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Impact of thermodynamic properties and heat loss on ignition of transportation fuels in rapid compression machines

Ahfaz Ahmed[a,*], Mireille Hantouche[b], Muneeb Khurshid[a], Samah Y. Mohamed[a], Ehson F. Nasir[a], Aamir Farooq[a], William L. Roberts[a], Omar M. Knio[c], S. Mani Sarathy[a,*]

[a] *Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*
[b] *Mechanical Engineering Department, Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*
[c] *Computer, Electrical, and Mathematical Science and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*

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ABSTRACT

Rapid compression machines (RCM) are extensively used to study autoignition of a wide variety of fuels at engine relevant conditions. Fuels ranging from pure species to full boiling range gasoline and diesel can be studied in an RCM to develop a better understanding of autoignition kinetics in low to intermediate temperature ranges. In an RCM, autoignition is achieved by compressing a fuel/oxidizer mixture to higher pressure and temperature, thereby initiating chemical reactions promoting ignition. During these experiments, the pressure is continuously monitored and is used to deduce significant events such as the end of compression and the onset of ignition. The pressure profile is also used to assess the temperature evolution of the gas mixture with time using the adiabatic core hypothesis and the heat capacity ratio of the gas mixture. In such RCM studies, real transportation fuels containing many components are often represented by simpler surrogate fuels. While simpler surrogates such as primary reference fuels (PRFs) and ternary primary reference fuel (TPRFs) can match research and motor octane number of transportation fuels, they may not accurately replicate thermodynamic properties (including heat capacity ratio). This non-conformity could exhibit significant discrepancies in the end of compression temperature, thereby affecting ignition delay (τ_{ign}) measurements. Another aspect of RCMs that can affect τ_{ign} measurement is post compression heat loss, which depends on various RCM parameters including geometry, extent of insulation, pre-heating temperature etc. To, better understand the effects of these non-chemical kinetic parameters on τ_{ign}, thermodynamic properties of a number of FACE G gasoline surrogates were calculated and simulated in a multi-zone RCM model. The problem was further investigated using a variance based analysis and individual sensitivities were calculated. This study highlights the effects on τ_{ign} due to thermodynamic properties of various surrogate fuels and differences in post compression heat loss over low, intermediate and high temperature region.

1. Introduction

Rapid compression machines (RCM) are routinely used to study autoignition of fuels under temperature and pressure of relevance to practical engines. A wide variety of fuels, ranging from pure hydrocarbons to regular gasoline and diesel [1–3] can be investigated in an RCM. Fig. 1 describes a typical RCM experiment where a fuel/oxidizer mixture is rapidly compressed to top dead center (TDC) thereby reaching a higher pressure and temperature. After TDC, the compressed gases experience heat loss (manifested as pressure decay), which is followed by a small pressure rise marking the onset of first stage ignition. Further, second stage or final ignition is recorded by a sharp pressure rise, and this duration between TDC and final ignition is designated as ignition delay (τ_{ign}). In this experiment, two parameters are of particular significance for the accurate determination of τ_{ign}: 1) The fuel/oxidizer mixture's temperature at TDC (T_{TDC}); and 2) Post compression heat loss, manifested as pressure decay.

The effect of T_{TDC} on τ_{ign} is well known from several RCM studies [4–7] and also the effect of post compression heat loss on τ_{ign} is well understood [5]. Briefly, higher T_{TDC} increases the rate of reactions promoting the ignition (except for negative temperature coefficient (NTC) region) and hence a shorter τ_{ign} is observed, while higher heat loss rate effectively reduces the bulk gas temperature thereby reducing the rate of reactions and yielding a longer τ_{ign}. Accurate temperature measurement in an RCM still remains a challenge, except for a few attempts [8–11]. The adiabatic core hypothesis [7] is largely used to

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[*] Corresponding authors at: Clean Combustion Research Center, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
E-mail addresses: ahfaz.ahmed@kaust.edu.sa (A. Ahmed), mani.sarathy@kaust.edu.sa (S.M. Sarathy).

