Narrative Progress Report

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Project Title: Fundamental understanding of stochastic ignition transition of hydrocarbon fuels
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Motivation and Background

Innovations in the operation of spark-ignition (SI) engines have dramatically reduced emissions to meet increasing standards but gains in the fuel economy of SI engines have comparatively trailed. Downsizing and super-charging (DSC) has emerged as a means to increase thermodynamic efficiency through the reduction of pumping and friction loads on an engine. However, the inhomogeneous ignition phenomena known as super knock has been found to be a limiting factor in the production of DSC engines.

Super knock is a rare event characterized by the formation of a high-pressure wave from an ignition kernel. This wave is sufficiently strong to yield in-cylinder pressures in excess of 300 bar and can destroy engine components in a single cycle. Super knock is far more severe than conventional knock with over-pressures that are usually an order of magnitude greater than the pressure at top-dead-center.

Due to the high peak pressures and wave speed, super knock is often considered to be a detonative event. Theory describing the development of a detonation from an exothermic reaction center (also known as a hot-spot) typically utilizes Zeldovich's scalings, which compares the acoustic speed to the reaction front gradient. This parameter states that self-excitement is possible when the chemical resonance is near unity. Lee et al. found experimentally using photochemical deposition that gradients in the induction time lead to detonation formation, which the authors deemed the Shock Wave Amplification by Coherent Energy Release (SWACER) mechanism. Sharpe and Short found through asymptotic analysis using a two-step chemical model that for sufficiently shallow induction gradients, the reaction wave propagates supersonically and is determinable only from initial conditions. Furthermore, Bradley and coworkers, extended the Zeldovich scaling to include an acoustic residence parameter, which characterizes the interaction of the heat release with the compression waves.

While significant evidence has been found to support the self-excitation description of super knock in one-dimension, recent visualizations of super knock in a rapid compression machine show a significant multi-dimensional interaction of the ignition kernel with the wall boundary, including the enhancement of the detonation wave through reflection. Hence, the parameters of Bradley are a useful but incomplete description of the super knock phenomena, and the predominant dynamics of the chemico-physical interaction in knock-to-super-knock transition is not well-understood at a fundamental level. That is, an understanding of the ignition kernel development and shock wave enhancement is needed.

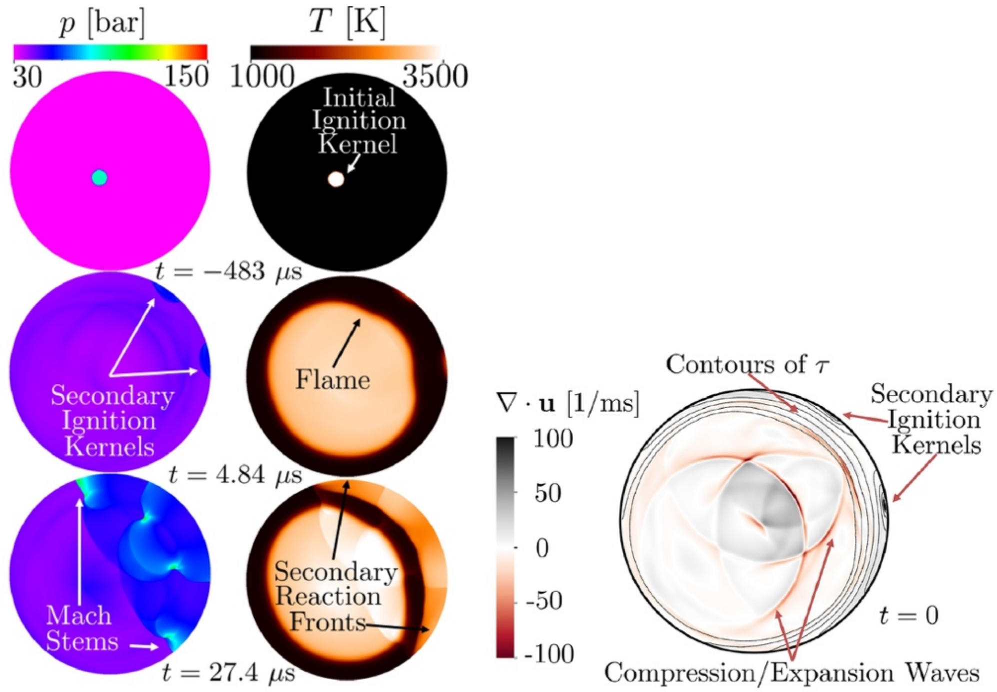
The objective of this work is two-fold: to develop a chemical model capable of simulating gas-dynamic ignition phenomena, and to employ this model for a multi-dimensional simulation of super knock.

Research Achievements and Key Results

A new ignition time model was developed [Grogan & Ihme 2019] to study super knock through zonal modeling and multi-dimensional simulation. The main research findings are as follows:

- It was demonstrated through the development of the ignition time model that the gas-dynamic forcing is exactly separable from the chemical self-excitement under the assumption of negligible diffusive effects.
- A zonal model was developed for the pre-ignition of a charge due to a flame as a relevant validation of the ignition time model. The flame acted to compress the unburned gas causing both the pressure and temperature to increase. For the case examined, a significant reduction in ignition delay was found. Furthermore, the ignition time model was found to yield a 0.2% difference in ignition delay compared to detailed chemistry indicating its applicability.
- A two-dimensional simulation was performed (see Figure below) to examine the complex shock-flame structures arising from pre-ignition in an RCM. The flame kernel was found to focus the shock wave yielding pressure in excess of 300 bar. Furthermore, the curvature of the wall was found to promote a Mach stem, which enhanced the shock wave. Since the pressure peaks found are in excess of 300 bar for the current configuration, it was concluded that the multi-dimensional simulation represented a super knock event.
- The simulation was found to be in agreement with the diagram of Gu et al. The combustion wave was found to be supersonic, propagating at 1100 m/s; however, it did not develop into a detonation during the course of the simulation.
- Since the simulation excluded diffusive effects in the ignition region, it was proposed that acoustic resonance the chamber is the primary driver of the development of super knock for the configuration under examination;

furthermore, it was argued that gas-dynamic compression due transient compression from the flame could be a key mechanism for super knock.



(a) Simulation Initial Condition and Ignition. (b) Compression and Ignition Onset.

Snapshots of the super knock ignition process. The time origin is the onset of ignition. The simulation condition matches the RCM experimental configuration of Wang et al. (2014). Contours in (b) are of the ignition time and are spaced logarithmically.

Impact

This research provided partial support for one PhD-student on the development of a novel ignition model for describing super knock. In addition, this research allowed the PI to generate preliminary results in support of a proposal application to the Energy Efficiency Renewable Energy Program at the Department of Energy with the goal of developing improved modeling capabilities for predicting multi-mode ignition in advanced low-emission internal combustion engines.

Reference

Grogan, K. P. and Ihme, M., "Development of an ignition time model with an application to super knock." Proceedings of the Combustion Institute, 37, 3487-3494, 2019.