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**Vaporization and Combustion Processes of Alcohols and
Acetone-Butanol-Ethanol (ABE) blended in n-Dodecane for
High Pressure-High Temperature Conditions:
Application to Compression Ignition Engine**

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ABSTRACT

This study investigates the effect of fuel properties on the spray and combustion process of Acetone-Butanol-Ethanol (ABE) mixture and alcohol fuels, blended with the diesel surrogate fuel, n-dodecane (n-Do100), in different volume ratio from 20% to 50%. These fuels were characterized in the High-Pressure and High-Temperature (HPHT) thermodynamic conditions, representing current common-rail diesel engine operating modes. For that, a new combustion chamber called “New One Shot Engine (NOSE)”, was designed and developed to provide a standard ambient condition, “Spray-A” (near 60 bar, 900 K and 22.8 kg/m³) defined by Engine Combustion Network (ECN). To validate NOSE achieved this condition, the ambient thermodynamic conditions (pressure and temperature) and gas field velocity were measured and characterized. The measured results demonstrated that NOSE can reach the standard Spray-A condition with a homogeneous ambient temperature field. Also, the simulated results and Particle Image Velocimetry (PIV) measurements confirmed that the ambient gas velocity was below 1 m/s as required by ECN Spray-A specifications. Moreover, by using the standard ambient condition, the spray and combustion parameters were characterized by using the standard optical techniques, post-processing and criteria recommended by ECN. The liquid and vapor spray parameters were characterized by Diffused-Back Illumination and Schlieren techniques in non-reactive condition (pure nitrogen), while the absolute ignition delay and lift-off length were measured by OH* chemiluminescence in reactive condition (15% oxygen). The experimental results show the spray and combustion parameters performed on NOSE have a good agreement with results from ECN database, which confirms the high accuracy of the experimental set-ups and post-processing obtained in this study.

The effect of fuel properties on the spray and combustion parameters of ABE-dodecane blends (ABE20, ABE30, ABE40 and ABE50) and alcohol-dodecane blends (Bu20, Bu40, Bu20Eth20 and Eth20) were investigated by these standard methods. The results show that the liquid length of ABE blends was shorter than n-Do100 and slightly decreased by increasing ABE ratio in the blend due to high volatility. In contrast, the longer liquid length was obtained

by increasing quantity of alcohol in the blend. As the slightly different density for all fuels, an only slight difference in the mass flow rate, vapor spray penetration and spray angle can be observed. For the combustion characteristics, the ignition delay and lift-off length were longer than n-Do100 and increased as a function of alcohol and ABE quantity in the blends. The auto-ignition ability influenced on the stabilized flame position as lift-off length presented the same order with the ignition delay. The linear relationship between the lift-off length and ignition delay for all conditions was verified for all fuels even if their oxygen content was different. Finally, the blending ratio of ABE 20%v (ABE20) performed similar spray and combustion characteristics to n-dodedance, indicating the high possibility of using ABE as Diesel substitute fuel with minor modification.

Keywords: Acetone-Butanol-Ethanol blend, Alcohol blend, Spray Characteristics, Lift-Off Length, Ignition Delay, High-Pressure High-Temperature Conditions.

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NOMENCLATURES

Symbols

θ	Spreading spray angle [degree]
ϕ	Equivalence ratio [-]
ρ_a	Ambient gas density [kg.m ⁻³]
ρ_f	Fuel density [kg.m ⁻³]
ρ_b	Density of bead thermocouple [kg.m ⁻³]
ρ_w	Density of wire thermocouple [kg.m ⁻³]
τ	Time constant [ms]
ε	Refractive angle [degree]
ϵ	Emissivity of the bead thermocouple [-]
σ	Stefan-Boltzmann constant .6703x10 ⁻⁸ [W.m ⁻² .K ⁻⁴]
γ	Specific heat capacities ratio [-]
a	Constant value [-]
A	Pre-exponential constant [μ s]
A_c	Cross sectional area [m ²]
A_p	Projected area of spray [pi ²]
b	Arbitrary constant value [-]
B	Transfer number [-]
B_M	Mass transfer number [-]
B_T	Heat transfer number [-]
Ca	Area coefficient [-]
Cd	Discharge coefficient [-]
Cv	Velocity coefficient [-]
C_w	Specific heat density of the thermocouple [J.kg ⁻¹ .K ⁻¹]
d_b	Bead thermocouple diameter [μ s]
d_w	Wire thermocouple diameter [μ s]

D	Injector hole diameter [m]
D_0	Sack chamber diameter of nozzle (m)
E_a	Apparent activation energy [kJ.mol ⁻¹]
h	heat transfer coefficient [W.m ⁻² .K ⁻¹]
I	Light intensity of image [-]
I_0	Light intensity of background image [-]
k	Thermal conductivity of gas [W.m ⁻¹ .K ⁻¹]
k_d	Gladstone-Dale coefficient [-]
K	Bulk modulus [bar]
KL	Optical thickness [-]
l	Length of the orifice [m]
L	Part length [m]
$\dot{m}$	Mass flow rate [g.s ⁻¹]
$\dot{m}_{ms}$	Measured mass flow rate [g.s ⁻¹]
$\dot{m}_{th}$	Theoretical mass flow rate [g.s ⁻¹]
$\dot{M}$	Spray momentum [g.m.s ⁻²]
n	Reflective index [-]
n_0	Surrounding refractive index
Nu	Nusselt number [-]
P	Pressure [bar]
P_b	Back pressure [bar]
P_{inj}	Injection pressure [bar]
$\dot{q}$	Volumetric flow rate [m ³ .s ⁻¹]
r	Round radius of nozzle [m]
R	Gas constant, 8.314 J .K ⁻¹ . mol ⁻¹
R^2	Coefficient of determination or R-squared [-]
t	Time [s]
t_b	Break-up time of spray [ms]
T_a	Ambient gas temperature [K]
T_{cor}	Corrected ambient gas temperature [K]

T_f	Fuel temperature [K]
T_s	Saturation temperature [K]
T_{ms}	Measured ambient gas temperature [K]
T_w	Wall temperature [K]
U	Flow velocity [m.s ⁻¹]
U_{th}	Theoretical flow velocity [m.s ⁻¹]
v	Speed of sound of fluid [m.s ⁻¹]
v_F	Fuel stoichiometric coefficients [-]
v_O	Oxygen stoichiometric coefficients [-]
V	Volume [m ³]
V_{BDC}	Cylinder volume at BDC [m ³]
V_{TDC}	Cylinder volume at TDC [m ³]
W_F	Species molecular weights of fuel [mol.g ⁻¹]
W_O	Species molecular weights of oxidizer [mol.g ⁻¹]
$Y_{F,0}$	Fuel mass fraction [-]
$Y_{O,0}$	Oxidizer mass fraction [-]
Z_{st}	Stoichiometric mixture fraction [-]

Abbreviations

A/F	Air-fuel ratio [-]
ABE	Acetone-Butanol-Ethanol
ABEXX	XX% in volume of ABE, blended in n-dodecane
BDC	Bottom Dead Center
BuXX	XX% in volume of butanol, blended in n-dodecane
CI	Compression Ignition
CN	Cetane Number [-]
CFD	Computational Fluid Dynamics
CPF	Constant-Pressure Flow chamber
CR	Compression Ratio [-]

CVP	Constant-preburn chamber
D100	100% Diesel fuel
DBI	Diffused Back-Illumination
ECN	Engine Combustion Network
EthXX	XX% in volume of ethanol, blended in n-dodecane
FWHM	Full Width at Half Maximum [nm]
HTHP	High-Pressure and High-Temperature
ICE	Internal Combustion Engine
ID	Ignition Delay [μ s]
LL	Liquid Length [m]
LOL	Lift-Off Length [m]
L_v	Latent heat of vaporization [kJ.kg^{-1}]
MFR	Mass flow rate [g.s^{-1}]
n-Do100	100% n-Dodecane
NOSE	New One Shot Engine
PAH	Polycyclic Aromatic Hydrocarbons
PIV	Particle Image Velocimetry
PM	Particulate Matter
RCYM	Rapid CYcling Machine
S	Vapor spray penetration [m]
SI	Spark Ignition engine
SEM	Scanning Electron Microscope
SOI	Start Of Injection
SOC	Start Of Combustion
STD	Standard deviation
TDC	Top Dead Center

BACKGROUND AND MOTIVATION

1. Energy and Environment Background

Concerns about climate change and energy security influence on the future energy policies in term of technology, regulations and investment in the energy sector. An increasing of global energy consumption by around 30% from 1990 to 2015 was related to a rising of the global population 28%, caused to increase CO₂ in atmospheric concentration around 13% [1]. As a result, the Earth's average surface temperature rose with them around 0.61 °C. By prediction, it could rise to 2 to 6 °C at the end of the 21st century. Based on this concerns, the global agreement to combat climate change called "Paris Agreement" was adopted under the United Nations Framework Convention on Climate Change (UNFCCC), which aims to hold global warming to well below 2 °C. For this reason, several policies have been driven to complement in this commitment.

