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# Flame lift-off length and soot production of oxygenated fuels in relation with ignition delay in a DI heavy-duty diesel engine

A.J. Donkerbroek<sup>a,\*</sup>, M.D. Boot<sup>b</sup>, C.C.M. Luijten<sup>b</sup>, N.J. Dam<sup>a,b</sup>, J.J. ter Meulen<sup>a</sup>

<sup>a</sup> Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands <sup>b</sup> Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

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#### ABSTRACT

The relation between ignition delay and flame lift-off length (based on OH\* chemiluminescence) has been studied in an optically accessible heavy-duty diesel engine. Soot production has been studied as well, using both exhaust soot data and high-speed imaging of the in-cylinder natural luminosity. Since the luminosity is estimated to scale with  $T^{13}$  for our experimental conditions, the local temperature becomes a decisive factor in the interpretation of natural luminosity images. The fuels used include regular diesel and blends of various oxygenates (cyclohexanone, anisole, and dibutyl maleate) with synthetic diesel, to cover a wide range of cetane numbers and oxygen content.

Based on a literature review, we hypothesize that the flame speed only determines an upper limit for the flame lift-off length (rather than its exact position). Under conditions that promote auto-ignition, the lift-off length may be shorter, and is likely governed by ignition chemistry.

For the oxygenated fuels, the flame lift-off length is found to increase with ignition delay. An inverse correlation is found between the soot luminosity and the oxygen ratio at the lift-off length. The anisole-blend does not produce measurable amounts of exhaust soot as long as the injection duration is shorter than the ignition delay. Under cooled EGR-like conditions, the ignition delay is so large that anisole is considered a candidate fuel for soot-free operation of heavy-duty diesel engines up to medium load.

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#### 1. Introduction

For more than a 100 years, engines have been optimised for the available fossil-based fuels. Meeting future emission legislation, however, should be reached in a two-way synergetic approach. In addition to adapting the engine hardware to the existing fuel, a fuel could be tailored to the engine. An important enabler for such tailored fuels in the future is the development of synthetic fuels (XTL = 'anything to liquid'). Basically, XTL entails the gasification of an arbitrary, preferably renewable, source of hydrocarbons into a desired liquid fuel via specialised catalytic routes. This opens the possibility to produce a dedicated fuel, on a large scale, tailored specifically for use in either conventional combustion engines or in modern concepts such as premixed charge compression ignition (PCCI).

This is not to say that fossil-based fuels have not improved over the years. For example, large investments have been made to cut the aromatic content of diesel fuel. Besides lower soot emissions, a result of the reduction in aromatic content is a higher cetane

\* Corresponding author. Fax: +31 24 3653311.

number (CN). In conventional diesel fuels, a higher CN typically results in smoother running of the (diesel) engine and lower soot emissions. It is stressed here that this reduction in soot is caused by the lower aromatic content. The fact that fewer aromatics (which are key soot precursors) in the fuel leads to a higher CN is a by-product. An increase in CN can either have a positive or negative effect on net soot production, depending on how it is realised. This dependency is discussed at length in [1].

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The dogma, however, of ever increasing requirements for the cetane number (CN) has come under pressure in light of amounting interest in premixed charge compression ignition (PCCI) combustion in diesel engines [2–4]. In PCCI mode, the combustion and injection processes do not overlap, thereby avoiding the formation of the (jet) diffusion flame responsible for soot and NO<sub>x</sub> in the fuel rich core and near-stoichiometric periphery, respectively. Instead, a more or less premixed mixture is created, which burns volumetrically, thereby largely avoiding fuel rich zones and hot pockets. Unfortunately, PCCI, which requires long ignition delays, is extremely difficult to achieve in a controlled way with the available high CN diesel fuels, especially at higher loads. Extreme measures (e.g. reduced compression ratio, or large amounts of exhaust gas recirculation) need to be employed in order to counteract the high reactivity of the fuel [2–5].

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E-mail address: Arjandonkerbroek@gmail.com (A.J. Donkerbroek).

Nomenclature							
CA CN EHPC EGR FLoL FSN FWHM ID IMEP PCCI PM	crank angle cetane number Eindhoven high-temperature high-pressure cell exhaust gas recirculation flame lift-off length filter smoke number full width half maximum ignition delay indicated mean effective pressure premixed charge compression ignition particulate matter	$\begin{array}{l} \text{RoHR} \\ \text{SLoL} \\ (a)\text{SodQ} \\ (a)\text{TDC} \\ P \\ T \\ \vartheta_{dQ} \\ \phi \\ \Omega \\ \Omega_f \\ \rho \end{array}$	rate of heat release soot lift-off length (after) start of rate of heat release (after) top dead centre pressure temperature timing of start of rate of heat release equivalence ratio oxygen ratio oxygen ratio of the fuel density (kg/m <sup>3</sup> )				

Alternatively, PCCI-like combustion can be achieved with more or less stock engine hardware when running on low CN fuels [1]. A lot of research has been performed by the authors on low CN fuels, particularly oxygenated (i.e. fuel-bonded oxygen) variants. This work, performed both on engines and burners, has recently been summarised in [6]. The results demonstrate that near-zero soot and NO<sub>x</sub> emissions can be achieved with low CN diesel-oxygenate blends. More importantly, both in the burner and engine experiments, a clear correlation was found between blend CN and soot, with the latter decreasing sharply with reduced CN. With respect to the engine experiments, the low soot production is believed to be linked to an increasing premixed burn fraction for lower CN blends, which exhibit longer ignition delays [1-4,6-8].

