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# Effect of initial temperature and fuel properties on knock characteristics in a rapid compression and expansion machine

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## Abstract

In this study, the effect of initial temperature and fuel properties (such as ignition delay time variation with temperature) on knock characteristics was investigated for methane and propane dual fuels via a rapid compression and expansion machine, which can emulate one compression and expansion stroke in a real engine. Numerical calculations using CHEMKIN-PRO with AramcoMech1.3 were carried out to obtain fuel properties. The correlation between flame propagation velocity at the moment of autoignition and knock intensity was confirmed. The findings revealed that unburned mass fraction and initial temperature did not directly affect knock intensity. Additionally, experimental results were analyzed based on theories proposed by Zeldovich and Bradley. The results of the analysis indicated that smaller gradients of autoignition delay time and temperature caused the higher flame propagation velocity and the resultant higher knock intensity. It was concluded that initial temperature affected both the gradient of autoignition delay time and that of temperature, which in turn indirectly influenced the knock intensities.

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*Keywords:* Knock intensity; Rapid compression expansion machine; Autoignition

## 1. Introduction

Currently, the “downsizing concept” forms a state-of-art technical trend given its high efficiency and low emission in engines. This can be realized by a high compression ratio and a highly boosted technology. A knock is likely to occur

when the pressure in both a high compression ratio and highly boosted engine increases. Particularly, a heavy knock produces unpleasant vibrations and sounds to the driver and causes damage to the engine. In order to circumvent this problem, several studies have focused on elucidating various aspects of the knock phenomenon, such as the prediction of knock occurrence.

As a knock is caused by autoignition, it can be classified in terms of autoignition modes, as pointed out by Maly [1]. There are different

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autoignition modes characterizing knock properties, including “deflagration,” “thermal explosion,” and “developing detonation,” which were originally proposed by Zeldovich [2] and Bradley [3–5]. According to Bradley [5], knock intensity is related to the autoignition modes, while the prediction of when autoignition will occur in an engine such as so-called Livengood–Wu integral [6] cannot predict the autoignition modes and the corresponding knock intensity. Therefore, investigating autoignition modes and their relation to knock intensity are important from both practical and scientific viewpoints.

Bradley et al. [3] investigated the coupling between a pressure wave and the corresponding reaction wave by 1-D simulation and elucidated the autoignition modes and resultant knock intensity. Dai et al. [7] extended the theory proposed by Zeldovich and Bradley with respect to autoignition modes to a negative temperature coefficient (NTC) region, where autoignition is initiated by a cold spot. They showed that the NTC behavior does not significantly affect the autoignition modes, and that the cool spot may also generate knock in engines within the NTC regime by using 1-D simulation.

However, experimental work to verify and reinforce the theory is still rare despite these theoretical and numerical pioneer studies. Rudloff et al. [8] extended the extant theory and introduced a new non-dimensional parameter to predict the violence of abnormal combustion in realistic engines. Nevertheless, they did not observe flame itself to identify the parameters.

A previous study [9] experimentally investigated the factor affecting knock intensity by using a rapid compression and expansion machine (RCEM) for various fuels. The results indicated that fuel properties (gradient of ignition delay time) affect knock intensity, which is consistent with the theory proposed by Zeldovich and Bradley. However, in the previous study, various fuels under the same initial condition were used to change the fuel properties and the effect of the initial condition on fuel properties was not taken into account.

In this study, we investigate the effect of initial temperature and resultant fuel properties on knock intensity for the same fuel based on the theoretical framework developed by Zeldovich and Bradley.

## 2. Zeldovich and Bradley’s theory

Zeldovich first analyzed different flame propagation modes for autoignition at a distinct “hot spot” [2]. The different modes included 1) thermal explosion, 2) supersonic autoignitive deflagration, 3) developing detonation, 4) subsonic autoignitive deflagration, and 5) conventional flame propagation. Gu and Bradley demonstrated the existence of these five modes through 1-D simulation and specified the initial conditions for each mode [3]. When

temperature distributions are non-uniform (that is, there are initial temperature gradients), autoignition occurs spatially in a continuous manner because of the distribution of different autoignition delay times,  $\tau$ , in space.

By assuming 1-D propagation, the autoignition propagation velocity relative to unburned gas,  $u$ , can be correlated with  $\tau$  as follows:

$$u = \frac{dx}{d\tau} = \left( \frac{d\tau}{dT} \frac{dT}{dx} \right)^{-1} \quad (1)$$

Given the expansion of the reacted gas and mass conservation, propagation speed relative to the fixed stationary coordinates,  $dx/dt$ , can be expressed as follows:

$$\frac{dx}{d\tau} = u\sigma \quad (2)$$

where  $\sigma$  is the ratio of the unburned gas density to the burned gas density.

When  $u = a$ , Eq. (1) gives the critical temperature gradient of a hot spot for developing detonation, as follows:

$$\left( \frac{dT}{dx} \right)_c = a^{-1} \left( \frac{d\tau}{dT} \right)^{-1} \quad (3)$$

By using the critical temperature gradient, the non-dimensional temperature gradient,  $\xi$ , can be defined as follows:

$$\xi = \left( \frac{dT}{dx} \right) / \left( \frac{dT}{dx} \right)_c = \frac{a}{u} \quad (4)$$

The other parameters affecting the characteristic of the pressure wave include the ratio of acoustic time to excitation time,  $\tau_e$ , which represents the dimensionless measurement of heat release supplied to the pressure wave corresponding to a residence time of a pressure wave in the hot spot. This can be expressed as follows:

$$\varepsilon = \frac{r_0/a}{\tau_e} \quad (5)$$

where  $r_0$  is the initial radius of the hot spot. Bradley et al. performed 1-D simulation to investigate the limits for detonation initiation in terms of  $\varepsilon$  and  $\xi$  and derived a detonation peninsular [3–5]. In addition, Bradley and Kalghatgi analyzed the ratio of the maximum value of instantaneous sound pressure  $Dp(t)_{\max}$  above the ambient at time  $t$  to ambient pressure,  $p$ , based on the simple acoustic theory [4]. They estimated that  $Dp(t)_{\max}/p$  is related to  $\xi^{-2}$ , although this is only valid in the absence of shock waves and detonations. This estimation is important because the factors affecting knock intensity were derived theoretically.

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