The transportation sector has been the major sector contributed CO₂ in the atmosphere since the last few decades, mainly by fossil fuel. Therefore, the vehicle manufacturers around the world have adopted policies requiring to improve the energy efficiency of new vehicles to reduce CO₂ and fuel consumption. For example, the EU has driven the policy to reduce CO₂ in a new passenger car in the commitment of 95 g/km in 2021 and decrease more in 2030 by 67 g/km, while the US and Canada provide on 99 g/km in 2025 [2]. Not only CO₂, other exhaust emissions, i.e., unburnt hydrocarbon (UHC), carbon monoxide (CO), oxides of nitrogen (NO_x) and particulate matter (PM) is also considered to put in the policy as presented in the stricter emission regulation standard, especially in PM and NO_x.

The biofuel is one powerful option to fulfill this commitment as it is renewable energy which can promote both CO₂ reduction and energy security. The International Renewable Energy Agency (IRENA) proposed the global roadmap "REmap" to drive the share of global renewable energy in the world's energy mix. Based on the projection, they observe that the renewable energy will be possible to increase the share in global energy from 18% in 2010 to

36% by 2030 and in transportation sector from 3% to 13% [3]. Also, the liquid biofuels, including both conventional and advanced forms of ethanol and biodiesel, could account for 10% of transport sector energy use by 2030, more than triple of the share in 2017.

However, even though there are several efforts to mitigate CO₂ emission and reduce energy consumption in the transportation sector. However, we need more technology to have high energy efficiency and new renewable energy to ensure that we will be the security of energy supply and efficient environmental protection in the future.

2. Technical Background

The spray characteristics of the diesel engine are the primary parameters that control the process of mixing formation, auto-ignition, combustion, subsequently emissions. Currently, the high development of injection technologies of modern diesel engine plays a significant role to improve engine performance, combustion and also mitigate exhaust emission without the penalty of engine performance. As a result, the better understanding on the complex phenomena of spray and combustion is necessary to improve in order to develop the next step of diesel engine technology and consider the new alternative fuel for CI engine.

Butanol is an exception renewable liquid biofuel for CI engine because of its superior properties compared to other alcohol fuels. It has higher energy content (up to 30%) induces a lower fuel consumption and also lower water solubility decreases the tendency to microbial-induced corrosion in fuel storage and pipelines during transportation [4], [5], [6]. Moreover, the higher Cetane Number of butanol (CN = 25) compared to ethanol (CN = 8) leads to an easier auto-ignition in the case of CI engines [4]. It is also more suitable for diesel injection systems thanks to its higher level of viscosity, more like diesel fuel and no water content. Moreover, due to its very good miscibility, it can be blended with diesel without any solvents addition. Last, by optimizing the rate of EGR, the butanol-diesel blends (up to 40%v) can significantly reduce the smoke and NO_x without the penalty on engine performance [7], [8], [9]. However, due to the low yield of production and high energy in separation process of butanol, related to the high production cost per unit, prohibits it to implement in the commercial scale as the fuel of transport vehicles.

An intermediate fermentation from butanol production, the Acetone-Butanol-Ethanol (ABE) mixture, is recently estimated as a new potential alternative fuel for CI engines, due to similar physical and chemical properties to those of butanol [10], [11]. By using *Clostridium* bacteria, *Clostridium beijerinckii* or *Clostridium acetobutylicum*, the fermentation of lignocellulosic hydrolysate sugars produces a mixture of ABE generally in a volume ratio of 3:6:1 [11], [12], [13]. ABE mixture needs to be distilled and dehydrated to extract pure butanol. Therefore, if ABE mixture can be used directly as fuel, the energy cost due to the separation would be eliminated and also it will be considered as a new alternative fuel for vehicles to promote the CO₂ reduction and energy security.

ABE-diesel blends up to 30%v can simultaneously reduce the soot precursors and PM. Also, by adding water (0.5%v in ABE-diesel blends 20%v), the brake thermal efficiency could be enhanced up to 8.65% and PM, NO_x, PAHs reduced up to 61.6%, 16.4% and 31.1%, respectively [11]. Moreover, the ABE-water mixture was blended with biodiesel-diesel to control NO_x and PM emissions. The results presented that the use of water containing-ABE-biodiesel-diesel blends could simultaneously reduce both PM and NO_x up to 30.7% and 63.1%, respectively [14].

Wu et al. [12] investigated the effect of butanol-diesel and ABE-diesel blends on LL in a Constant Volume Preburnt. They found that the spray feature of the pure ABE (3:6:1) and butanol are narrower and shorter than pure diesel one due to higher volatility values, especially at the lowest ambient temperature. In another study [13], various volume fractions of ABE(3:6:1) in diesel blends, (20, 50 and 80%v), were investigated on the spray and combustion characteristics. The results showed that LL decreases as a function of ABE proportion, but ABE20 and D100 have similar spray characteristics while ABE50 and ABE80 are shorter and narrower ones.

The combustion of ABE mixtures (3:6:1 and 6:3:1) blended with diesel was also compared with pure diesel [12], [13], [16]. They found that the liquid and flame lift-off lengths are shorter and longer than D100 as a function of the ABE proportion. The longer ID and longer “gap” between liquid length and flame lift-off length of ABE mixture provide more time and space to favor droplets vaporization and mixing with ambient gas, also due to better volatility. As the results, ABE-diesel blends not only promote soot oxidation due to the oxygen content but also

lower soot formation itself. In the last, they concluded that ABE20 (3:6:1) displayed similar spray characteristics to diesel, while ABE50(3:6:1) performed the combustion characteristics close to diesel, the ABE ratio between 20%v and 50%v would be a good potential to use in CI engine with minor modification as it could be maintained combustion characteristic similar to conventional diesel fuel.

3. Research Objective

Although several studies have investigated in ABE and butanol diesel blends as their potential of to reduce soot and NO_x simultaneously, there is not yet a complete comparative study of these fuels on spray and combustion behaviors to understand better the effect of fuel properties. Also, this is no research fully comparison of the currently interested alcohol-diesel blend fuels on the spray and combustion characteristics, such as an ethanol-diesel blend of 20%v and butanol-ethanol-diesel blends (20%v of butanol, 20%v of ethanol and 60%v of diesel). As these fuels also have a high potential for CI engine as presented the low soot and NO_x emission due to high oxygen content in the molecule.

Moreover, there is ambiguous on the suitable blending ratio of ABE, as Wu et al. suggested that the suitable ratio of ABE in ABE-diesel blend for CI engine is between 20% and 50%, which need more research to identify. In the last, even though the spray and combustion parameter has been characterized as presented in some literature reviews, the optical techniques to measure as well as a criterion of post-processing to characterize these parameters were not suitable as seen by the low quality of raw images. Therefore, the standard condition, technical measurement and post-processing are required in order to obtain the accurate result for considering new alternative fuel and improving simulation model.

