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# Investigation of *iso*-octane combustion in a homogeneous charge compression ignition engine seeded by ozone, nitric oxide and nitrogen dioxide

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## Abstract

The homogeneous charge compression ignition (HCCI) engine is well known as an alternative engine which could replace conventional engines (spark ignition (SI) and combustion ignition (CI) engines) in order to meet pollutant requirements and reduce fuel consumption. However, controlling this kind of combustion remains difficult and represents a real challenge. The present investigation focussed on the use of different oxidizing chemical species (ozone, nitric oxide and nitrogen dioxide) which can modify the chemical kinetic governing HCCI combustion. Experiments were conducted on a single cylinder HCCI engine fuelled with iso-octane, for constant engine parameters and for oxidizing species concentrations varying from 0 up to 100 ppm. These experimental results are coupled with kinetic analyses in a homogeneous constant volume reactor performed with a detailed kinetic mechanism. The effects of ozone, nitric oxide and nitrogen dioxide were initially studied and compared when they separately seed the intake of the engine. Results showed that all the molecules improve HCCI iso-octane combustion. The highest effect on CA50 phasing was observed for ozone while the lowest was for nitrogen dioxide. These results were confirmed and explained by a kinetic interpretation. HCCI experiments were then carried out with ozone and nitric oxide injected together in the intake of the engine. Experimental results show a combustion enhancement when these two molecules are present but a delay in CA50 phasing was observed for low ozone concentrations and a constant nitric oxide concentration until the ozone concentration becomes higher. A kinetic interpretation, through two-step computations, showed that there is a strong oxidizing reaction between nitric oxide and ozone, yielding nitrogen dioxide. Therefore, the presence of nitrogen dioxide can explain the CA50 delay observed due to its low effect among all the oxidizing chemical species studied.


*Keywords:* HCCI; Iso-octane combustion; Ozone ($O_3$); Nitric oxide (NO); Nitrogen dioxide ($NO_2$)

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## 1. Introduction

Nowadays, limitations on pollutant emissions are increasing drastically and reducing fuel consumption has become a real challenge for the future due to the depletion in fossil fuel reserves. Currently, internal combustion engines are mostly dominated by two different conventional combustion modes, spark ignition (SI) and compression ignition (CI), but it becomes hard for these kinds of engines to meet these requirements. Consequently, other combustion strategies must be explored, such as homogeneous charge compression ignition (HCCI). This combustion mode, which is considered as an alternative engine to replace conventional engines, yields efficiencies similar to those of a CI engine, coupled with low nitrogen oxide ($NO_x$) and particulate matter (PM) emissions. However, controlling HCCI combustion, which is dominated by chemical kinetics, remains the greatest issue to be solved and has been the main topic of research in recent years [1].

Many studies have been conducted with different fuels or fuel mixtures [2–5] and results showed that the HCCI engine presents a major advantage through its fuel flexibility. Other studies involve the use of exhaust gas recirculation (EGR) as a means of combustion control [6–8] and some investigations focussed on EGR components [9,10]. Among the numerous species composing EGR, nitric oxide (NO) has received particular attention. Contino et al. [11] performed HCCI experiments and computations for NO concentrations varying from 0 to 500 ppm and observed that this chemical species has a promoting effect on combustion. Dubreuil et al. [12] explored its effect on n-heptane and two alternative fuels using an HCCI engine. The results on cool and main flame ignition delays showed that the addition of NO advances the combustion. However, for concentrations higher than 100 ppm, the cool flame phasing is delayed while a lower effect is observed on the main flame. Moreover, another recent study on three gasoline surrogate fuels [13] also presented similar results, but with pressure and temperature dependencies. Finally, the oxidation of a n-heptane/toluene blend fuel was studied in a jet stirred reactor (JSR) by Anderlohr et al. [14]. Results demonstrated that the promoting effect of NO is due to the reaction with hydroperoxyl radicals ($HO_2$) coming from the fuel oxidation to yield a nitrogen dioxide ($NO_2$) and a hydroxyl radical (OH). The same reactions were also identified by Dayma et al. [15] on methanol oxidation when NO is added.

Recently, the use of ozone as a good combustion promoter was investigated and several studies on HCCI engines were carried out with this oxidizing species. Foucher et al. [16] explored the effect of ozone on n-heptane combustion and Masurier et al. [17] extended the investigation to primary reference fuels (PRF), i.e. n-heptane, iso-octane and mixtures of these two fuels. Both studies showed that ozone concentrations lower than 50 ppm can strongly enhance and advance PRF combustion. Moreover, results on kinetic computations established that the promoting effect comes from the decomposition of ozone into oxygen ($O_2$) and O-atoms followed by rapid oxidation of the fuel. Another study on a cooperative fuel research (CFR) Diesel engine [18] showed that ozone decreases the ignition delay and consequently, changes the effective fuel cetane number (CN). Finally, HCCI experiments conducted with natural gas [19,20] as well as dimethyl ester (DME) [21] also confirmed that ozone improves self-ignition and can control combustion phasing.

Ozone and nitric oxide, as well as other species such as nitrogen dioxide ($NO_2$), are the main oxidizing species produced by dielectric barrier discharge (DBD) or corona discharge (CD) supplied with air [22,23]. Moreover, the size of these devices is approximately the one of intake engine lines, sometimes smaller, implementations can therefore be easily considered at the entrance of intake manifolds to keep homogeneous inlet conditions. Consequently, the impact of these species may be considered and studies must be conducted.

The aim of the present investigation was to study the effect of three different oxidizing chemical species (ozone ($O_3$), nitric oxide (NO) and nitrogen dioxide ($NO_2$)) on an HCCI engine fuelled with iso-octane when they are separately seeded in the intake of the engine. Since the interactions between $O_3$ and NO when simultaneously injected have not been studied yet, experiments with these two species were also conducted. Finally, computations on ignition delays with a detailed kinetic mechanism were performed to give a kinetic interpretation of the effect of the oxidizing species studied.

## 2. Experimental setup

The experimental setup used for this study is presented in Fig. 1. It is a single-cylinder conventional Diesel engine, modified to run in HCCI mode and coupled to an electric motor to maintain a constant rotation speed. Details and validation of the HCCI setup are described by Dubreuil et al. [10] and the main characteristics of this engine are given in Table 1. In the present study, each flow of gases and liquids was controlled by mass flow controllers and introduced inside a plenum upstream the combustion chamber to prepare a perfectly homogeneous mixture. The air flow came from an air compressor and was divided into two flows: one directly supplies the intake and the other is employed to dilute and