Shock-wave initiation of detonations in propane/air mixtures

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Introduction

Functioning of propulsion devices based on supersonic combustion modes is usually accompanied by the formation and propagation of shock waves, which produce the necessary level of thermal excitation of the mixture to maintain high rate of energy release in the system. In some cases, apparatus design can be considered as a single self-consistent device in which interactions of shock waves with confinement walls and inner flow structure sustain the propagation of fast deflagrations and detonations along a certain trajectory. Under such approach, the confinement geometry can facilitate substantially the mixture re-ignition inside combustion chamber due to the effects of shock focusing [1-5]. This work addresses to systematic experimental and numerical investigations of auto-ignition phenomena at shock wave interaction with reflecting ducts of different geometry in propane/air mixtures, which are used as a model fuel for many studies of detonations. Under this studies the self-ignition and initiation domains in stoichiometric propane-air mixtures have been investigated under shock wave focusing in 1 - hemi-spherical and hemi-cylindrical reflectors with radii R= 38 mm; 2 - wedge and cone reflectors with apex angles of 90 ^{0}; 3 - parabolic and paraboloidal reflectors.

Experimental Setup

Stainless steel shock tubes of 76 and 50 mm in diameter were used in experiments. The runs were performed in stoichiometric $\phi = 1$ propane/air mixtures at mean post-reflected shock pressures of 3 $\pm$ 0.2 atm. Pressure variations in different cross-sections were recorded by piezoelectric pressure gauges with a 1.5-mm spatial resolution. The pressures at the cavity bottom were measured by high-frequency pressure sensors. Stainless steel test sections for shock focusing are mated to the end flanges of shock tubes. To measure ignition delays inside reflecting cavities, 5-mm transparent quartz rods were passed through the models near the cavity bottom. The flame emission in selected spectral band was registered by means of the photo-multiplier. In all shock wave focusing tests in propane/air mixtures the luminosity of C_2 radicals (λ=516.5 nm) was detected using a narrow-band interferometric filter. The identification of initiation modes was performed by comparing reflected shock wave velocity and post- shock pressures at different distances from the cavity bottom.

To obtain reference data for propane-air oxidation, the ignition delay times and direct initiation modes were established behind normally reflected shock wave. Critical Mach numbers demarcating different self-ignition domains for plane reflection case are plotted in Fig.1 and provide the basis for the following performance analysis of axisymmetric and two-dimensional profiles in propane/air mixtures.

Computational model

The unsteady Reynolds Averaged Navier Stokes (RANS) equations are solved using a coupled, unstructured Total Variation diminishing (TVD) solver [6], which is second-order accurate in space and a nonlinear Riemann solver, namely HLLC (Harten, Lax and van Lear with Contact discontinuity). Dual time-stepping and algebraic multigrid methods were used for convergence acceleration. Perfect gas assumption and variable thermal and transport properties were used to model the participating gas mixtures, and a realizable k-ε model was used for modeling turbulence

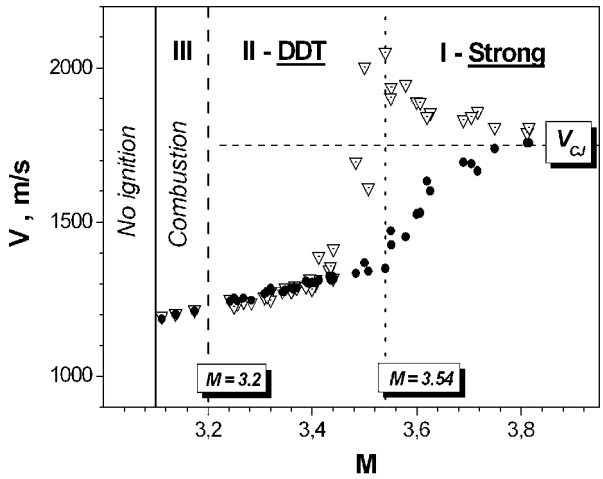

Fig. 1. Diagrams of self-ignition mode behind normally reflected shock wave in propane/air mixtures. Mean post-shock pressure is P = 3.1 $\pm$ 0.2 atm.

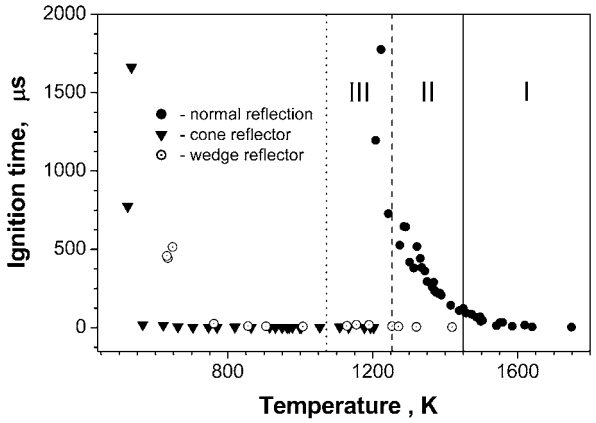

Fig. 2. Ignition time vs. mean post-shock temperature at shock wave reflections from a plane wall, two-dimensional, and axisymmetric profiles. Strong ignitions for: I – plane wall; II - wedge; III - cone. Mean post-shock pressure is P = 3.1 $\pm$ 0.5 atm.

processes. In these simulations, heat transfer to the walls is neglected. For all the simulations reported here, viscous terms are included because they are important for simulating boundary layer-shock interactions and boundary layer-detonation interactions.