Therefore, the effect of fuel properties on the spray and combustion process of ABE mixture and alcohol fuels, blended with the diesel surrogate fuel, n-dodecane, in different volume ratio will be investigated. The objectives of this study are:

- To design and develop a high-pressure and high-temperature combustion chamber in order to simulate the thermodynamic condition similar to the diesel engine.

- To characterize and validate the ambient condition to reach a standard ambient condition of the Engine Combustion Network (ECN) called “Spray-A”.
- To characterize and validate the spray and combustion parameters with the ECN database, available on the ECN website by using the standard optical technique measurements and post-processing recommended by ECN.
- To characterize the spray and combustion parameters of ABE-dodecane blends and alcohol-dodecane blends by the standard condition, optical technique measurement and post-processing recommended by the ECN to investigate the effect of fuel properties.
- To characterize the ABE-dodecane blends in different ABE ratio between 20%v to 50% by volume to reveal the suitable ratio of CI engine.

4. Thesis Outline

This manuscript consists of 6 chapters. In this chapter, general information about energy and environment concerning is given, to introduce the interest of using ABE mixture as an alternative fuel for CI engine. In **Chapter 1**, the background of the spray and combustion parameters is introduced to emphasize on how these parameters are important. Moreover, the review of using alcohol-diesel and ABE-diesel blends in the diesel engine is presented to reveal the lack of research and how we can fulfill. **Chapter 2** describes the details of design and development of the high-pressure and high-temperature chamber as well as the details of the combustion chamber characterizations to achieve the standard Spray-A ambient condition of ECN. For **Chapter 3**, the results of spray and combustion parameters measured by standard condition, optical technique and post-processing are presented. A discussion based on the comparison with the ECN database proves the quality of the NOSE set-up.

In **Chapter 4**, the spray and combustion parameters of alcohol-dodecane blends and ABE-dodecane blend (20%v) are characterized to analyze the effect of fuel properties, especially viscosity, density and oxygen content. Meanwhile, in **Chapter 5**, the effect of the volume ratio of ABE (from 20%v to 50%v) in ABE-dodecane blends is investigated in order to

reveal the suitable ratio of ABE for CI engine. In the last chapter, the conclusion of this study is summarized and presents the future research perspective.

CHAPTER 1

LITERATURE REVIEW

1.1 Energy Consumption and CO₂ Distribution Outlook

Over the last two decades, an increase of the global population by 28% has boosted the global energy consumption around 30%, remaining increase by prediction approximately 2% per year till 2040 [1]. As a results, the greenhouse gases (GHG), i.e. carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O) have significantly increased concertation in the atmosphere, mainly from fossil fuel emissions. In 2011, the concentration of these GHG was higher than the pre-industrial period (during 1750 to 1850) around 40%, 150% and 20% for CO₂, CH₄, and N₂O, respectively [17]. Consequently, the Earth's average surface temperature increases with these GHG concentrations, warming by 0.61 °C from 1850-1900 to 1985-2005, as seen in **Figure 1**. Some predictions announce the average surface temperature could rise between 2 °C and 6 °C by the end of the 21st century. Concerning on this point of view, a new global agreement to combat climate change called “Paris Agreement” was adopted under the United Nations Framework Convention on Climate Change (UNFCCC) in December 2015. The Paris climate agreement aims at holding global warming to well below 2 °C and to “pursue efforts” to limit it to 2 °C. In preparation of this agreement, countries submitted national plans that spell out their intentions for addressing the climate change challenge after 2020 [18], [19].

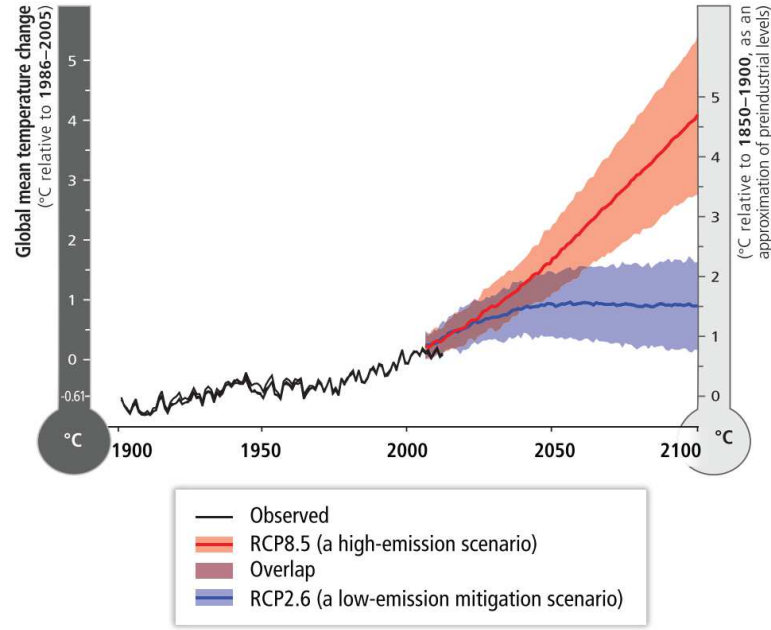


Figure 1 Observed and projected future global annual average temperature relative to 1886–2005 [20].

The transportation sector is the second largest sector of energy consumer with around 30% of total energy since 2010 and a predicted increase by 1.4% per year until 2040, mainly due to the use of gasoline and diesel [1], [21] (see **Figure 2** (a)). This relates to CO₂ contribution, released CO₂ in atmosphere around 20% of total amount since the last two decades as seen in **Figure 2** (b). By forecasting in 2030, transport emissions will be expected to increase by roughly two-thirds to 15 billion metric tons of CO₂ (GtCO₂) related to 8.8 GtCO₂ in 2010 [2]. Based on this assessment, nine countries (USA, Canada, China, EU, Japan, Brazil, India, South Korea and Mexico) have adopted policies requiring vehicle manufacturers to improve the energy efficiency of new Light-Duty Vehicles (LDV) by almost 1.5 GtCO₂ in 2030. Only four of them (Japan, US, Canada and China) have adopted the reduction also for Heavy-Duty Vehicle (HDV) by 0.26 GtCO₂ in 2030. The policies of these governments take different approaches to design their regulations. **Figure 3** presents the comparative policy of reducing CO₂ emission and fuel consumption of the passenger cars for different countries, normalized to NEDC (New European Driving Cycle) testing standard. The EU has the policy to reach 95 gCO₂/km in 2021 and 67 gCO₂/km in 2030, while the US and Canada fixed their objective to 99 gCO₂/km in 2025.

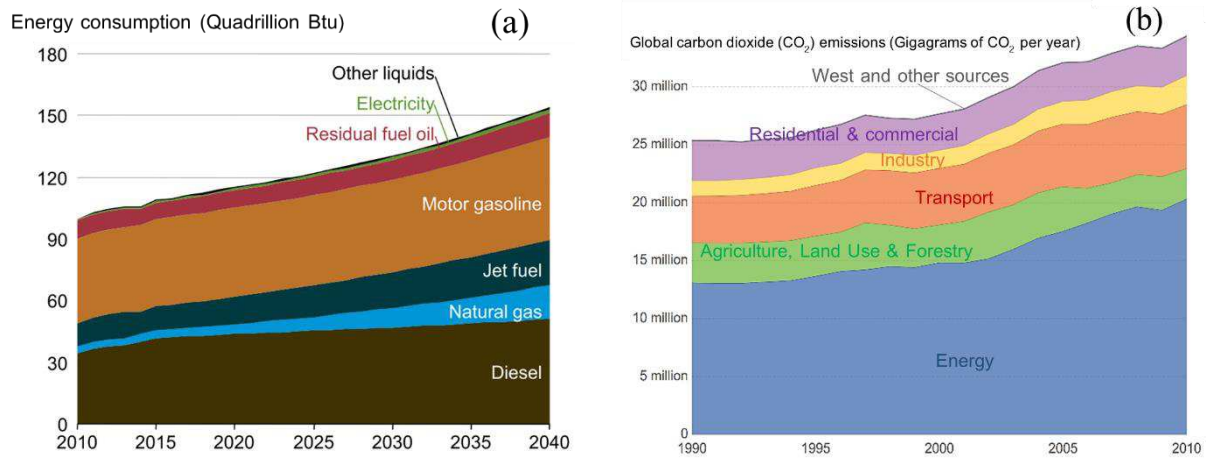


Figure 2 Energy and CO₂ in transportation: (a) world transportation sector delivered energy consumption by energy source, 2010 to 2040 [21], (b) global CO₂ emission by sector [22].