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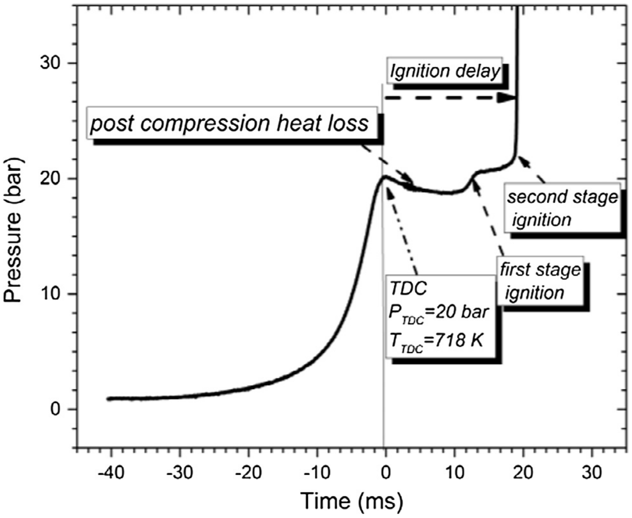

Fig. 1. RCM pressure profile for a gasoline/air mixture at equivalence ratio $\varnothing = 1$ and $P_{TDC} = 20\,bar\ T_{TDC} = 718\,K$ [3].

estimate the temperature profile from the measured pressure trace. Eq. (1) describes the relation between P_{TDC}, T_{TDC} of the adiabatic core and its dependence on γ, defined as the ratio of specific heats $\left(\frac{C_p}{C_v}\right)$ of the fuel/oxidizer mixture.

$$\int_{T_1}^{T_2} \frac{\gamma}{\gamma-1}\frac{dT}{T} = ln\left(\frac{P_2}{P_1}\right) \tag{1}$$

Eq. (1) implies that γ needs to be well known to estimate T_{TDC} precisely. Fig. 2 presents the effect of T_{TDC} on measured τ_{ign} in an RCM for iso-octane from the data set of Atef *et al.* [12] at $P_{TDC} = 20$ bar and $T_{TDC} = 803, 841, 884\,K$. The measurements from these experiments demonstrate a reduction in τ_{ign} with increase in temperature, a well-known fact reiterated to substantiate the arguments in this study. In later sections, it is shown that the differences in T_{TDC} could be introduced by dissimilarities in γ of surrogates, in line with Eq. (1). Such surrogates could have identical ignition delays across a range of experimental conditions but due to the differences in γ, they could show dissimilarities in τ_{ign} in RCM.

It must be noted that differences in T_{TDC} in Fig. 2 are not due to dissimilar γ, but is attained through variation in initial experimental conditions and is presented solely to substantiate the effect of T_{TDC} on τ_{ign}.

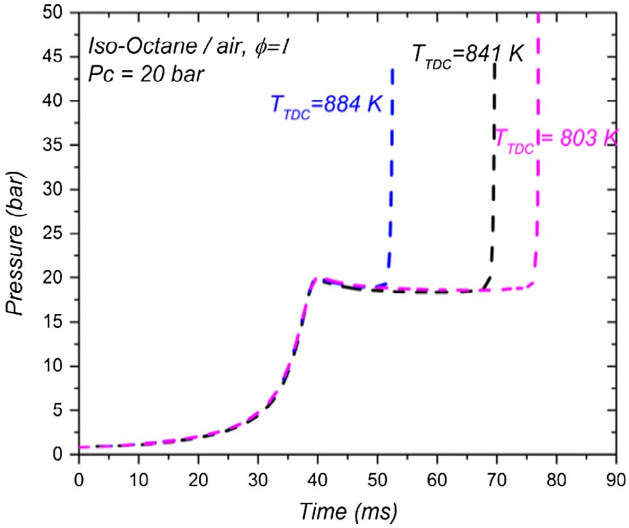

Fig. 2. The effect of T_{TDC} on measured ignition delay for iso-octane in air at $\varnothing = 1$ (O_2: N_2 = 1: 3.76) at $P_{TDC} = 20$ bar.

