol , were used with quite coarse computational mesh (cell size of 5 cm) nevertheless allowing for reasonable agreement with theoretical predictions of detonation velocity and maximum overpressure based on *Chapman-Jouguet* (C-J) model of planar detonation. *Advection Upstream Splitting Method* (AUSM+) enabling precise shock capture [*Liou, 2009*] was utilized in the simulations along with 4-stage *Runge-Kutta* time stepping algorithm. The time step was varied in the course of simulation within the limit of *Courant-Friedrichs-Lewy* conditions (CFL < 1).

Validation: Test Conditions and Simulation Results

The large scale open–space test results reported by *Groethe et al.* [2007] were used for validation of the modeling approach in this work. A 300 m³ hemispherical balloon filled with hydrogen premixed with air in nearly stoichiometric proportion (30% vol. H₂) was detonated with the aid of 10g of high explosive (C-4) booster charge placed at the center of the balloon in this test. The overpressure caused by the blast wave was measured at the distance of 15.6 m from the epicenter. The measured flame front speed agreed with C-J theoretical value for stoichiometric hydrogen-air mixture. (1968 m/s, [cf. *Bjerketvedt et al., 1997*]).

In order to limit the computational costs axial symmetry was assumed and 2D mesh covering distance of 40 m from the center of the balloon was prepared for the simulation. The cell size in the detonation area (the balloon) was approx. 5 cm (refined to 2 cm around the ignition point) and 10 - 17 cm outside the balloon in the area of blast wave propagation. The gas was assumed to be initially at 27°C and 101.325 kPa. The calculated location of flame front an overpressure profiles are shown in the Fig. 1 and 2.

The detonation wave front reached the balloon surface during the test at 2588 μs as recorded with a high speed camera, which agrees with the time of 2552 μs observed during the CFD simulation and the theoretical value of *Chapman-Jouguet* detonation velocity (Fig. 1.).

The value of peak overpressure in the simulated detonation wave reached 16.6 bar, which is also close to the value of P_{CJ} = 15.8 bar predicted by the *Chapman-Joguet* theory for the stoichiometric hydrogen –air mixture [cf. *Bjerketvedt et al., 1997*].

The calculated overpressure and temperature fields during blast wave propagation (after the detonation) are shown in the Fig. 3 and 4 respectively.
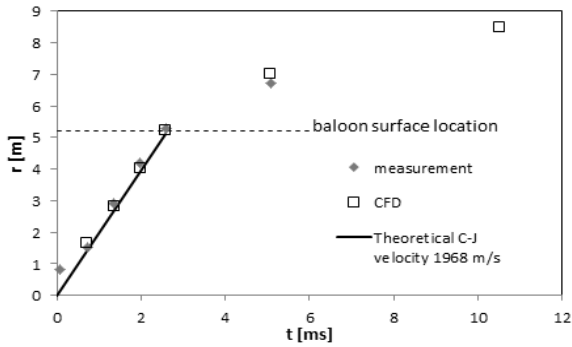
Fig. 1. Location of flame front (fireball surface) at various time instants after ignition. Measurement results were taken from [*Groethe et al., 2007*]
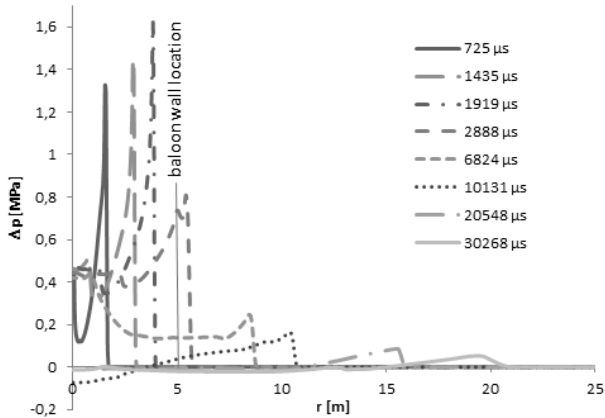

Fig. 2. Overpressure profiles at various time instants after ignition
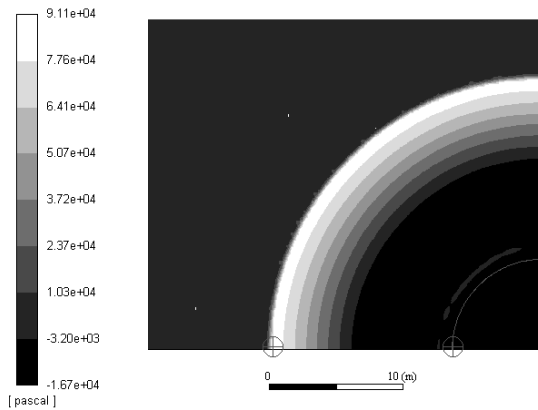