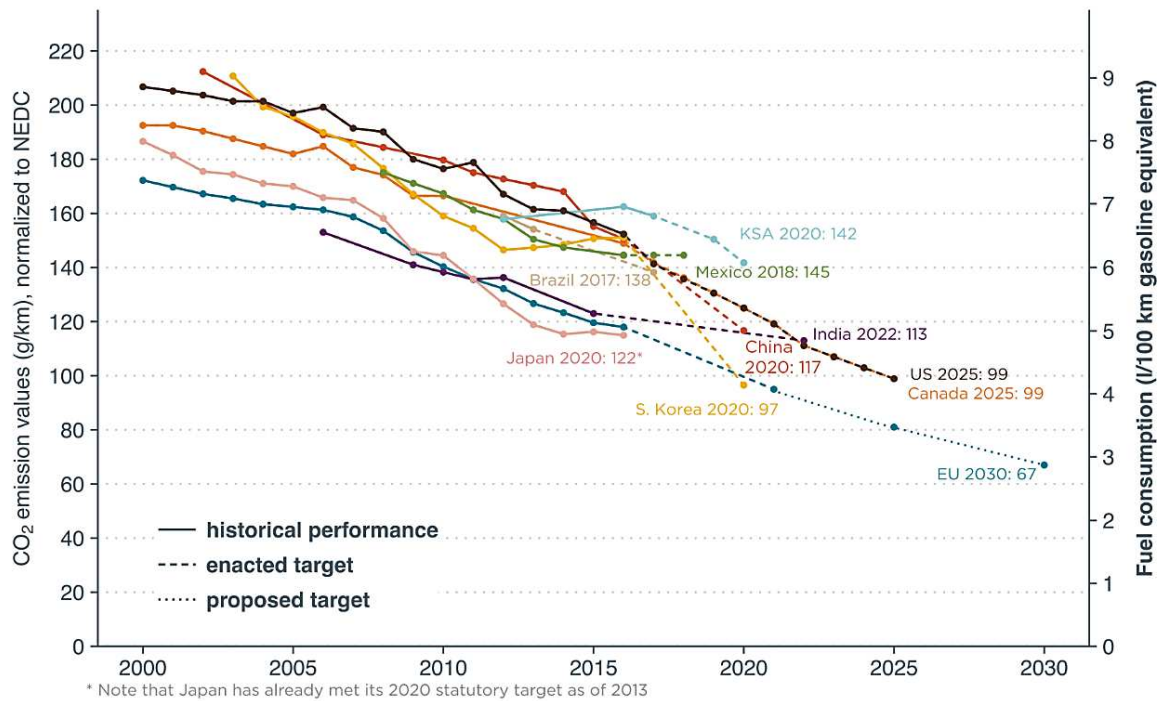


Figure 3 CO₂ emissions and fuel consumption for passenger cars [23].

There is not only the effort to mitigate CO₂ emission and reduce energy consumption, but other exhaust emissions as unburnt hydrocarbon (UHC), carbon monoxide (CO), oxides of nitrogen (NO_x) and particulate matter (PM) have also been considered in the government policies. The EU and USA have developed the emission regulation for vehicle emissions and fuel quality to provide a pathway that other countries can follow to improve the environmental performance of their vehicle fleets [2]. For example, the regulations for light-duty vehicles in the EU progress from Euro I to Euro VI and in the USA EPA Tier 1 to Tier 3, which set more strict for PM and NO_x, as shown an example in **Figure 4**.

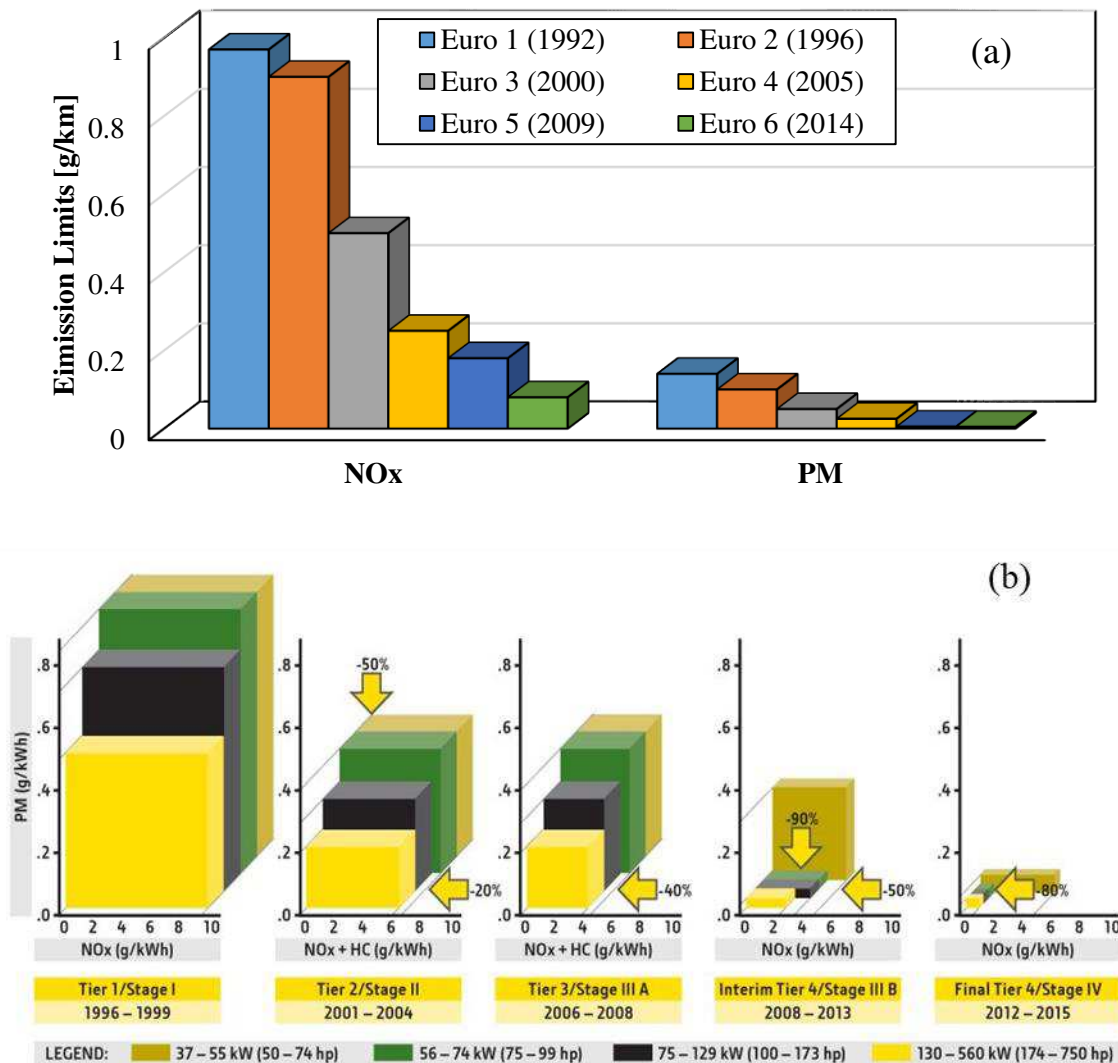


Figure 4 Emission standards: (a) European emission standard for diesel passenger cars (sourced by <https://www.dieselnr.com/>), (b) United States Environmental Protection Agency (EPA) nonroad emission regulation: 37-560 kW (sourced by <https://www.deere.com/>).

