



# Combustion and emissions characteristics of toluene/n-heptane and 1-octene/n-octane binary mixtures in a direct injection compression ignition engine



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## ABSTRACT

Successfully designing and making effective use of the next generation of liquid fuels, which will be derived from a range of biomass and fossil sources, requires an understanding of the interactions between structurally similar and dissimilar fuel components when utilised in current engine technology. Interactions between fuel components can influence the release of energy and production of harmful emissions in compression ignition combustion through determination of the autoignition behavior of the fuel. This paper presents experimental studies carried out in a single-cylinder engine supplied with a range of binary mixture fuels to investigate the effect of fuel component interactions on autoignition in direct injection compression ignition. A range of binary mixtures consisting of toluene and n-heptane and also 1-octene and n-octane were tested so as to observe respectively the effect of an aromatic compound and an alkene on n-alkane combustion and emissions. The engine tests were carried out at constant injection timing and they were repeated at constant ignition timing and at constant ignition delay, the latter being achieved through the addition to the various fuels of small quantities of ignition improver (2-ethylhexyl nitrate). Increasing the presence of toluene in the toluene/n-heptane binary mixtures resulted in an increased ignition delay time and generated a distinct two stage ignition process. An increased level of 1-octene in the binary mixtures of 1-octene/n-octane was also found to increase ignition delay, though to a much lesser extent than toluene in the case of the toluene/n-heptane mixtures. Interactions between the fuel components during the ignition delay period appear important in the case of the toluene/n-heptane mixtures but not those of 1-octene/n-octane. At constant injection and constant ignition timings, the combustion phasing and the level of emissions produced by each binary mixture were primarily driven by the ignition delay time. With ignition delay equalised, an effect of adiabatic flame temperature on NO<sub>x</sub> production was visible.

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## 1. Introduction

There is consensus that anthropogenic release of CO<sub>2</sub> is resulting in global climate change [1], and this coupled with fears regarding security of supply of traditional fossil fuels is driving the move towards more sustainable future fuels. In addition, emissions legislation [2] reflects the need to reduce the levels of other environmentally harmful emissions from combustion of liquid fuels, such as NO<sub>x</sub> [3] and particulate matter; optimising the efficiency of energy release, while decreasing pollutant emissions, will be key to the success of future fuels.

Such fuels will likely come from both refined fossil sources and biomass. In either case, the resulting fuel will be a mixture of many

compounds of dissimilar chemical structure. Manipulation of the composition of a fuel is already routinely used, for example in fossil diesel, to meet specifications regarding cold flow properties and cetane number. Varying proportions of fuel components has also been employed to better control homogeneous charge compression ignition (HCCI) combustion [4–6]. However, when designing a future fuel, a deeper understanding of how individual components are interacting to dictate combustion phasing and contributing to the production of emissions is invaluable.

Key to determining combustion phasing in compression ignition combustion is the ignition delay time exhibited by a fuel. Therefore, studying the autoignition properties of binary fuel mixtures has long been of interest in combustion research and, in particular, mixtures containing toluene have received much attention. As an aromatic compound, toluene is representative of the many such compounds found in fossil fuels, and of compounds produced

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### Nomenclature

NO <sub>x</sub>	nitrogen oxides	SOC2	start of 2nd phase of combustion and point between SOC and the time of peak heat release rate at which $d(\tan^{-1}(dHRR/dCAD))$ is at a minimum and dHRR is positive
CO <sub>2</sub>	carbon dioxide	2 EHN	2 ethyl hexyl nitrate
IQT	ignition quality testing	CID	constant ignition delay
DCN	derived cetane number	IMEP	indicated mean effective pressure
CO	carbon monoxide	PPM	parts per million
THC	total hydrocarbons	FAME	fatty acid methyl ester
CAD	crank angle degree	HCCI	homogeneous charge compression ignition
PID	proportional integral derivative	RCM	rapid compression machine
DAQ	data acquisition	HRR	heat release rate
O <sub>2</sub>	oxygen	CFR	Cooperative Fuel Research
SOI	start of injection	SMD	Sauter mean diameter
BTDC	before top-dead-centre	CFD	computational fluid dynamics
TDC	top-dead-centre		
SOC	start of combustion		

from the catalytic cracking of crude renewable oils and the hydrothermal treatment of algal biomass [7,8]. Fuels suitable for compression ignition combustion nearly always require components that possess long alkyl chains in order to be of significant ignition quality, and several studies have investigated the interactions of toluene with n-heptane in differing proportions and at varying conditions.

