Detonation Initiation in the Reflected Shock Experiments: 1-Dim Benchmark Case for the Reactive CFD Models used in the PDE Applications

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1 Introduction

Development of the detonation-based hybrid engines, including the Pulsed Detonation Engines (PDE), can be more effective (in terms of spent time and efforts), if a whole PDE development lifecycle will be supported by a set of the validated modeling and simulation tools.

Now, specifically for the PDE applications, there are exists the ample sets of the 0-dim and 2-dim data. Ignition delay time is a typical representative of the 0-dim data. The traces of detonation evolution on the smoked foils or the video captured in the shock tubes are the typical representatives of the 2-dim data. For systematic validation of the reactive CFD models, targeted to simulation of the detonation life cycle (from initiation to quenching), a well documented 1-dimensional benchmark case is required. Vital need in 1-dim benchmark for detonation is dictated by the following reasons. Successful validation against the available experimental 0-dim data, for example on ignition delay times, gives evidence that only the chemical kinetic scheme, incorporated into the reactive CFD model, is valid. Capability to simulate a complex interaction of the kinetic, gasdynamic and transport (including turbulence) processes, which take place during detonation wave evolution within PDE, can be, in principle, validated in the 2-dim or 3-dim simulations. However, in current practice, the multi-dimensional simulations are extremely expensive for the large scale, high fidelity engineering simulations (if ever possible, for situations, where the multi-step chemistry is essential – critical phenomena, environmental compliance, etc.). Before starting the expensive multi-dimensional simulations, it will be worth while to check validity of the reactive CFD model to reproduce a 1-dim situation. The well known experimental case of steady deflagration in tube is not satisfactory, since it represents only early stage of detonation formation process. The widely known theoretical case of the steady ZND detonation wave do no have a direct measurable experimental counterparts.

In our work on validation of the reactive CFD model, customized for the Jet A-air-fueled PDE application, we guess that the experimental results of the detonation initiation in reflected shock wave experiments can play a role of a model case (benchmark) for the 1-dimensional validation of the reactive CFD models. This report is focused on the pro-and contra arguments for using the experiments on reflected shock wave velocity upon initial incident shock wave Mach number using the results of 1-dim simulation of the experimental data of Penyazkov [1], using detailed mutli-step chemical model of Jet A-air combustion [2].

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2 Problem formulation and numerical setup

The schematic representations of the experimental setup [1] and 1D grid with specified pressure sensors are shown on the Fig 1a and 1b, respectively. In the experiment, an arrival of the wave were detected by the three pressure sensors, located at the wall PS0, at the distance 7.3 cm from the wall PS1 and at the distance 17.2 cm from the wall PS2 (see Fig 1a for schematic).

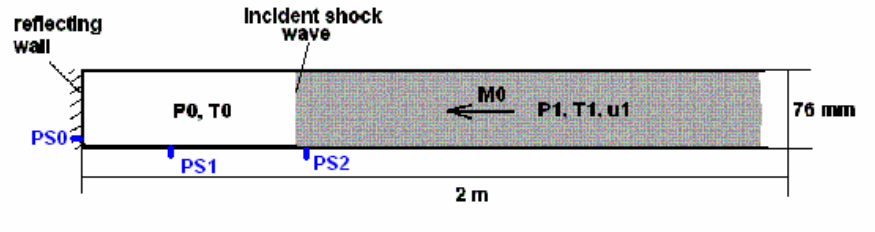

Figure 1a. Shock wave tube geometry in experiments [1]. PS0 - pressure sensor at the reflecting wall, PS1 - pressure sensor on the distance of 7.3 cm from reflecting wall, PS2 - pressure sensor on the distance of 17.2 cm from reflecting wall.

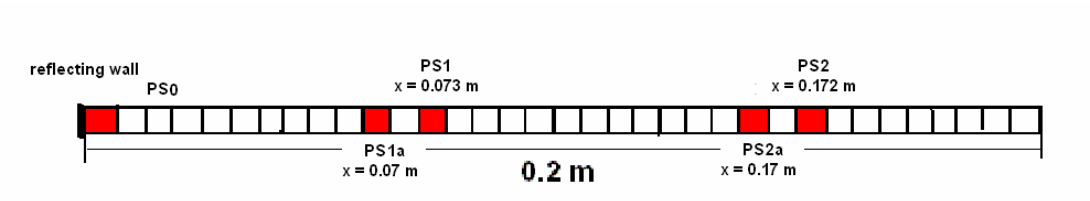

Figure 1b. 1D grid used in computations with specified pressure sensor locations.

