LES of a Large-Scale Detonation Experiment in the RUT Facility

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1 Introduction

Safety provisions are key issues for emerging hydrogen economy. Transition from deflagration to detonation is a worst case scenario for hydrogen safety engineering. Although hydrogen-air mixtures are more likely to deflagrate at many practical scenarios, detonations can not be excluded and assessment of consequences is necessary. The contemporary tools such as computational fluid dynamics should be developed to be available for engineers designing hydrogen infrastructures and mitigating risks.

Most of numerical detonation studies are devoted to resolution of details at real scales of underlying physical phenomena. This makes simulation of detonation at industrial scales of tens and hundreds of meters impractical. Recently authors published the large eddy simulation (LES) model of large scale hydrogen-air planar detonation and results of its verification by the Zel'dovich - von Neumann - Doring (ZND) detonation theory [1]. This detonation model features similar approach to the LES deflagration model published elsewhere [2][3][4]. The model has been previously applied to simulate propagation of blast wave in a fare field from detonation [5]

Prediction of detonation parameters in complex geometries is very important for hydrogen safety engineering. This paper presents the comparison of a numerical simulation by the LES model [1] with unique large-scale experiment in the RUT facility [6] performed in Russia by Kurchatov Institute as a part of an international collaborative project.

2 The model

The governing equations are described in detail elsewhere [3] and include 3D filtered mass, momentum and energy equations for a compressible Newtonian fluid. The progress variable equation is the same as for the deflagration model accept for the source term. The sub-grid scale turbulence is modeled by the renormalization group (RNG) approach [7]. Reaction front in the detonation wave is defined by the progress variable where c=0 for unburned mixture and c=1 for combustion products. The propagation of combustion is modeled by the progress variable equation first introduced in [8]

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{c}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{c}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial\tilde{c}}{\partial x_j}\right)+\bar{S}_c$$

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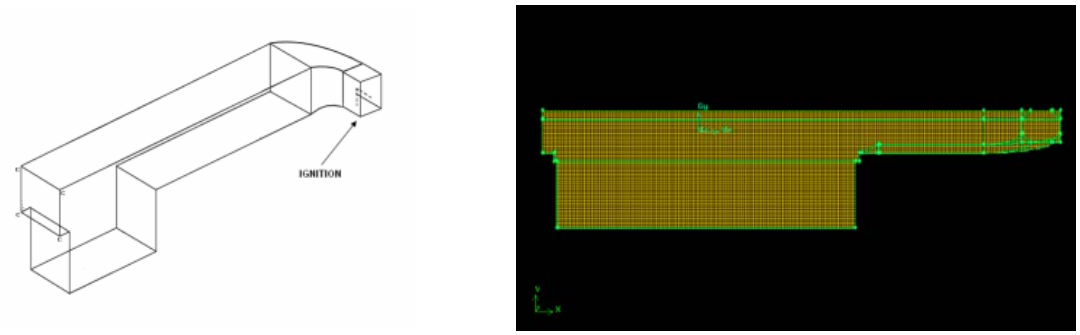
The difference between deflagration and detonation mathematical models is the substitution of the turbulent burning velocity by the detonation velocity in the source term, $S_c = \rho_u \cdot D \cdot \left|\nabla \tilde{c}\right|$, where ρ_u is density of unburned mixture in front of a shock, ∇c is a gradient of the progress variable. Integration across the reaction front gives a correct values of mass burning rate per unit area of the detonation wave $\rho_u \cdot D$. Detonation velocity is pre-calculated with Shock & Detonation (SD) Toolbox [9] which uses CANTERA software [10]. The source term in the energy equation is connected with the source term in the progress variable equation $S_e = \Delta H_c \cdot S_c$, where ΔH_c is the standard heat of combustion which is calculated by CANTERA [10]. Specific heats of unburned and burnt mixtures were approximated as piecewise-polynomial functions of temperature with polynomial coefficients calculated according to mass-weighted mixing law of composing species.

The gradient method by definition does not track the exact location of the reaction front but represents change of the progress variable through control volumes (CV) [11] and numerical requirement is for the flame front to occupy 4-5 CV [12]. This requirement is valid for shock front too. In calculations the realistic detonation front scales are given up. However, to reproduce in simulations the von Neumann peak, i.e. to achieve propagation of leading shock with correct velocity equal to detonation speed, the numerical combustion front is "kept behind" the numerical shock front to feed the first by energy released during combustion.

3 Calculation settings

A series of large scale hydrogen-air detonation experiments were carried out in the RUT facility [1], designed as a blast wave generator. A detonation test with 25.5% of hydrogen in air was chosen in this study. The initial temperature and initial pressure were 293 K and 101325 Pa, respectively. The facility is 18.2 m in length; enclosure's volume is 192 m^3 (see Fig. 1).



a) b)

Figure 1. Experimental scheme and calculation domain.

