



WPI

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Zoom Meeting ID:

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PhD Dissertation Defense Presentation

Investigation into the Controlling Physics of the Deflagration-to-Detonation Transition



Abstract: The deflagration-to-detonation transition (DDT) poses a significant explosion hazard in combustible gas mixtures. Understanding how fundamental mixture properties affect flame runaway and DDT will enable development of generally applicable modeling approaches. The sensitivity of DDT to two mixture properties are investigated. First is the auto-ignition propensity of the mixture, which varies significantly across fuels, and also changes with small changes in fuel composition, like what exists between samples from different natural gas sources. Second is the thermo-diffusive stability, which can play a dominant role in the flame evolution of lean H₂/air mixtures and rich heavy hydrocarbon/air mixtures. This dissertation utilizes a combined experimental and modeling approach to investigate if auto-ignition is a rate limiting step, and whether thermo-diffusive stability of the mixture and the attendant flame acceleration has an influence on DDT.

Experiments conducted in a smooth, closed cylindrical tube with mixtures of similar deflagrative properties revealed a negligible sensitivity of the critical velocity at which the detonation ignited to the ignition delay of the mixture. This result suggests that auto-ignition of the mixture in hot-spots may not be rate limiting in the conditions studied. Experiments conducted with thermo-diffusively stable and unstable mixtures displayed a sensitivity of the critical velocity to flame wrinkling induced by instability onset. Turbulence induced flame wrinkling displayed similar behavior to the unstable experiments, with an increased propensity for detonation onset. The influence of flame wrinkling on DDT is not captured by existing theoretical models.

To understand the gas-dynamic environment ahead of the accelerating flame, two-dimensional numerical simulations of flame acceleration and DDT were performed for a stoichiometric H₂/O₂ mixture using detailed chemistry. The simulations revealed significant pressure buildup at the flame tip prior to flame runaway and DDT. However, to investigate the complex coupling between the flame and the gas-dynamic field a reduced-order model was developed.

To this end, a one-dimensional Lagrangian model solving the Euler equations with an accelerating piston boundary was developed to reconstruct the gas-dynamic state ahead of accelerating flames using experimentally measured flame velocity as input. Testing against the two-dimensional simulations revealed that using the flame displacement velocity as the piston velocity overpredicted the thermodynamic state ahead of the flame. This was corrected through implementing a semi-porous piston, allowing mass flux through the boundary, bringing the model predictions into agreement with the simulations. Application of the model to the experimental results revealed two distinct pathways to DDT for thermo-diffusively stable and unstable mixtures. For TD-stable mixtures, DDT required significant flame acceleration and elevated pressures and temperatures ahead of the flame. In contrast, TD-unstable mixtures underwent DDT at substantially lower pressures and temperatures, and without the rapid acceleration observed in TD-stable mixtures. These results provide a novel insight into the gas-dynamic evolution ahead of accelerating flames prior to flame runaway.

Collectively, the results indicate that auto-ignition is not rate-limiting for DDT in the configurations studied. Instead, the results point to the critical role of flame wrinkling in DDT. The reduced-order model revealed that thermo-diffusively stable and unstable mixtures undergo DDT through different pathways, the mechanisms of which warrant further investigation.