The ignition delay mechanism, however, does not explain the occurrence of the same CN-soot trend in (co-flow diffusion) burner experiments [6]. In the utilised burners, combustion is continuous, with experiments lasting an average of over 30 minutes. Any effects of ignition delay are therefore irrelevant as the flame is ignited by an external agent such as a match or a lighter. A potential mechanism might involve the flame lift-off length (FLoL, i.e. the location downstream of the injector where the reaction zone stabilises after autoignition), which indicates to a large extent how much air is entrained upstream of the diffusion flame [6]. A longer FLoL means more air entrainment. Consequently, a lower equivalence ratio is established in the jet core, ultimately leading to the formation of less soot [9,10]. The question addressed here is whether the FLoL is governed by flame propagation velocity or by ignition processes.

#### 1.1. Summary of literature study

Table 1 provides a summary of the reviewed literature. In all studies the authors conclude that the FLoL is governed largely by ignition processes rather than by flame propagation. This conclusion appears to hold for a wide range of liquid and gaseous fuels irrespective of operating pressure, but is not in agreement with

Table 1		
Summation	of FLoL literature	review

the widely accepted flame propagation model [11,12]. Why this is the case requires further investigation, but the applied air/co-flow temperature might be of significance. While in [11,12] the air was at room temperature, the air/co-flow temperature in [9,13–18] was elevated to 750–1500 K. At the former conditions, auto-ignition processes are not supported and hence it is improbable that auto-ignition behaviour will influence the FLoL. In all like-lihood, the FLoL will then be governed by flame propagation. At the latter conditions, however, temperatures are high enough to facilitate auto-ignition chemistry and indeed it appears from [9,13–18] that this chemistry influences the FLoL.

A hypothesis based on the literature review is that the prevailing oxidizer temperature determines whether or not auto-ignition behaviour upstream of the FLoL is important with respect to the location of FLoL. Herein, a combination of effects is imaginable, with upstream auto-ignition events driving the 'nominal' FLoL, as determined by flame propagation, closer to the injector. In other words, the balance between flame speed and injection velocity determines an upper limit for the FLoL. In the event of upstream ignition events, however, the FLoL will be 'pulled' closer to the injector orifice and ignition chemistry will, along with flame propagation, determine the location of the FLoL.

An analogy can be drawn to knock in spark-ignition engines. The normal mode of combustion in spark-ignition engines is flame propagation. In some cases, however, the unburnt mixture, downstream of the moving flame front, can heat up (due to compression via expansion of the burnt products) to such an extent that undesired auto-ignition (or knock) occurs. In the event of knock, the propagating flame front will be strongly influenced by this autoignition process.

#### 1.2. Objective

Although a lot of data on the relationship between FLoL and ignition behaviour can be found in literature, the associated

Ref.	Setup	Fuel properties		Conditions			Observation	Conclusion
		Phase	CN	$T_g(\mathbf{K})$	p <sub>g</sub> (bar)	$ ho_g  (kg/m^3)$	Ignition precursors upstream of FLoL	Does FLoL correlate with ignition delay?
[9]	CVV <sup>a</sup>	L	42-80	800-1300	-	7.3–30	-	Yes, but no one-to-one correlation
[13]	CVV <sup>a</sup>	L	43-80	800-1300	-	7.3-30	CH <sub>2</sub> O and kernels of OH	Yes, but no one-to-one correlation
[14]	CVV <sup>a</sup>	L	41-56	800	50	-	Kernels of OH	Yes
[15]	CFB <sup>b</sup>	G	-	1045	1	-	HO <sub>2</sub>	Yes
[16]	CFB <sup>b</sup>	G	<0	1355-1475	1	-	CH <sub>2</sub> O and kernels of OH	Yes
[17]	CFB <sup>b</sup>	G	<0	1600	1	-	Kernels of OH	Yes
[18]	CVV <sup>a</sup>	L	46	750-900	-	14.8	Kernels of OH	Yes
[55]	CVV <sup>a</sup>	L	34-70	900-1000	60-67	22.8		Yes, and not with fuel volatility

CN = cetane number, CVV = constant volume vessel, CFB = co-flow (turbulent diffusion) burner, G = gas, L = liquid.

<sup>a</sup>  $T_g$  refers to gas temperature in vessel.

<sup>b</sup>  $T_g$  refers to co-flow temperature.

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