Numerical prediction of shock induced ignition in the presence of fluctuations

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Previous experiments of deflagration to detonation transition have established that hot spots stemming from hydrodynamic fluctuations in a reactive mixture play an important role. The current study addresses the classic problem of shock induced ignition and transition to detonation in 1D. Fluctuations are introduced in the reactive medium by allowing speed modulations of the piston driving the shock wave, with prescribed frequency and amplitude. This gives rise to acoustic oscillations in the medium, as it undergoes ignition and DDT.

The problem is treated numerically with a newly developed Lagrangian code with full chemistry. The Lagrangian description permits to simply implement the piston speed evolution. The convective terms are solved by an exact Riemann solver, while the chemical kinetic evolution is integrated with Cantera. We studied mixtures of hydrogen and ethylene with oxygen, under the experimental conditions of the fast flame experiments recently published by Saif et al. (PROCI 2017). The San Diego mechanism was used for both mixtures. The code was first verified on steady ZND detonations. The code reproduced well the exact ZND structure with full chemistry.

Preliminary results studied the role of the fluctuation amplitude and wavelength on ignition in hydrogen and ethylene. For the hydrogen mixture, the numerical simulations identified the different ignition regimes predicted by Sharpe with a much simpler two-step model . At temperatures above the cross-over temperature, the ignition and detonation formation were more gradual. At low temperatures, the ignition gave rise to a strong shock prior to transition to detonation. The ignition regimes correlated well with the χ parameter, defined as the product of the effective activation energy and ratio of induction to reaction. The fluctuations induced by the piston were found to have a stronger effect on mixtures with large χ. In these cases, ignition delays were lowered and the transition to detonation was more rapid.

Numerical simulations in the ethylene mixture revealed that the ignition was always accompanied by very strong pressure waves and the establishment of internal detonation waves. This was found compatible with the larger sensitivity to hot spot ignition in this mixture, and larger χ parameter. In all cases studied, the fluctuations were found to significantly shorten the ignition delay.