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# Three-stage autoignition of gasoline in an HCCI engine: An experimental and chemical kinetic modeling investigation

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## Abstract

The alternative HCCI combustion mode presents a possible means for decreasing the pollution with respect to conventional gasoline or diesel engines, while maintaining the efficiency of a diesel engine or even increasing it. This paper investigates the possibility of using gasoline in an HCCI engine and analyzes the autoignition of gasoline in such an engine. The compression ratio that has been used is 13.5, keeping the inlet temperature at 70 °C, varying the equivalence ratio from 0.3 to 0.54, and the EGR (represented by $N_2$) ratio from 0 to 37 vol%. For comparison, a PRF95 and a surrogate containing 11 vol% $n$-heptane, 59 vol% iso-octane, and 30 vol% toluene are used. A previously validated kinetic surrogate mechanism is used to analyze the experiments and to yield possible explanations to kinetic phenomena. From this work, it seems quite possible to use the high octane-rated gasoline for autoignition purposes, even under lean inlet conditions. Furthermore, it appeared that gasoline and its surrogate, unlike PRF95, show a three-stage autoignition. Since the PRF95 does not contain toluene, it is suggested by the kinetic mechanism that the benzyl radical, issued from toluene, causes this so-defined "obstructed preignition" and delaying thereby the final ignition for gasoline and its surrogate. The results of the kinetic mechanism supporting this explanation are shown in this paper.

*Keywords:* Three-stage autoignition of gasoline; HCCI engine; Combustion; Kinetic mechanism; Obstructed preignition

## 1. Introduction

The HCCI combustion has been proposed as an interesting alternative combustion technology for the reduction of automobile pollution. This technology has not been implemented in the real market, mainly due to the lack of sufficient control of the ignition delay. For this purpose, several physical parameters that affect the quality of the HCCI combustion and the ignition delay have been studied in the literature [1–11]: mixture homogeneity, inlet temperature of air and fuel, fuel composition, and kinetics of the fuel oxidation at lower temperatures. Since the operating conditions of an HCCI engine are dependent on the

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fuel that is to be used, special attention is given to fuel autoignition research, both experimentally and numerically: primary reference fuels (PRF) [2], aliphatic hydrocarbons [4,5,12,13], aromatics [7,8], light hydrocarbons and gaseous fuels [14–17], diesel fuels [18–24], and gasoline fuels [25–27], to mention a few. Before any alternative fuels will be used, the use of conventional fuels, such as gasoline and diesel, in HCCI engines is of importance. Therefore, the autoignition of such fuels should be investigated. The first part of this paper analyzes the kinetics of the autoignition of gasoline in an HCCI engine with a compression ratio of 13.5, an inlet temperature of 70 °C, varying the equivalence ratio from 0.3 to 0.54, and the EGR ratio (represented by $N_2$) from 0 to 37 vol%.

Gasoline is a multicomponent fuel. Hydrocarbon interaction during the combustion can occur, where the intermediary products of one fuel component intervene with the intermediary products of another fuel component. Some investigations [28–30] have been performed, studying such interactions between hydrocarbons. They state that interactions can take place through a radical pool of OH, H, and O radicals. They also note the possibility that chemical interactions can take place between different fuel components and their radicals. An example is presented in [28], concerning the reaction between respectively an alkyl- or alkylperoxy radical from one fuel component with an alkane from another fuel component. As such, there is a possibility that interactions between fuel components and their intermediary species can take place that can influence the autoignition process. This necessitates the use of chemical kinetic mechanisms for multicomponent fuels for the analysis of such interactions as is done by [28–30]. The second part of this paper aims at analyzing the hydrocarbon interaction taking place in gasoline, by the use of a surrogate fuel and a corresponding experimentally validated surrogate mechanism [31,32], included in Appendix A.

## 2. Experimental

The experimental setup is presented elaborately in previous work [32]. The essentials are reported in this section. The complete experimental setup comprises an HCCI engine, the air inlet system, the fuel injection system, a premixture tank for inlet mixture homogeneity purposes, and an EGR installation. In this paper, the EGR installation provides for the dilution by nitrogen, which is used as a parameter for the gasoline autoignition investigation. A premixture tank serves to mix the injected fuel with the entering air and subsequently with the EGR flow. Before the fuel/air/EGR mixture enters the engine, it passes through a tube, the geometry (several 90° bends) of which enhances the homogeneity of the mixture.

The HCCI engine's compression ratio is set to be 13.5 for this study. The engine has a bore of 82.55 mm, a stroke of 114.5 mm, and a displacement volume of 612 $cm^3$. The ratio of the connecting rod to crank radius is 4.44. The exhaust valve opens at 140° after top dead center (ATDC) and closes at 15° ATDC. The intake valve opens at 10° ATDC and closes at 146° BTDC. The measurements of the equivalence ratio, measured by the flow rates of the fuel and the air, present an error of ±0.005, while the compression ratio shows an error of ±0.5. The temperatures of the cooling water (50 °C) and the oil (40 °C) as well as that at the inlet of the engine show an error of ±1 °C. The composition of the fuel has an error of ±1 vol%, while that of the EGR flow exhibits an error of ±2%.

Three fuels are used in this work: a commercial gasoline with octane number 95; a gasoline surrogate that consists of a mixture of *n*-heptane, iso-octane, and toluene; and a primary reference fuel (PRF), containing 95 vol% iso-octane and 5 vol% *n*-heptane, referred to as PRF95. In order to generalize this study and broaden the range at which it is performed, the gasoline autoignition process is done at different equivalence ratios and EGR ratios. These are parameters that influence considerably the energy of the system. The cylinder pressure is measured by a pressure sensor and the heat release is calculated from this measured pressure. The ignition delays are calculated from the heat release maxima. The cool flame delay is defined as the crank angle degrees' (CAD) interval from bottom dead center (BDC) until the first heat release maximum and the final ignition is defined as CAD interval from BDC until the last heat release maximum. The autoignition process is a result of various complex chemical, physical, and energetic processes that take place during the autoignition process. The ignition delays represent the chemistry; the pressure and the heat release represent the power, work, energy, and heat involved. The experimental findings are analyzed, using the same experimentally validated kinetic surrogate mechanism that is used in previous work [31,32]. This mechanism has been obtained by reducing detailed individual *n*-heptane, iso-octane, and toluene kinetic mechanisms, using the quasi-steady-state assumption and the partial equilibrium assumption. Furthermore, by leaving the reactions that are important to simulate the autoignition under HCCI operating conditions, the mechanisms were reduced even more. Finally, these mechanisms were merged into a ternary reduced kinetic mechanism for gasoline and diesel surrogates. The surrogate mechanism has been validated experimentally in a constant volume environment for temperatures be-