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# Effects of flame propagation speed and chamber size on end-gas autoignition

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#### Abstract

End-gas autoignition has direct relevance to engine knock and thereby has been extensively studied. However, in the literature there are still some contradictions on how different factors affect end-gas autoignition and knock intensity. Specifically, there is contradictory literature on (1) whether faster combustion may promote or inhibit end-gas autoignition and engine knock, and (2) whether knock intensity increases or decreases with burned mass fraction (BMF). To answer these two questions, one-dimensional flame propagation and end-gas autoignition in a closed cylindrical chamber are investigated and the effects of flame propagation speed and chamber size on end-gas autoignition are examined in this study. In the transient numerical simulation, two fuels, hydrogen and iso-octane, are studied; and detailed chemistry is considered. It is shown that if the flame propagation is fast enough or the chamber is small enough, end-gas autoignition and knock can be prevented; otherwise, the knock intensity may increase as the flame propagation speed increases or as the chamber size decreases. The maximum pressure is found to change non-monotonically with the BMF as well as the flame propagation speed and chamber size. This helps to explain why there is contradictory literature on those two questions mentioned above. The answers to these two questions depend on the amount of unburned mixture at the moment of end-gas autoignition: if there is enough unburned mixture before end-gas autoignition, the maximum pressure increases with the flame propagation speed and BMF; otherwise, the opposite trend occurs. Besides, comparison between the results for hydrogen and iso-octane indicates that end-gas chemical reaction and heat release occurring before autoignition can greatly reduce the maximum pressure.

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Keywords: Autoignition; End-gas; Flame propagation speed; Chamber size; Maximum pressure

#### 1. Introduction

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When a premixed flame propagates in a closed chamber, the unburned gas (end-gas) is progressively compressed and its temperature and pressure continuously increase. Under certain conditions, the ignition delay time of end-gas might be shorter

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than the time taken by the propagating flame to consume all the unburned mixture, and thereby autoignition might occur in end-gas.

End-gas autoignition has direct relevance to knock in spark ignition engines (SIE) [1–3]. Therefore, there are many studies on end-gas autoignition in the literature. Previous theoretical (e.g., [4– 6]), experimental (e.g., [7, 8]) and numerical (e.g., [9-11]) works on end-gas autoignition were described in our recent paper [12] and thereby is not repeated here. Besides, direct numerical simulations (DNS) were conducted to study the combustion in Homogeneous Charge Compression-Ignition (HCCI), Spark-Assisted HCCI (SACI), and Reactivity Controlled Compression Ignition (RCCI) conditions. For examples, Bhagatwala et al. [26] conducted DNS of an autoignitive ethanol/air mixture in HCCI and SACI modes. In their simulation, source terms were included to emulate the compression and expansion due to piston motion. They demonstrated that compression heating has great impact on hear release profile. Bhagatwala et al. [27] conducted 1D and 2D DNS under RCCI conditions of a primary reference fuel (PRF) mixture. They observed both deflagration and spontaneous ignition fronts and analyzed the influence of n-heptane concentration, fuel-concentration stratification and pressure on the combustion modes. Yoo and coworkers [28, 29] examined the influence of temperature inhomogeneities and turbulence on the ignition in PRF HCCI combustion. They found that the influence of fuel composition on the ignition characteristics of PRF/air decreases greatly with thermal stratification. These studies are related to end-gas autoignition since both deflagration and autoignition modes are included.

Despite the extensive attention devoted to understanding end-gas autoignition and engine knock, there are still some disagreements or even contradictions on how different factors affect end-gas autoignition and knock intensity. For example, Chen and Raine [13] found that there is contradictory literature about whether faster combustion may promote or inhibit end-gas autoignition and engine knock. On one hand, faster flame propagation results in less time for end-gas autoignition and thereby knock may be suppressed (e.g., [14]). On the other hand, increasing the flame propagation speed makes the end-gas pressure and temperature rise more rapidly and thereby reduces the ignition delay time, which is favorable for endgas autoignition and knock (e.g., [15]). Therefore, there is a need to investigate how flame propagation speed affect end-gas autoignition and knock intensity.

Besides, the knock intensity is considered to be strongly correlated with the amount of unburned or burned mixture at the moment of end-gas autoignition. Burned Mass Fraction (BMF, the mass fraction of burned gas at the moment of end-gas autoignition) is often used as an indicator for knock severity. However, there is contradictory literature on whether knock intensity increases or decreases with BMF. For examples, Robert et al. [16] demonstrated that the knock intensity increases as BMF decreases; while Kagan et al. [4] and Kagan and Sivashinsky [5] showed that knock intensity increases when BMF increases. It is therefore of interest to investigate how knock intensity changes with BMF.

The above-mentioned two contradictions constitute the motivation of the present work. The objective of this study is to clarify these contradictions. One-dimensional (1D) flame propagation and end-gas autoignition in a closed cylindrical chamber were investigated here. It is noted that autoignition in practical engines is a highly nonhomogeneous phenomenon. Since, turbulence variable chamber volume, boundary layer and wall heat transfer are not considered in the 1D model, engine combustion and knock cannot be fully represented by the present 1D model (therefore, 'maximum pressure' instead of 'knock intensity' is used for present simulation results). Nevertheless, such simple 1D model still helps to clarify the contradictions mentioned above since different effects can be isolated and quantified individually.

Besides the flame propagation speed, we also considered the chamber size since it also affects end-gas autoignition and BMF. Both theoretical analysis and numerical simulations were conducted to examine the effects of flame propagation speed and chamber size on end-gas autoignition and to elucidate the relationship between maximum pressure and BMF.

#### 2. Theoretical analysis

We analyzed 1D laminar flame propagation and end-gas autoignition in a closed chamber: only 1D cylindrical geometry was considered here and similar analysis can be easily extended to planar and spherical geometries. It is noted that similar analysis was conducted before for laminar flame speed measurement using propagating spherical flames in a closed spherical chamber [17, 18] (but not for endgas autoignition). The premixture with initial temperature  $T_0$  and pressure  $P_0$  is ignited from the center line in a 1D cylindrical chamber whose inner radius is  $R_W$ . Since, the end-gas is progressively compressed by the propagating flame, its temperature  $T_u$  and pressure P continuously increase. Similar to [17], the following assumptions were adopted in the present analysis: the 1D cylindrical flame is thin and smooth; the pressure is spatially uniform and changes only with time, i.e., P = P(t); the burned and unburned gases behave as ideal gases; the unburned gas is compressed isentropically; and heat loss and buoyancy effects are negligible. Moreover,

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