Inside the computational domain, five pressure sensors were placed at a fixed distances from the left wall: PS0 – 0.0001 m, PS1a – 0.07 m, PS1 – 0.073 m, PS2a – 0.17 m, PS2 – 0.172 m, instead of the three pressure sensors in real experiments (pressure sensors PS1a and PS2a were added). The main reason for such allocation of the pressure sensors is to obtain not only wave speed, averaged over some interval in space, but local wave speeds as well. The stoichiometric Jet-A/air was chosen as a fuel-oxidizer mixture. Jet-A is described by brutto formula $C_{12}H_{23}$ and its thermo-chemical data are taken Burcat's internet database. The kinetic mechanism of a Jet A combustion contains 15 substances and 13 reactions [2]. A commercially available numerical solver, Metacomptech Inc. CFD++, was used to obtain time-resolved predictions of the processes presented in this paper.

3 Simulation results: comparison with experiment

In experiments [1] two different types of the results were obtained. First, ignition delay times, which were used for validation of the detailed kinetic schema in [2]. Second type of the results is the measurement of the reflected shock wave speed at a given distance from the reflecting wall.

On the Figs 2a and 2b the speed of the reflected shock wave relative to moving gas ($\overline{D}_{PS1}+u_1, \overline{D}_{PS2}+u_1$) is plotted vs. incident shock Mach number. This speed was calculated according to relations given by Eqs. (1):

$$\overline{D}_{PS1} = \frac{x_{PS1}-x_{PS0}}{t_{PS1}-t_{PS0}}\, m/s \qquad \overline{D}_{PS2} = \frac{x_{PS2}-x_{PS1}}{t_{PS2}-t_{PS1}}\, m/s \tag{1}$$

and represents averaged speed between two pressure transducers (the superscript line reflects this fact). In these formulas x_{PSi} and t_{PSi} is a distance from the reflecting wall to the pressure sensor *PS*i and time of arrival of the reflected shock wave to pressure sensor *PS*i (first pressure jump) respectively. For both pressure sensors (*PS*1 –

x = 0.073 m and *PS*2 – x = 0.172 m) for the Mach numbers below 2.75, the speed of the reflected wave coincides with the value for the inert medium. For pressure sensor *PS*1 in the intermediate range 2.8 < M0 <3.0 the speed of the reflected wave gradually increases (in simulation as well as in experiment), attaining CJ value. The most discrepancy in experimental and simulated wave speeds is in this range of incident shock Mach numbers. The same behavior is observed for pressure sensor *PS*2.

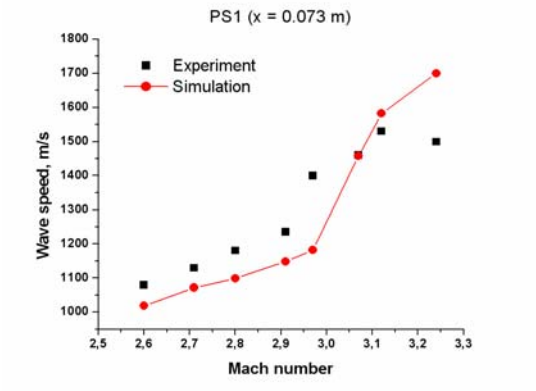

Figure 2a. Reflected shock wave speed vs. Incident shock wave Mach number. Prediction (circle) vs test measurement (square) at the *PS*1.

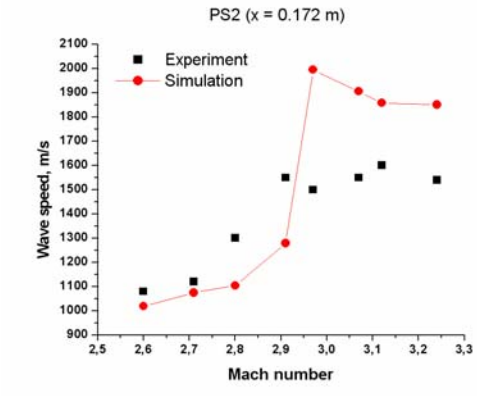

Figure 2b. Reflected shock wave speed vs. Incident shock wave Mach number. Prediction (circle) vs test measurement (square) at the *PS*2.

4 Discussion

In case of the low mach numbers of the incident shock, the temperatures behind reflected shock are relatively small as well and induction time *tind* (see Fig. 4), required for the mixture to ignite are large. After the induction time is finished, the ignition at the wall starts and after some transitional process the overdriven detonation is formed. The time scale *tf* and spatial scale *xf* of the formation process are small in comparison with the induction time (*th* << *tind*) and distance, traveled by reflected shock wave to this time (*xf* << (*tind* + *tf*)·D_r, where D_r is a speed of the reflected shock in the Lab frame). The detonation formed, attains its steady CJ speed value D_{CJ2} (where D_{CJ2} is a speed of the detonation wave in the Lab frame). After some time *tp* (propagation time) this detonation wave overtakes reflected shock wave (corresponding distance is *xp*) and forms overdriven detonation wave, propagating through the gas, compressed by incident shock wave. Its CJ speed is D_{CJ1} (in the Lab frame). The sequence of the events, described above remains valid up to sufficiently high temperatures and is illustrated on the *x*-*t* diagram of the Fig. 4.