Another powerful option to reduce pollutant and CO₂ emissions is the use of alternative biofuels. According to the global roadmap, called “REmap report”, of the International Renewable Energy Agency (IRENA) projects, the share of global renewable energy will be possible to increase in the world’s energy mix from 18% in 2010 to 36% by 2030 and from 3% to 13% in transportation sector [24] (see **Figure 5** (a)). The passenger transport would have the share in 18% in 2030, which is the largest share of all transport sections, as shown in **Figure 5** (b). The liquid biofuels, including both conventional and advanced forms of ethanol and biodiesel, could account for 10% of energy use in the transport sector by 2030, more than the triple of the share in 2017.

From this point of view, even though there are several efforts to mitigate CO₂ emission and reduce energy consumption in the transportation sector, more technologies are needed to increase energy efficiency to ensure the security of energy supply and efficient environmental protection in the future. The biofuel is one of the high potential solutions to solve both of the climate change and energy security.

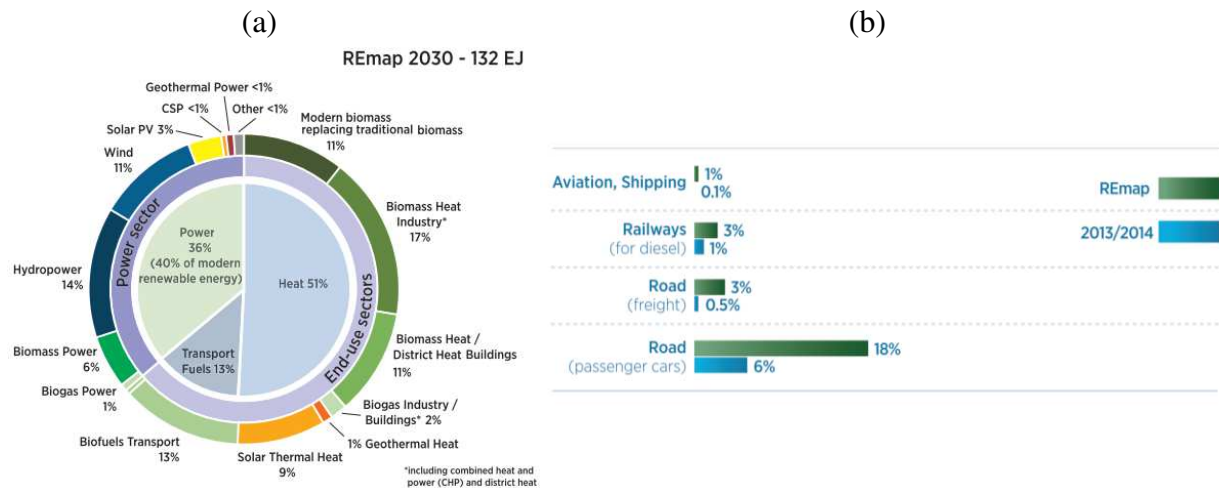


Figure 5 REmap global roadmap for 2030: (a) breakdown of global renewable energy use in 2010 and REmap 2030, by technology and sector [24], (b) renewable energy share by transport mode in 2013/2014 and 2030 according to REmap [25].

1.2 Compression Ignition (CI) Engine

Diesel or Compression Ignition (CI) engines are widely used as power unit of vehicles such as passenger car, truck, bus as well as the ship. One of the most significant advantages of a diesel engine compared to Spark Ignition (SI) engines is that CI engines are significantly more efficient in term of fuel consumption and thermal efficiency due to its higher compression ratio and no effect on pumping losses. Moreover, they are higher reliability and durability of usability lead to the most of heavy-duty engines for trucks, buses and ships are Diesel. However, there are some drawbacks: due to its operating on diffusion-controlled combustion, NO_x and Soot emissions reduction are challenging and requiring an expensive special catalytic converter.

The CI engine is based on the auto-ignition of fuel due to the thermodynamic conditions generated by the high compression ratio. As there is no ignition device, the ability of auto-ignition is depended on the auto-ignition characteristic, mainly indicated by the Cetane Number (CN) of fuel. In the last few decades, diesel engines were strongly improved to respect more and more stringent emissions regulations, especially for NO_x and Soot [4], [26]. On the other hand, it was improved the combustion efficiency to reduce the fuel consumption, leading to reduce the CO₂ emission as well. As seen in **Figure 6**, the injection and spray characteristics are the primary parameters that control the process of mixing formation, auto-ignition, combustion and subsequently emissions. Therefore, numerous engineers have developed and improved in the injection system such as designing an injection system, developing an injection strategy, etc. The increase of injection pressure in modern diesel engines due to the development of the common-rail significantly improves the spray and atomization processes, inducing the increase of the engine performance and the emissions reduction. The injection strategies (as multiple injections) play a significant role to mitigate exhaust emissions without the penalty of engine performance [27], [28]. However, the recent development of injection technologies contributes to accentuate the complex phenomena, which govern spray and combustion processes. It is then still necessary to perform studies to develop as accurate as possible the models to improve the compression ignition engine technology. This conclusion was made 10 years ago by the Sandia National Laboratories, Institut Francais du Petrole energies nouvelles (IFPen) and Centro di Motores Termicos (CMT) led to the Engine Combustion Network (ECN, <https://ecn.sandia.gov/>). ECN is an international collaboration dedicated to sharing the highly

accurate experimental data of spray and combustion for gasoline and diesel engines in order to improve the Computational Fluid Dynamics (CFD) model.

