A Model for Numerical Simulations of Large-Scale Deflagrations and Detonations

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1 Introduction

Introduction of hydrogen as an energy carrier of the near future poses many challenges, including safety, which may be considered as a major barrier to emerging hydrogen economy. There are several properties of hydrogen air mixtures, which are different from ordinary hydrocarbon air mixtures, like for example low ignition energy, wide flammability and detonability limits, and high burning velocity. There is a need for a better understanding of special, hydrogen related phenomena like spontaneous ignition during high pressure releases and the stronger tendency of a DDT transition. One way for an approval of a better understanding is the development of predictive tools and its validation with existing experimental data. Transition from deflagration to detonation during an accident drastically changes safety requirements, particularly safety distances.

The paper presents a model, which is under development at the University of Ulster and based on Large Eddy Simulation (LES) approach. So far the model has been successfully applied to simulate large-scale hydrogen-air deflagrations. In particular, the model was validated against experimental data on hydrogen-air deflagrations in closed vessel [1], the open atmosphere [2], vented vessel [3]. In this study the model is extended further to predict detonation wave propagation and explosion blast wave.

2 Deflagration model

Description of the deflagration model is given elsewhere [1-3]. The governing equations include filtered mass, momentum and energy conservation equation. The RNG turbulence model by Yakhot et al. [4], capable to describe transitional and laminar flow regimes, is employed to model sub-grid scale (SGS) turbulence. Combustion model utilises the filtered progress variable equation to model flame front propagation:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{c}\right)+\frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{u}_j\widetilde{c}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \widetilde{c}}{\partial x_j}\right)+\overline{S}_c\,. \tag{1}$$

The additional conservation equation for air mass fraction is required if flame propagates through non-uniform mixture, e.g. during dilution of initial hydrogen-air mixture with surrounding air in the open atmosphere. The gradient method is used to model the mass burning rate:

$$\overline{S_c} = \rho_u S_t \left|grad\,\widetilde{c}\right|\,. \tag{2}$$

The concept of burning velocity S_t together with the gradient method provides a way to ensure that the prescribed mass burning rate $\rho_u S_t$ takes place in simulations irrespective of the grid resolution. Effects of small-scale turbulence, generated by the flame front itself, and flow turbulence on the turbulent burning velocity are modelled in the following way. An increase of the burning velocity on SGS level due to flame front induced

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turbulence is accounted for according to the theory of Karlovits [5], when the maximum increase of flame front area is characterized by the factor $(E_i - 1)/\sqrt{3}$ depending on the expansion coefficient E_i, and the observations of Gostintsev et al. [6], which state that the self-similar regime of flame propagation is established at characteristic flame radius equal to R_*=1.0-1.2 m for stoichiometric hydrogen-air mixture. The effect of flow turbulence is accounted for by the RNG turbulent premixed combustion model [7]: $S_t = S_u \exp(u'/S_t)^2$, where u' - root-mean square of the SGS velocity.

3 Extension of the model to detonations

A scale of industrial explosions may be hundred meters. This makes numerical simulation of detonation wave propagation, pressure loads and impulse of explosion blast wave a complicated task. Characteristic size of the control volume in such a problem may be of the order of meter. An approach to tackle this problem may be a use of the detonation velocity in the source term of the progress variable equation. Indeed, the detonation velocity can be calculated beforehand from the theory, e.g. the Chapman-Jouguet detonation velocity can be calculated as described in [8]. Thus, the source term for the progress variable equation for detonation modelling is:

$$\overline{S_c} = r_u D_{CJ} \left| grad \tilde{c} \right| , \qquad (3)$$

where D_{CJ} is the Chapman-Jouguet detonation velocity. The product $r_u D_{CJ}$ represents mass reaction rate per unit area in the case of detonation. The value of D_{CJ} is a function of the initial pressure, temperature and fuel concentration. The source term in the energy conservation equation is equal to the source term in the progress variable equation multiplied by the heat of combustion.

4 Comparison with large-scale detonation experiments

The approach to a detonation wave propagation model described above was validated against experimental data [9], where a series of tests with directly initiated detonations is described. The hemispherical detonation of 30% hydrogen-air mixture of radius R_0=5.23 m, propagating through unobstructed environment was chosen for simulation.

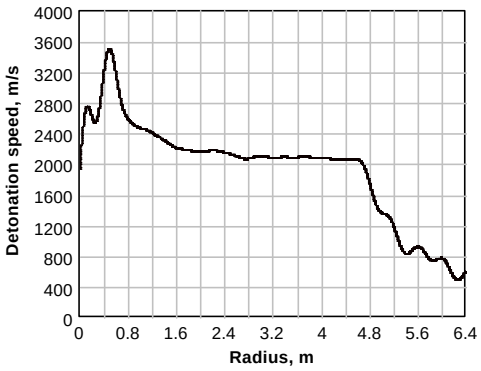

Figure 1. Smoothed simulated detonation propagation velocity.

The detonation velocity for the mixture, determined according to [8], is D_{CJ}=1977 m/s. Mixture ignition was achieved in the same way as for deflagration simulation, i.e. by increase of the progress variable in the control volume, corresponding to position of ignition source, from value 0 to 1. The period of ignition corresponds to the combustion wave propagation through half of the ignition control volume. Calculation domain was meshed using tetrahedral control volumes close to ignition area and hexahedral control volumes in the rest of the calculation domain.