A two-step reduced chemical mechanism was used to model ignition chemistry required to simulate detonation initiation [7,8]. The equilibrium parameters required for use in these two-step mechanisms as defined in [7,8].

Experimental Results

Two-dimensional wedge, parabola, and corresponding axisymmetric ducts were used as the focusing elements. We have categorized four different regimes of the self-ignition at focusing conditions in the following terms: no ignition, weak ignition (deflagration), transient ignition resulting in DDT upstream the reflector and strong ignition (detonation) [3, 5]. Particular attention has been paid to determining the critical ISW intensity required for initiation of different self-ignition modes. The measured values of ignition delays vs. mean post-shock temperature are plotted in the Figure 2. As is seen in the figure, the shock wave focusing in two-dimensional and axisymmetric profiles significantly decrease the ignition thresholds of propane/air mixture as compared with the case of the normal reflection. The focusing results in a substantial decrease of ignition times in a wide range of post-shock temperatures. For self-ignition of the mixture, 3D axisymmetric reflectors are much more efficient than two-dimensional ones.

Figure 3 shows absolute velocities of the reflected wave at different parts of the tube from the cone apex vs. ISW intensity. The critical Mach numbers required for direct initiation in the cone and paraboloidal reflectors are 2.76 and 2.69, respectively. For paraboloid case, the transient regimes have not been observed experimentally, and as the ISW intensity decreasing, the weak ignition immediately follows the strong ignition mode. For cone reflector, the transient domain extends to lower Mach numbers and occurs at critical shock strengths of M > 2.36. So, one can conclude that cone reflector with apex angle of 90^0 is more efficient than paraboloidal one to generate the gaseous explosions via DDT or direct initiation at a studied range of conditions.

Computational Results

The computational simulations were performed using (i) a 2D axisymmetric CFD model and (ii) a 3D CFD model for a cone reflector. These simulations include a strong as well as a transient

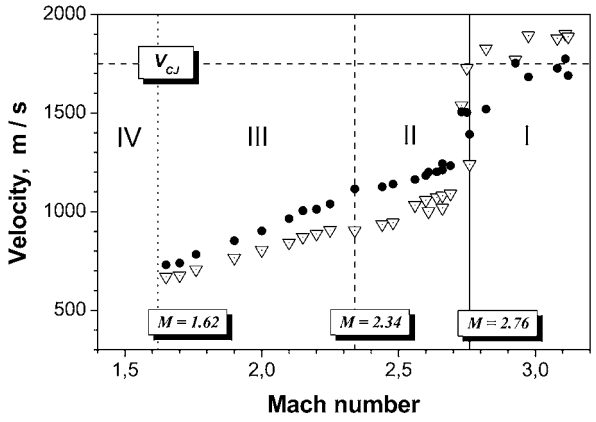

Fig. 3. Absolute velocity of reflected shock wave at different bases along the tube vs. ISW Mach number in cone reflector: I - strong ignition; II - transient ignition; III - weak ignition; VI - no ignition.

initiation in a stoichiometric C_3H_8-air mixture.

The 3D CFD simulation of a strong initiation event (M = 3.07) is shown in Fig. 4. Figure 4 (i)-(ii) presents the progression of this simulation, which shows axial variation of schlieren with fuel mass fraction values and contours of U-velocity. The simulations show that the initiation occurs at the apex of the cone reflector very rapid detonation initiation immediately after the reflected wave passes by the probe location (with in ~ 50 μs). An explosion that occurred at the apex of the cone can be seen in contours of schlieren in Figure 5(i). Figure 4(i) shows the butter fly structure of the detonation diffraction as seen in U-velocity contours in the diverging section of the cone reflector and Fig. 4(ii) shows a fully-developed planar detonation front.

The predicted pressure-time traces at three distinct but separate locations show good agreement with test measurements. The comparisons of the 2D axisymmetric and 3D CFD simulations show that the 2D axisymmetric simulations predict the occurrence of the detonation initiation and the progression of events leading to a quasi-steady detonation wave propagation reasonably well for the case of strong initiation. For the case of the transient initiation case, the 3D simulations show evolution of the events from reflection of the shock wave to formation of the detonation wave front exhibit local three dimensional flow effects.