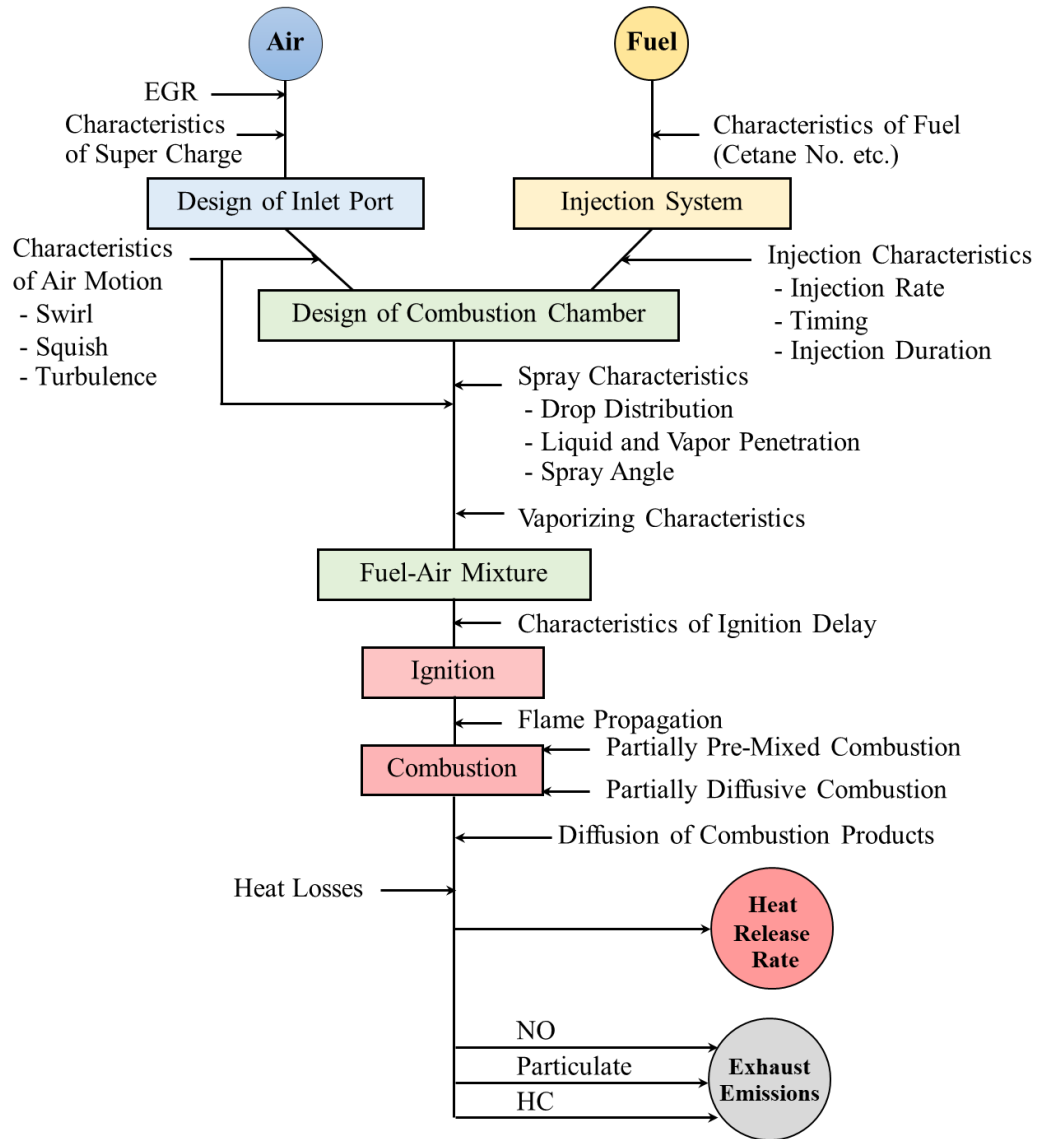


Figure 6 Block diagram of diesel combustion (modified from Hiroyasu and Arai [29]).

1.3 Diesel Spray and Combustion Characteristics

Over the last two decades, the diesel spray characteristics have been intensively studied at High-Pressure and High-Temperature conditions, representing the conditions reachable inside the combustion chamber of a diesel engine. Thanks to optical technique measurements, all complex phenomena between flow mechanics and kinetics are better described for a better understanding [30], [31]. As a result, few conceptual models of diesel spray and its combustion were proposed [32], [33], [34] as briefly described below. First, the highly pressurized fuel is injected into the combustion chamber where the ambient air is dense due to high-pressure and high-temperature conditions. This generates resistance and produces shear of the liquid fuel. Then, the fuel starts to be broken up and groups of droplets are formed around the spray jet. Due to the entrainment by the hot air, they are vaporized, as it can be seen in **Figure 7**. At the same time, the liquid fuel spray continues to penetrate to downstream until the total fuel evaporation rate inside the spray equals the fuel injection rate [35]. Only the vaporized fuel is penetrated beyond to downstream and mixed with air, forming a rich mixture, i.e., a local equivalence ratio (ϕ) ~ 2 to 4.

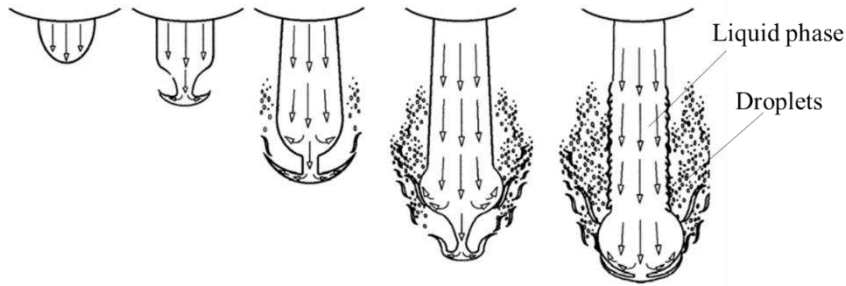


Figure 7 Scheme of an initial break-up model of liquid fuel [33].

The hot gases continue to entrain the mixture until the auto-ignition process starts and the rich mixture burns as premixed combustion (as represented by a light blue color in **Figure 8**). Shortly after the ignition, the OH production grows to form a diffusion flame on the periphery of the jet, as presented in the orange layer. The distance between the injector tip and the location of the stabilized diffusion flame is defined as the lift-off length. The soot formation begins to be

formed downstream of the premixed flame, representing in gray, due to the transport of the product gases of incomplete initial phase combustion, consisting in soot precursors i.e. polycyclic aromatic hydrocarbons (PAHs). Then the soot particles are transported until the diffusion flame at the periphery of the jet where they can be oxidized by oxygen in hot ambient gases as presented in **Figure 8** (soot oxidation zone). At the periphery jet, the mixture is near the stoichiometry, the high temperature of combustion induces NO_x production in the oxidizer side of the diffusion flame (green region).

Even though some conceptual processes of the spray and combustion phenomena were developed from observation with optical techniques, quantitative and accurate experimental results are still needed to improve the models to simulate and predict spray and combustion processes in the case of engine designs. Moreover, as the effect of fuels characteristic parameters is not well considered in these models, the behavior in the case of new alternative fuel has to be studied.

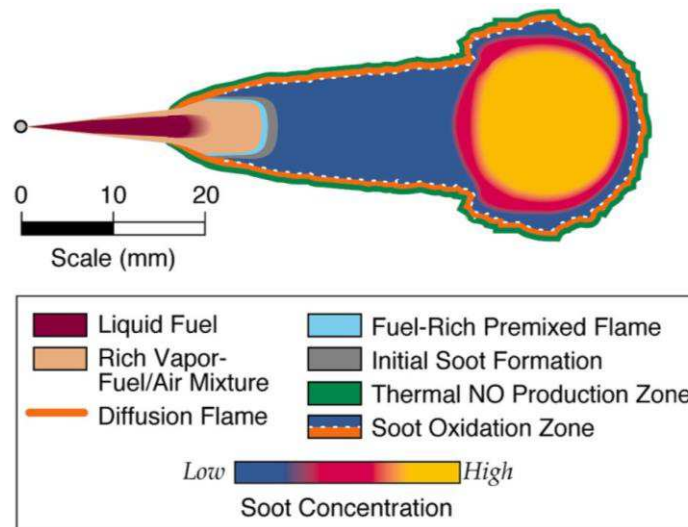


Figure 8 Dec's conceptual model for conventional diesel combustion during the quasi-steady period [32], [36].

1.3.1 Mass flow rate of fuel

The fuel Mass Flow Rate (MFR) is the first parameter which influences on the spray characteristics, the air-fuel mixture formation, the combustion efficiency as well as the exhaust emissions [37], [38], [39]. By modifying the injection rate shape, the fuel consumption and gas

emissions were significantly reduced, due to its effects on the atomization and the fuel-air mixing, [40] [41], [42]. Moreover, some studies indicated the initial rise of MFR profile has a significant effect on the exhaust gas emissions (NO_x and Soot) and noise emission [38], [43]. Tanabe et al. [40] suggested a new conceptual injection model, called “Next-generation Common Rail System” (NCRS), in order to switch the fuel pressure supplied to the injector from the low to high rail pressure during the injection period, resulting in control the injection rate shape. The difference between conventional Common Rail System (CRS) and NCRS is highlighted in **Figure 9** (a) when the injection rates are plotted. By varying a wide range of the low injection pressure common rail (LPCR) from 22 to 40 MPa and the high pressure common rail (HPCR) from 80 to 120 MPa, the results showed that it was possible to control combustion by controlling the injection rate by using the NCRS and to improve the NO_x-fuel consumption and NO_x-PM trade-offs. Some experimental results of the engine performance and emissions are presented in **Figure 9** (b). In comparison with the conventional CRS at the LPCR pressure 40 MPa and HPCR pressure 80 MPa, NO_x was reduced by 22% for the same fuel consumption. While by adjusting the fuel consumption to provide constant NO_x, the fuel consumption was reduced by 2.6%, at lower PM levels. Moreover, Desantes et al. [37] modified a pump-line-nozzle system, which is able to modulate the instantaneous fuel injection rate, “boot-type injection,” in order to study the effects of injection rate shaping on the combustion process and exhaust emissions of a single cylinder, direct-injection diesel engine. They observed that by changing the initial injection rate shape, a significant reduction in NO_x emissions is reached, which is greater as the boot length is increased or the boot pressure is reduced.