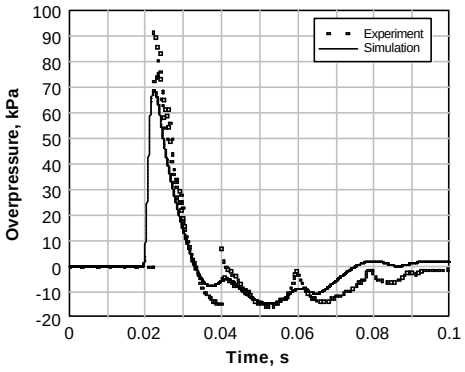

Figure 2. Comparison of experimental and simulated pressure dynamics at R=15.61 m

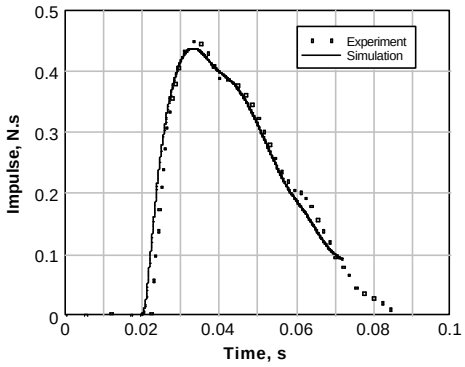

Figure 3. Comparison of experimental and simulated impulse at R=15.61 m

The smoothed simulated velocity of detonation wave propagation is shown in Fig.1. It corresponds to the Chapmen-Jouguet velocity, which is an input parameter for simulations. Higher values of simulated detonation propagation velocity at the beginning could be attributed to the detonation initiation procedure and/or a numerical procedure for calculation of the detonation front location. Comparison of the simulated pressure dynamics and experimental pressure in the decaying blast wave, obtained at radius R=15.61 m from the detonation initiation point, is given in Fig.2, which is in agreement with the experiment.

Neither von Neumann (p=28.5 atm) nor Chapman-Jouguet (p=15.3 atm) pressure peaks were resolved in the simulations. This is due to the disparity between physical scales of the detonation front thickness and large size of the calculation mesh. The maximum peak overpressure achieved in simulations is about p=9 atm. However, the calculated impulse is in an excellent agreement with the experimental data, see Fig.3, as the correct energy release was provided by the model.

Structure of pressure distribution within the detonation area is in agreement with detonation theory [10]. The Tailor expansion wave occupies about 50% of the burnt mixture radius with the overpressure at the end of the expansion wave about p=4 atm.

5 Modelling of explosion dynamics with deflagration followed by detonation

The common approach enables simultaneous simulation of deflagration and detonation. One of the Fraunhofer-ICT experiments [11] on DDT was simulated. In test IA4, 22,5% hydrogen-air mixture was ignited in 3.0x1.5x1.5 m^3 vented vessel. The transition to detonation happened outside the vessel in a 12x3x3 m^3 lane, filled with the same mixture. Fig.4 shows comparison between simulated and experimental pressure dynamics inside the vessel. “Slow” deflagration dynamics during initial 60 ms of explosion development is well reproduced by the model, including the decrease of the pressure inside the vessel when combustion products start to flow out of the vessel to the lane. A sharp pressure peak at about 61 ms (experiment) is a pressure wave originating from the detonation, which is triggered within the lane. The maximum of the experimental pressure is not correct, because of the type of pressure transducer used there, which is not suitable for short pressure rise times; however similarities in the pressure behaviour are evident.

The model for simultaneous simulation of deflagration and detonation wave propagation is as follows. The source term in the progress variable equation is S_t for deflagration and D_{CJ} for detonation. This is realised by introducing additional scalar transport equation to trace detonation wave propagation, having the meaning of a “detonation marker”. The “detonation marker” equation has the same form as (1) with the source term (3). Once solution for the progress variable equation and “detonation marker” are known, then the highest value and the highest source term supersedes in the progress variable equation, making it enable to trace both deflagration and detonation waves propagation.

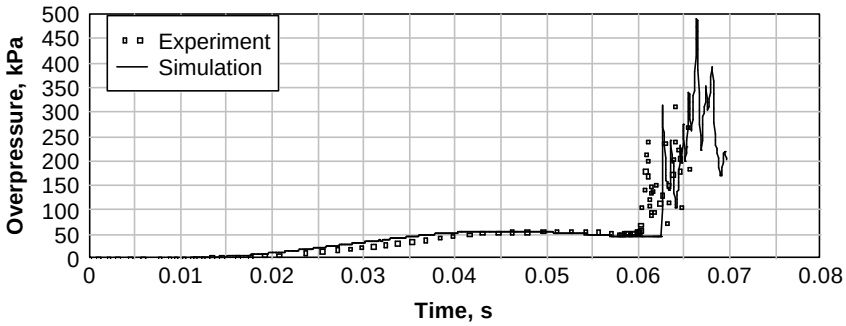

Fig.4. Comparison of experimental and simulated pressure dynamics inside vented vessel [10].

6 Conclusions

The LES model applied previously to large-scale deflagrations has been extended to simulate large-scale detonations. The simulations are compared with experimental data of hemispherical 30% hydrogen-air mixture detonation, propagating in an unobstructed environment. The velocity of the detonation wave propagation could be accurately simulated, and the structure of the pressure wave within the detonation area and of the decaying blast wave were obtained. The impulse of the outgoing explosion blast wave is reproduced by the model in agreement with experiment in spite of some under prediction of maximum pressure peak. It is demonstrated that with this model the simultaneous simulation of the deflagration and detonation wave propagation is possible.

Acknowledgement*:* The authors would like to acknowledge valuable and greatly appreciated input from Sergey Dorofeev (FM Global Research, USA).

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