The calculation domain was created and meshed using Gambit 2.2 tool of the CFD package Fluent. Hexahedral grid was built of control volumes with size 0.1x0.1x0.1 m (237005 CVs). Numerically detonation was initiated at the whole one end of the enclosure (see Figure 1a). Such initiation decreases the amplitude of reflected and interfering shocks. At the walls we imposed the non-slip boundary conditions for the momentum equations, adiabatic boundary conditions for the energy equation, and zero flux boundary conditions for the progress variable equation. Mixture is quiescent at ignition, u=0 m/s. Hydrogen and air mass fractions are Y_{H2}= 0.024 and Y_a= 0.976, respectively. The progress variable is set to c=0 in the whole domain except the area of detonation initiation.

The Fluent 6.3 software was used as an engine for the LES model simulations. The double precision parallel version of the solver was used with explicit linearization of the governing equations.

To compute the convective fluxes the Advection Upstream Splitting Method (AUSM+) [13] and the central difference scheme for diffusion terms were applied. The 4-order Runge–Kutta scheme was used for time stepping. The Courant–Friedrichs–Lewy (CFL) number was equal to CFL=0.05. This number was found to provide solution stability and convergence for simulation when the detonation speed is higher than the speed of sound used in the standard CFL number definition.

4 Results

Comparison between detonation experiment and numerical simulations is shown in Figure 1. Two pressure gauges (P08 and P10) were chosen to compare pressure histories (Figure 1a and 1b) and propagation of the detonation front (Figure 1d).