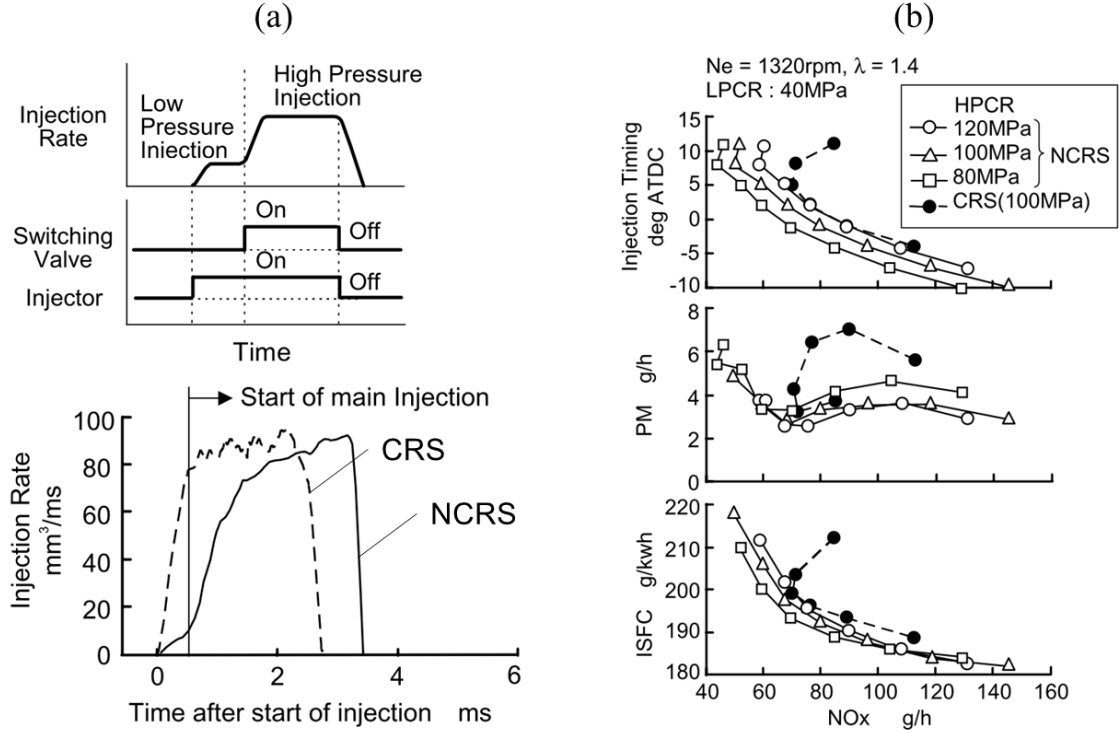


Figure 9 The effect of injection rate on the engine performance and emissions studied by Tanabe et al. [40]: (a) schematic injection rate of NCRS (top) and real injection rate of NCRS compared to conventional CRS (bottom) and (b) engine performance and emission results for different injection pressures at engine speed 1320 rpm and $\lambda = 1.4$.

The theoretical mass flow rate ($\dot{m}_{th}$) can be derived by the continuity and Bernoulli's equations as in **Eq. 1** to **Eq. 3**, with A_c the outlet cross-section area of injector hole, ρ_f the fuel density, U_{th} the theoretical injection velocity at the outlet injector hole, and P_b the back-pressures. The discharge coefficient, Cd is the ratio between the mean measured MFR ($\dot{m}_{ms}$) and theoretical MFR as presented in **Eq. 4**.

$$\dot{m}_{th} = \rho_f \cdot A_c \cdot U_{th} \quad \text{Eq. 1}$$

$$U_{th} = \sqrt{\frac{2 \cdot \Delta P}{\rho_f}} \quad \text{Eq. 2}$$

$$\dot{m}_{th} = A_c \cdot \sqrt{(P_j - P_b) \cdot \rho_f} \quad \text{Eq. 3}$$

$$Cd = \frac{\dot{m}_{ms}}{\dot{m}_{th}} \quad \text{Eq. 4}$$

1.3.2 Liquid length penetration

The liquid length (LL) is one important parameter considered to design the engine as directly effects on the formation of emissions. LL needs to be optimized to avoid impingements and liquid fuel deposits on the piston bowl or cylinder wall, which causes stronger HC and particle emissions [35]. Also, the knowledge of this parameter provides information on the mixing field near the injector tip, which governs the mixing and vaporizing processes inside the combustion chamber. Based on the experimental results, Dec [32] also presented the conceptual model of the LL evolution as seen in **Figure 10**. First, the liquid fuel is injected into the chamber and covers the cross-section (1.0° after the start of injection (SOI)). Then a vapor-fuel region begins to develop along the sides of the jet beyond the extent of the liquid droplets (2.0° after SOI). The vapor region at the sides grows thicker as the jet continues to penetrate because the width of the liquid region increases more slowly than does the width of the overall jet. At 3.0° after SOI the liquid reaches its maximum penetration length around 23 mm, where the total fuel evaporation rate in the spray equals the fuel injection rate [35]. When this condition occurs, the tip of the liquid region stops penetrating and begins fluctuating about a mean axial location. After that, the energy to vaporize the fuel comes mainly from the hot air entrained into the spray, but does not energy released by combustion. At 4.5° after SOI, the vapor jet is continuously penetrated to about 34 mm, and the leading portion contains a relatively uniform fuel-air mixture. The full evolution of liquid phase fuel is presented by Siebers et al.'s experimental results [35], [44], as seen in **Figure 10** (b).

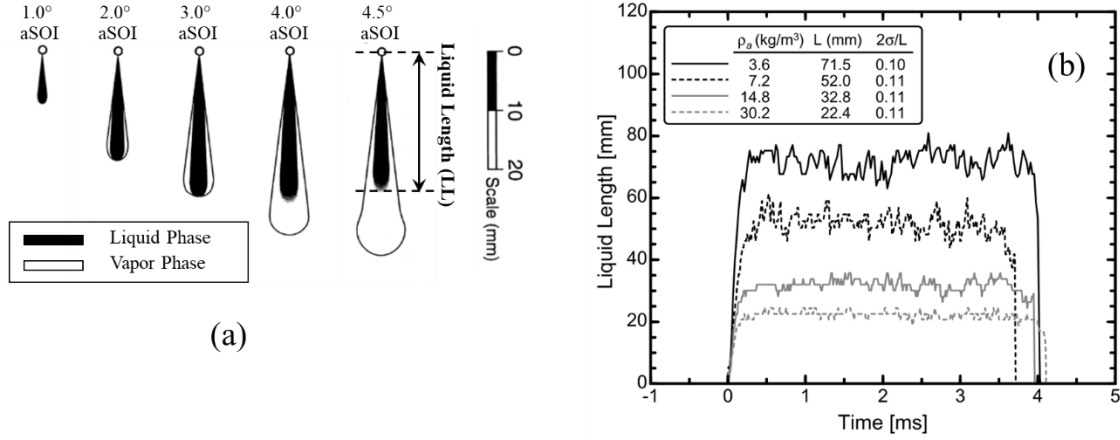


Figure 10 Liquid phase evolution: (a) temporal sequence of a schematic model of the liquid phase fuel proposed by Dec [32] and (b) the maximum axial penetration of LL on the spray axis as a function of time for four ambient gas densities obtained by Mie-scattering [35].

Generally, LL is defined as the maximum distance of the liquid-phase from the injector tip to liquid phase fuel penetration [34], [35], [45], [46], as seen in **Figure 10** (b). LL is influenced by many parameters such as the ambient condition, injector configuration, injection condition and fuel properties. By using the Mie-scattering technique, Siebers [35] characterized the liquid phase of fuel as a function of ambient and injection conditions, as well as fuel properties. As seen in **Figure 11**, LL shorten when the orifice diameter decreases but increases with the decreasing of ambient density and temperature. The fuel temperature has the opposite effect as LL shorten by increasing fuel temperature, whereas no significant effect of the injection pressure was founded in the range of 40 to 160 MPa (see **Figure 11** (b)). Fuel volatility also plays an important role in LL while the viscosity is less important. The effect of different parameters on LL is summarized in **Table 1**.