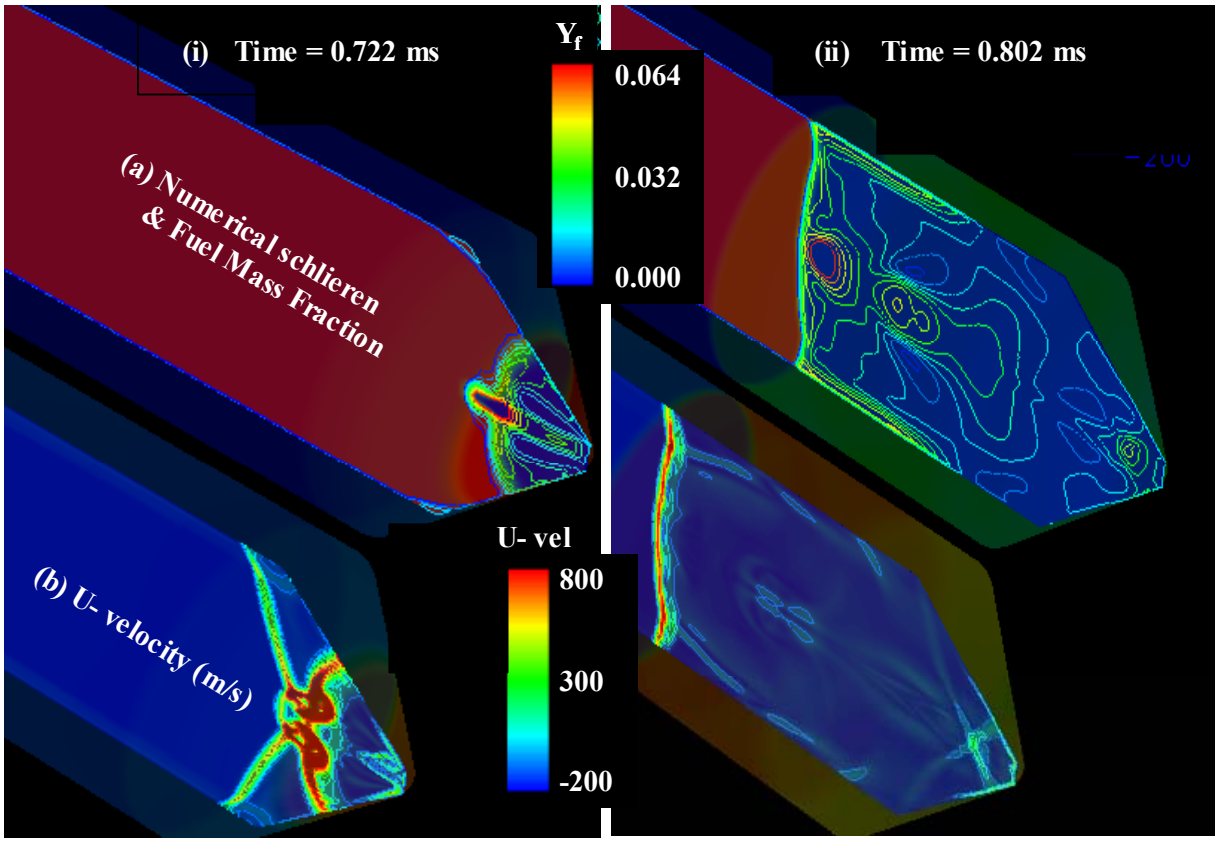

Fig. 4. Progression of detonation initiation events for the case of strong initiation at (i) t = 0.722 ms and (ii) t = 0802 ms, shows axial variation of (a) numerical schlieren rendered with fuel mass fraction and (b) contours of U-velocity as a function of time for the case of a cone reflector, obtained using a 3D CFD model.

Conclusions

The self-ignition and initiation domains in stoichiometric propane-air mixtures at post shock pressures of P = 3.2 $\pm$ 0.5 atm were determined at shock wave focusing in 1 – hemi-spherical and hemi-cylindrical reflectors with radii R= 38 mm; 2- wedge and cone reflectors with apex angles of 90^0; 3 - parabolic and paraboloidal reflectors. The critical Mach numbers required for direct initiation are 2.76 and 2.69 in cone and parabaloidal reflectors, respectively. For cone reflector, the transient ignition resulting to DDT occurs at critical shock strengths of M > 2.32.

Multidimensional (2D axisymmetric and 3D) computational simulations are reported for two-specific cases namely strong initiation and transient initiation for the case of a cone reflector. Simulations show, while the detonation initiation occurs in a very short duration of time for the case of strong initiation (approximately 55 μs after the incident shock wave is reflected from the wall), reflected-shock-to-detonation transition occurs over a relatively longer duration of time (1.6 ms after the incident shock wave is reflected from the wall) for the case of transient initiation. Simulations also show that while the wall-bound, corner convective flows induced by reflected shock boundary layer interactions have no impact on the occurrence of the detonation initiation in the strong initiation case, these flows may have significant impact on the occurrence of the detonation initiation in the transient initiation case. Comparisons of predicted and measured pressure-time traces show reasonable agreement.

Acknowledgements

This work were sponsored by State Scientific Program «Energy 18» (Republic of Belarus) and GE Global Research Center.

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