The implications of this observation lie in the practice of using surrogate fuels to represent transportation fuels in RCM simulations and experiments. Traditional surrogates for gasoline-type fuels are primary reference fuels (PRF) and ternary primary reference fuels (TPRF), which are comprised of iso-octane/*n*-heptane and iso-octane/*n*-heptane/toluene respectively. The PRFs and TPRFs are prepared to match research and motor octane numbers of the target fuel, while they do not necessarily match other fuel properties, including specific heat ratio (γ over the temperature range). If such discrepancies exists, they could introduce uncertainty in T_{TDC}, eventually affecting τ_{ign} measurements and simulations.

The other parameter considered in this study with a potential effect on τ_{ign} measurements in RCM is the post-compression heat loss which is specific to an RCM facility. In Fig. 3, RCM pressure traces from the National University of Galway, Ireland (NUIG) and the University of Connecticut, USA (UCONN), are shown under identical TDC conditions from the data set of Atef *et al.* [12].

In both the cases, measurements from UCONN show higher pressure decay, indicating higher rate of heat loss, and hence a longer τ_{ign}. Fig. 3 interestingly points out that even under identical experimental conditions, different heat loss attributes of the RCM facility can result in different ignition delays for identical fuel/oxidizer mixtures. This observation also implies that, while studying a fuel across RCM facilities, the data must be interpreted in conjunction with the employed RCM's heat loss attributes, as earlier discussed by Mittal and Sung [7].

RCM exhibits a complex reactive flow problem, and there are several experimental factors that could affect the processes leading to ignition. Apart from differences arising from γ, temperature in the RCM is affected by experimental factors such as pressure, fuel mixing procedure, and diagnostic measurements techniques as shown by Weber *et al.* [13]. They also show that the initial temperature and pressure are the major sources of uncertainty in T_{TDC} estimation. RCM experiments often use diluents in ignition studies which leads to differences in ignition delay measurements. Wulmer *et al.* [14] conducted such an investigation on shock tube and RCM with different diluent mixtures and concluded that ignition delay strongly depends on diluent's properties such as thermal conductivity, thermal diffusivity and heat capacity. In a similar investigation, Wagnon *et al.* [12] discussed the effect of four different diluent gases: argon, nitrogen, water, and carbon dioxide, on ignition delay measurements for three different fuels in an RCM. The heat release rates and τ_{ign} were found to be sensitive to diluents; the study also discussed the significance of diluents on low-temperature kinetics. Recently, Goldsborough *et al.* [5] conducted a detailed review of RCM studies and also discussed about parameters that could significantly affect τ_{ign} measurements and simulations in RCMs. Some of the earlier investigations (and comparisons in Fig. 3) have also shown that the RCM heat loss affects the τ_{ign} [4,15] measurements and different RCM facilities could report different values of τ_{ign} under identical experimental conditions. However, to the authors' knowledge none of the earlier studies have conducted a detailed analysis of such effects of variation in T_{TDC} (due to γ) and heat loss on τ_{ign} in RCM, and therefore a detailed investigation is warranted. To study this problem in detail, three surrogates of FACE G [16] gasoline with different γ resulting in different T_{TDC} are considered. The effect of heat loss on ignition delay has been accounted for by building a simplified multi-zone RCM model to allow variation in the heat loss rate for fuels with single and multi-stage ignition delays. Furthermore, a numerical experiment was designed with τ_{ign} as a function of T_{TDC} (a strong function of γ) and RCM heat loss rates. Investigations were conducted with a variance based analysis to decouple the effects of these parameters on τ_{ign} and identify individual sensitivities.