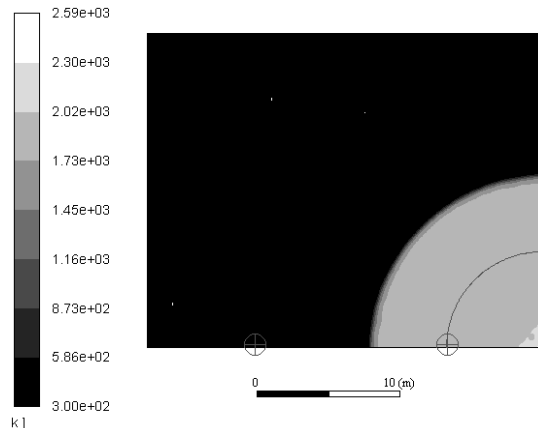Fig. 3. Overpressure field [Pa] at t = 20.55 ms after ignition

Fig. 4. Temperature field [K] at t = 20.55 ms after ignition
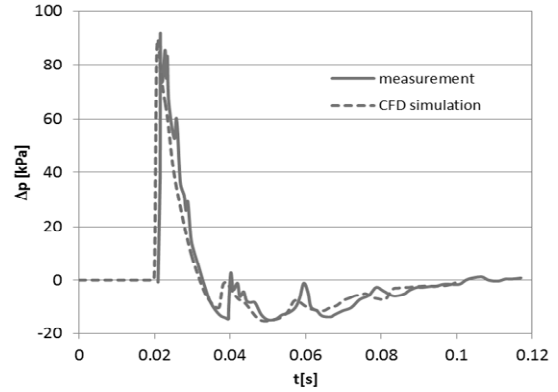

Fig. 5. Evolution of overpressure at the distance of 15.61 m from the measurement results were taken from *Groethe et al. 2007*]

The calculated temperature field at the instant detonation wave reaches balloon wall indicates that combustion products during detonation remain very hot (2500K - 3500K) but the spatial range of high temperature gases behind the shock propagating outside the balloon is rather limited (Fig. 4) being much shorter than the distance covered by the blast wave outside the balloon (Fig. 3).

The time instant (20.55 ms) the simulated blast wave reached pressure probe location point (at 15.61m from the epicenter, see label marks in the Fig. 3) is in good agreement with the measured delay of peak overpressure shown in the Fig.5. Also the peak height and the recorded time evolution of overpressure at this location is in fair agreement with simulation results (Fig. 5). Pressure variations during Taylor wave passage (expansion wave behind the shock) visible in the Fig. 5 at time > 0.03s, were caused by interference with reflected shock waves and quite well reproduced in the simulation results.

Conclusions

A simplified model of hydrogen-air mixture detonation based on one-step *Arrhenius* kinetics utilizing tuned parameters and CFD methodology allows for satisfactory prediction of overpressure field and detonation front velocity during large scale open-space detonation of hydrogen-air mixtures, at moderate computational cost owing to the possibility of using coarse meshes.

The model implemented within reliable CFD software package can be a valuable to for analyzing accident scenarios, and consequences of flammable gas detonation and resulting pressure loads in 2D and 3D geometries of industrial scale.

LITERATURE

Bjerketvedt D., Bakke J.R., van Wingerden K., (1997). Gas explosion handbook, *J. Hazardous Materials*, 52, 1-150. DOI: 10.1016/S0304-3894(97)81620-2

Groethe M., Merilo E., Colton J., Chiba S., Sato Y., Iwabuchi H., (2007) . Large-scale hydrogen deflagrations and detonations. *Int. J. Hydr. Energy,* 32, 2125-2133. DOI: /10.1016/j.ijhydene.2007.04.016.

Heidari A., Ferraris S. , Wen J.X., Tam V.H.Y., (2011) . Numerical simulation of large scale hydrogen detonation. *International*. *Int. J. Hydr. Energy,* 36, 2538-2544. DOI: 10.1016/j.ijhydene.2010.05.093

Liou M. S., (1996). A sequel to AUSM: AUSM+. *J. Comp. Phys.,* 129. 364-382. DOI: 10.1006/jcph.1996.0256.

Yanez J., Kotchourko A., Lelyakin A., Gavrikov A., Efimenko A., Zbikowski M. , Makarov D., Molkov V., (2011). A comparison exercise on the CFD detonation simulation in large-scale confined volumes. *Int. J. Hydr. Energy,* 36, 2613-2619. DOI: 10.1016/j.ijhydene.2010.04.133