THEORY OF DIRECT INITIATION OF DETONATION

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In this work, we discuss an application of a nonlinear evolution equation that we have developed for the dynamics of slowly evolving weakly-curved detonations [1] to a problem of direct initiation of detonation. The evolution equation is

$$\dot{D} = a_1\omega_* - a_2\kappa \,, \qquad (1)$$

where a_1, a_2 are certain positive functions of D, ω_* is the reaction rate at the sonic locus, κ is the lead-shock curvature. The evolution equation exhibits competing effects of the heat release, curvature, and shock acceleration. For a spherical detonation, Eq. 1 is a second-order ordinary differential equation in the shock radius $R = 2/\kappa$. Solutions of the equation for spherical detonation in stoichiometric hydrogen-oxygen are shown in left Fig. 1. The variables are scaled based on the half-reaction length, initial pressure, and initial density. Dashed line is the quasi-steady solution obtained from $a_1\omega_* = a_2\kappa$, thin solid lines are solutions of Eq. 1 for different initial speed of the lead shock D_0 at fixed initial radius $R_0 = 200$, dash-dot line is the reactive blast wave solution of Taylor-Sedov-Korobeinikov [2] at critical energy $E_c = 1.48\cdot 10^8$ and radius $R_s = 89.5$.

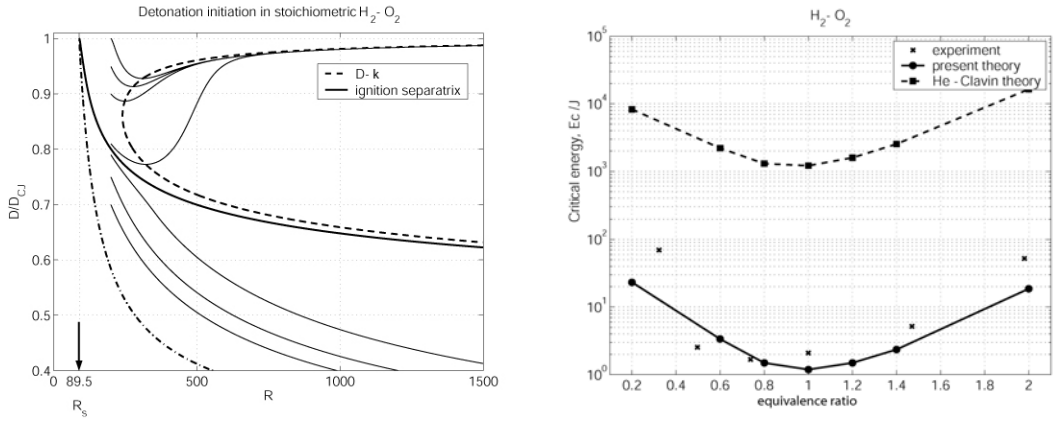

Fig. 1. The dynamics of initiation (left) and critical energies (right) for spherical detonation in H_2-O_2

An important feature to point out is that integral curves $D(R)$ that start from large D_0 suffer an initial drop in velocity, pass through a minimum, and then increase, asymptotically approaching D_{CJ} as $R \to \infty$. But solutions corresponding to low D_0 decay with R and recover only at extremely large distances (on the order of 10^8 in the scales of the reaction zone). This critical behavior is strikingly similar to what is observed in experiments and numerical simulations of direct initiation. Thick solid curve in left Fig. 1, which we call the "ignition separatrix"', defines critical conditions; it separates initial states that lead to ignition (above the curve) from those that lead to failure (below the curve).

By using the reactive blast wave solution and global kinetic data from Caltech detonation database, which are derived from detailed chemical calculations, we calculated critical energies for hydrogen-oxygen (shown in right Fig. 1) for a range of equivalence ratios, compared the predictions with

experimental data of Matsui and Lee [3] and found excellent agreement. Also shown is the prediction based on the quasi-steady theory of He and Clavin [4], which is seen to over-predict critical energies by 3-4 orders of magnitude in agreement with findings by Eckett, Quirk, and Shepherd [5]. We have also calculated critical energies for hydrogen-air and ethylene-air mixtures with similar conclusions. Present theory that considers higher-order unsteady effects (shock acceleration) successfully describes basic features of the initiation process observed in experiments and numerical simulations and allows one to calculate initiation energies based on the explosive chemical and thermodynamic properties only, without having to invoke significant modeling assumptions. It is shown that detonation dynamics during initiation depends on the relative strength of the heat-release "force" ($a_1\omega_*$) and flow-divergence "force" ($a_2\kappa$), resulting in successful initiation of self-sustained detonation if the heat release is sufficiently stronger than divergence or in failure if otherwise. The theory demonstrates the importance of unsteady effects in the initiation dynamics as was also pointed out by Eckett, Quirk, and Shepherd [5] and Lee and Higgins [6] in earlier studies.

Generally, the theory is applicable to multi-dimensional detonations that have small curvature on the scale of the reaction-zone size and propagate so that the lead-shock speed changes very slowly on the reaction-zone time scales. A very important aspect of the evolution equation (1) is that it does not rely on any assumption regarding the shock-speed variation about planar CJ speed, D-D_{CJ}, so that D can deviate from D_{CJ} by O(1) amount. This property allows one to investigate the detonation failure dynamics that occurs at significantly below-CJ speeds. Comparisons with two-dimensional simulations of detonation diffraction around a 90-degree corner also demonstrate the ability of the theory to predict detonation failure and re-initiation under more general conditions.

Acknowledgements

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