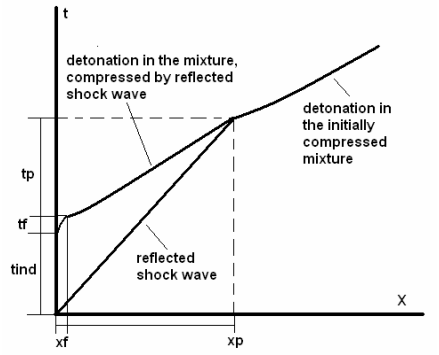

Figure 2. *x*-*t* diagramm of the processes behind reflected shock wave. See the section 4 for explanations

Correlation of the point *xp* with the positions of the pressure sensors x_{PS1} and x_{PS2} throw the light on the dependences of the Figs. 2a and 2b.

For the pressure sensor *PS*1:

1) if *xp* > x_{PS1}, then $\overline{D}_{PS1} = D_r$ (reflected shock wave passes through *PS*1);

2) if *xp* < x_{PS1}, than the average speed $\overline{D}_{PS1}$ is given by Eq. (2):

$$\overline{D}_{PS1} = D_{CJ1} - \frac{D_r D_{CJ2}\left(D_{CJ1} - D_r\right)}{D_{CJ2} - D_r} \cdot \frac{tind}{x_{PS1}}. \qquad (2)$$

It follows from Eq. (2), that the dependence $\overline{D}_{PS1}\left(M_0\right)$ is a monotonous, see Fig. 2a.

For the pressure sensor *PS*2:

1) if *xp* < x_{PS1}, than $\overline{D}_{PS2} \geq D_{CJ1}$ (overdriven detonation passes through *PS*2);

2) if $xp > x_{PS2,}$ than $\overline{D}_{PS2} = D_r$ (reflected shock wave passes through *PS*2);

3) if $x_{PS1} < xp < x_{PS1}$, than there is no simple expression like Eq. (3) for $\overline{D}_{PS2}$, but estimation is

$$\overline{D}_{PS2} \approx f(xp) \cdot D_{CJ1} \frac{x_{PS2} - D_r \cdot tind}{x_{PS2} - x_{PS1}}, \quad (3)$$

where $f(xp) > 1$ is an average overdrive factor of the detonation wave between point *xp* and pressure sensor *PS*2. Expression reveals, the for a long induction periods *tind* (low temperatures) $\overline{D}_{PS2}$ is small and is compared with D_r. For very small induction periods (high temperatures behind reflected shock) $\overline{D}_{PS2}$ is large enough $\overline{D}_{PS2}/D_{CJ1} \approx f(xp) \cdot x_{PS2}/(x_{PS2} - x_{PS1}) > 1$, i.e. dependence $\overline{D}_{PS2}(M_0)$ could exhibit maximum, as on the Fig. 2b.

While Eq. (3) gives a rough estimation for average speed of the reflected shock involving such an undefined parameter as $f(xp)$, the relation (2) is sufficiently accurate.

The equation (2) in Arrhenius coordinates ($\ln(D_{CJ1} - \overline{D}_{PS1}), 1/T_2$) will be a straight line with the inclination of E_a/R, where T_2 is temperature behind reflected shock wave, E_a is activation energy in Arrhenius law for induction time and R is universal gas constant. Using this type of the coordinates, the dependence $\overline{D}_{PS1}(M_0)$ exhibits fundamental property, which does not depend on parameters of the experimental setup, but only depend on kinetics of the chemical reaction in the system, i.e. effective activation energy, and serves as a support for direct ignition time measurements.

Contrary, the average speed of the reflected shock wave for the second pressure sensor (calculated according to Eq. (1)) is not so useful; it strongly depends on the relative positions of the pressure sensors and does not depend on the kinetics of the reactions directly

5 Conclusions

In the present work the mechanism of Jet-A combustion developed in [2] was applied for simulation of the detonation initiation by reflection of the plane shock waves in 1D approach. Results of the simulations agreed well with the experimental data and reproduce experimentally measured speeds with the accuracy 10 – 15% in the range of incident shock Mach numbers of 2.6 – 3.0. Investigation of the pressure and temperature spatial evolution in time allowed to describe sequence of events in the system, to show presence of an overdriven detonation in the system and quantitatively describe dependences of the measured in experiments averaged reflected shock speeds on incident shock wave strength. Possibility of the reflected wave speed maximum at the second pressure sensor was revealed. Nevertheless the specific form of the plots, obtained from experiments or simulations are strongly dependent on specific features of the setup. The measurement of the reflected wave speed at the first pressure sensor can be used as a support for direct measurements of the ignition delay times because of its direct relation with the kinetics of the combustion, as shown in the previous section.

6 Acknowlegments

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References

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