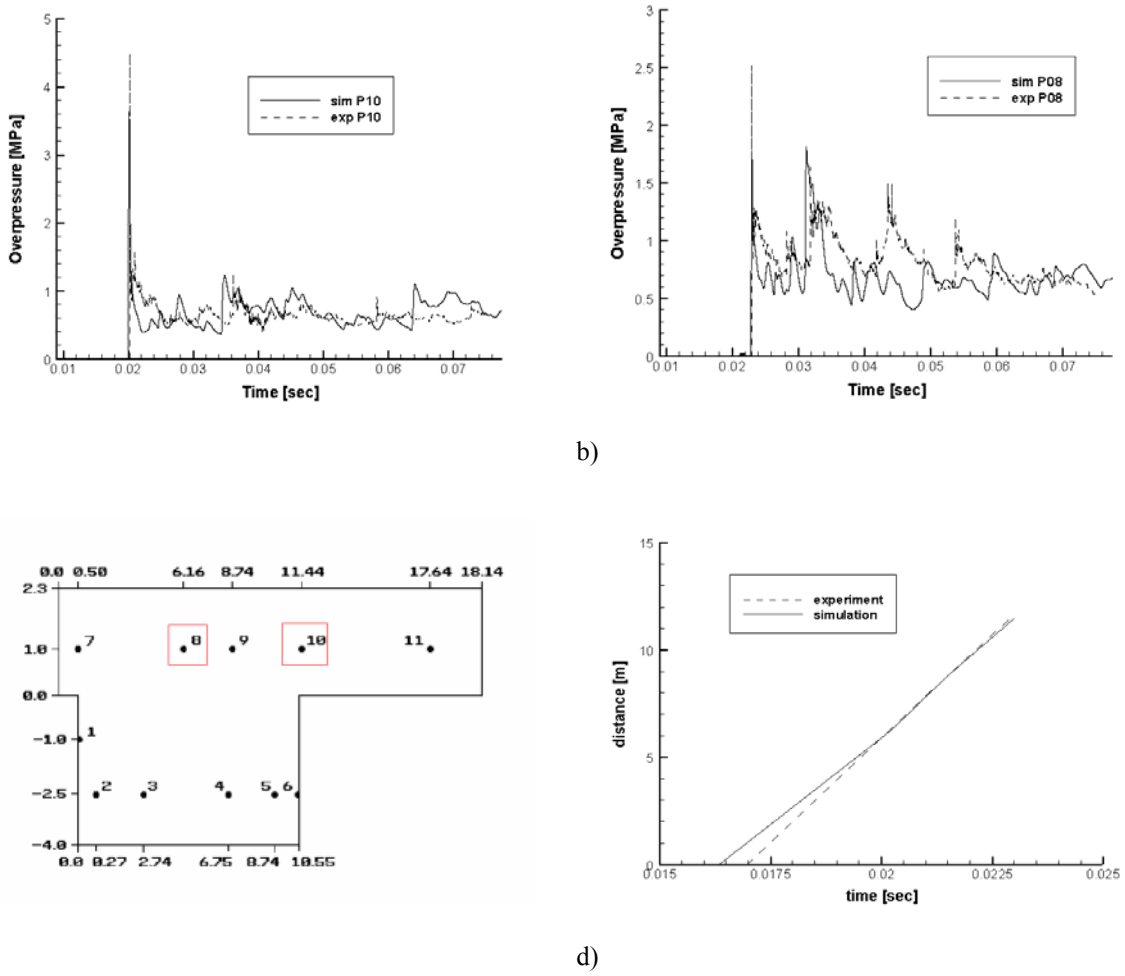


Figure 2. Comparison between experiment and simulations: a) pressure dynamics at location of pressure gauge P10, b) pressure pressure dynamics at location of pressure gauge P08, c) location of pressure gauges, d) propagation of detonation front.

Pre-calculated by CANTERA [10] detonation velocity of 25.5% hydrogen-air mixture, D=1873 m/s, is very close to the average velocity of the detonation front propagating in the experiment (see Figure 1d). Initiation of detonation in the experiment was done by "point" high explosive charge (200 g) and in simulations the progress variable was set to c=1 and high pressure (20 MPa) and temperature (6000 K) were defined in a slice of control volumes along the whole end wall where experimental

initiation took place (planar initiation). Theoretical value of von Neumann peak for 25.5% mixture is 2.6 MPa while in real detonation wave this value is changing constantly due to three dimensional structure of the detonation wave. In simulations detonation structure is given up due to coarse mesh. Still the maximum peak of pressure and pressure in the expansion wave is in a reasonable agreement with experimental data for such complex geometry (Figure 1a and 1b). The shape of the Taylor wave is naturally not smooth as in a planar detonation [1] due to reflections of shock waves. Difference in details of pressure dynamics could be attributed mainly to difference in experimental and numerical initiation of detonation.

5 Conclusions

The previously developed and verified against the ZND theory LES model for planar detonation is applied to simulate experimental data in the complex geometry of the RUT facility of 192 m^3 volume. The model does not require Arrhenius chemistry what essentially decreases computational time for large scales problems. Simulation results are in a reasonable agreement with experiment to satisfy requirements for hydrogen safety engineering.

References

[1] Zbikowski M, Makarov D, Molkov V (2008). LES Model of Large Scale Hydrogen-Air Planar Detonations: Verification by the ZND Theory. International Journal of Hydrogen Energy, 33:4884–4892.

[2] Makarov D, Molkov V, Gostintsev Yu (2004). Comparison between RNG and fractal combustion models for LES of unconfined explosions. Combustion Science and Technology, 179:1.

[3] Molkov VV, Makarov DV, Schneider H (2006). LES modelling of an unconfined large-scale hydrogen-air deflagration. Journal of Physics D: Applied Physics, 39:4366.

[4] Makarov D, Verbecke F, Molkov V (2007) Numerical Analysis of Hydrogen Deflagration Mitigation by Venting Through a Duct. Journal of Loss Prevention in the Process Industries, 20:433-438.

[5] Makarov D, Molkov V, Zbikowski M, Schneider H (2007). The Model for Numerical Simulations of Large-Scale Deflagrations and Detonations. 21st ICDERS, July 23-27, 2007, Poitiers, France.

[6] Efimenko A, Gavrikov A (2007). Large Scale Hydrogen-Air Detonation Experiments. The Effect of Ignition Location and Hydrogen Concentration on Loads. Description of HySafe SBEP V13.

[7] Yakhot V, Orszag S (1986). Renormalization group analysis of turbulence. I. Basic theory. Journal of Scientific Computingб 1:3.

[8] Prudnikov, A.G. Combustion of homogeneous fuel-air mixtures in turbulent flows. In B.V. Raushenbakh, editor, Physical Principles of the Working Process in Combustion Chambers of Jet Engines, Chapter 5, pp.244-336. Clearing House for Federal Scientific & Technical Information, Springfield, 1967..

[9] http://www.galcit.caltech.edu/EDL/public/cantera/html/SD_Toolbox/index.html

[10] Goodwin D. CANTERA (2005) – Object-oriented software for reacting flows. Technical report, California Institute of Technology.

[11] Oran ES, Boris JP (2001). Numerical Simulation of Reactive Flow. Cambridge University Press, Second edition.

[12] Hawkes ER, Cant RS (2001). Implication of a flame surface density approach to large eddy simulation of premixed turbulent combustion. Combustion and Flame, 126:1617–1629.

[13] Liou MS (1996). A sequel to AUSM: AUSM+. Journal of Computational Physics; 129:364-382.