Such investigations have in general focused on identifying the autoignition properties of toluene and n-heptane mixtures so as to further understanding of fuel effects on the phenomena of knock in SI engines and the rate of combustion in HCCI engines. One such means of doing so has been the rapid pressurisation of fuel and air mixtures in high pressure shock tubes. Herzler et al. [9] studied the ignition delay times of a mixture comprising 65% toluene and 35% n-heptane (by volume) at compression pressures of 10, 30 and 50 bar. While increasing the pressure consistently reduced ignition delay times, the effect of doing so became less important at higher pressures. For example, increasing the pressure from 10 to 30 bar resulted in a larger decrease in ignition delay than the same magnitude of pressure increase from 30 to 50 bar. Comparison of the data for the 65% toluene blend to that of pure n-heptane from a previous study [10] showed reduced negative temperature coefficient (NTC) reactivity for the toluene containing mixture. Hartman et al. [11] investigated the behavior of toluene and n-heptane blends containing up to 40% (volume) toluene in a high pressure shock tube at 40 bar and a temperature range of 700–1200 K. Above 20% toluene, further addition of toluene retarded the point of ignition and reduced the NTC region. Kinetic modelling suggested that the inhibiting effect of toluene on ignition of the mixtures to be highly temperature dependent and of greatest influence at 850 K for the conditions studied.

In studying HCCI in a rapid compression machine (RCM) with a peak compression ratio pressure of 4 bar, Tanaka et al. [4] observed the significantly longer ignition delay of a fully premixed blend comprising 74% toluene and 26% n-heptane compared to that of pure n-heptane. Andrae et al. [12] considered the autoignition of two toluene and n-heptane blends in a HCCI engine, both experimentally and through simulation. In engine tests, the blend containing a higher proportion of toluene exhibited longer ignition delays and initially the numerical simulation only accurately predicted these results when co-oxidation of the reactants was included. In addition to reactions involving the shared pool of radicals created by the oxidation of toluene and n-heptane, it

was suggested that reactions between the resulting benzyl and heptyl radicals were also important. However, a later refinement of the detailed model [13], utilising more accurate rate constants for the experimental conditions studied, found such reactions to be of less significance than originally considered.

Subsequently, Andrae et al. [14] in conducting semi-detailed kinetic modelling of toluene and n-heptane fuel mixtures, found the importance of cross reactions between the respective radicals of each fuel species to be dependent on the reaction conditions. In shock tube combustion at temperatures below 800 K, the inclusion of such reactions increased the model reactivity, but had no effect at higher temperatures or in HCCI simulations. Similarly, in conducting detailed kinetic modelling of surrogate gasoline fuels in a HCCI engine, Naik et al. [15] found that including cross reactions between the fuel components, which included toluene and n-heptane, had no effect on the model accuracy. Co-oxidation reactions between toluene and n-heptane were included in the modelling work of Anderlohr et al. [16], who found the reactivity of toluene to be influenced by the presence of NO<sub>x</sub>, with hydrogen abstraction from toluene by NO<sub>2</sub> found to promote low temperature radical branching.

In a more recent RCM study, Di Sante [17] investigated the ignition delay times of a range of toluene and n-heptane mixtures in different proportions and at final compression temperatures. It was found that increasing the percentage of toluene present in the blend increased both the 1st and 2nd stage ignition delay times, though the influence of toluene addition diminished with increasing temperature.

Vanhove et al. [18] conducted a series of RCM experiments with a range of binary mixtures, including a 1/1 (% mols) toluene and n-heptane blend, at a range of temperatures between 650 and 900 K and a compression pressure of 3–5 bar. Analysis of the reaction mixtures during the ignition delay period revealed that in addition to n-heptane, toluene also underwent oxidation prior to autoignition. A similar mixture of benzene and n-heptane produced a similar profile of ignition delay with temperature, but sampling of the reaction mixture revealed that benzene had not reacted, suggesting that the inhibiting effect of toluene may not be chemical. Further mixtures of iso-octane and toluene did show a decrease in reactivity relative to pure iso-octane that was attributable to competition for radicals between the fuel components. This was attributed to the lesser reactivity of iso-octane relative to n-heptane, thus placing greater demand on the available radicals.

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