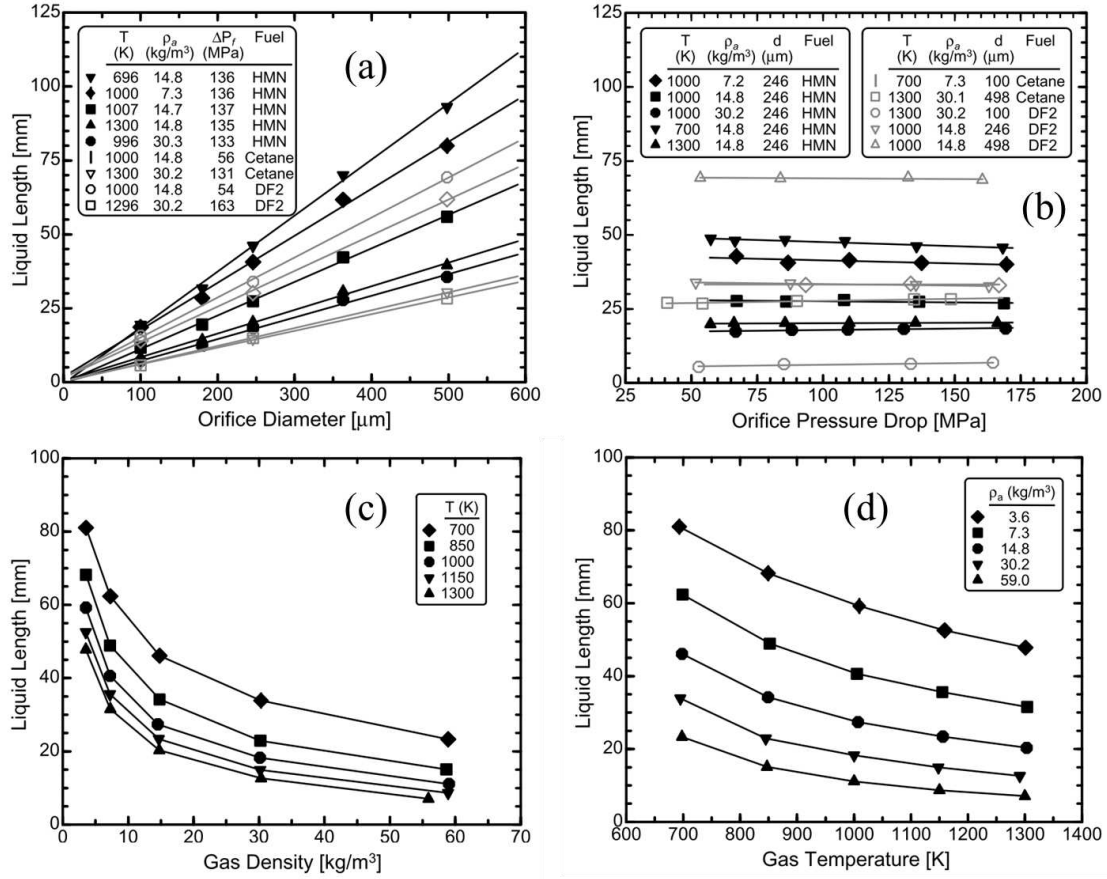


Figure 11 Liquid length evolution as a function of, (a) orifice diameter, (b) orifice pressure, (c) ambient gas density and (d) ambient gas temperature [35].

Table 1 Summary of main parameters on macroscopic spray characteristics.

Parameters	Liquid Length (LL)	Spray Angle (θ) (at steady state)	Vapor Spray Penetration (S)
↑ Ambient density	↓ ([35], [44], [47], [48])	↑ ([49], [33], [50])	↓ ([33], [49], [50])
↑ Ambient temperature	↓ ([35], [44], [47], [48])	↓ Slightly ([47])	NE : [47], [51] (same density)
↑ Injection pressure	NE ([35], [48])	↑ ([50])	↑ ([50], [51])
↑ Injection temperature	↓ ([52])	-	-
↑ Injector hole diameter	↑ ([35], [47], [48])	NE ([49]) ↑ ([33])	↑ ([33], [49], [47])
↑ Fuel density	↑ ([53])	NE ([53]) ↑ Slightly ([50])	NE ([53]) ↑ Slightly ([50])

Parameters	Liquid Length (LL)	Spray Angle (θ) (at steady state)	Vapor Spray Penetration (S)
↑ Fuel viscosity	-	NE ([53])	NE ([53]) ↑ Slightly ([50])
↑ Fuel volatility (↓ Boiling point) (↑ Vapor pressure)	↓ ([35], [44], [53])	-	NE ([53])

Note: ↑ = Increase; ↓ = Decrease; NE = No effect

Based on experimental results, different models have been developed to predict LL as a function of conditions. Hiroyasu and Arai [29] proposed the empirical correlation for a complete spray region for the high injection velocity (more than 100 m/s related to diesel injection), as presented in **Eq. 5**. This correlation takes into account the ambient and injection conditions and the injector geometry, such as injector hole diameter (D), round radius (r), nozzle length (l) and injection velocity (U) and the ambient air and fuel densities (noted ρ_a and ρ_f).

$$LL = 7D \cdot \left(1 + 0.4 \frac{r}{D}\right) \cdot \left(\frac{\rho_a}{\rho_f \cdot U}\right)^{0.05} \cdot \left(\frac{l}{D}\right)^{0.13} \cdot \left(\frac{\rho_f}{\rho_a}\right)^{0.5} \quad \text{Eq. 5}$$

Later, Naber and Siebers ([34], [35], [44]) proposed a scaling law correlation developed from a theoretical diesel spray model by using mass, momentum and energy conservation equations. The physical spray is assumed to be a quasi-steady flow with a uniform growth rate, with a constant spreading spray angle (α). The spray boundary is simplified, as the mixing, the velocity, the fuel concentration and the temperature profile are considered perfect inside the boundary. The fuel vapor phase is in thermodynamic equilibrium with the entrained ambient gases, therefore the fuel in liquid phase, vapor phase and ambient gases are also assumed to be at the same temperature. The gas absorption in the liquid phase and the recovery of kinetic energy in fuel vaporization region of the spray are also neglected. Also, no process of atomization is considered. Therefore, the liquid length is given by a dimensional scaling law as in **Eq. 6**. More details are given in [34].

$$LL = \frac{b}{a} \cdot \sqrt{\frac{\rho_f}{\rho_a}} \cdot \frac{\sqrt{Ca} \cdot D}{\tan\left(\frac{\theta}{2}\right)} \cdot \sqrt{\left(\frac{2}{B(T_a, P_a, T_f)} + 1\right)^2 - 1} \quad \text{Eq. 6}$$

where a is a constant coefficient between the tangent real spray angle (α) and the measured spray angle (θ), $\tan(\alpha) = a \cdot \tan(\theta)$. b is an arbitrary constant to adjust the predicted value due to different simplifying assumptions, determined by the best fit from the experimental data. The density ratio, ρ_f/ρ_a , represents the effect of mass and momentum transport on LL. The specificity of the injector is included in the orifice area-contraction coefficient (Ca) and the orifice diameter (D). In the main square-root, the transfer number (B) takes into account the effect of parameters involved in the energy transport on LL, which is a function of the ambient gas temperature (T_a) and pressure (P_a) and fuel temperature (T_f).

1.3.3 Vapor spray penetration

The vapor spray penetration, S , is an ‘indirect’ parameter to qualify the fuel-air mixing process, necessary for engine design. Indeed, it has to be optimized to avoid the adverse effects of impingement on the combustion chamber wall and piston head, one source of unburned hydrocarbons (UHC) and soot formation [54], [55], [56]. Generally, the vapor spray penetration is defined as the furthest spray distance along the spray axis from the injector tip to the boundary of the spray [49]. As investigated by numerous studies (S) is strongly affected by the spray momentum of injected fuel [29], ambient conditions [49], injector geometrical characteristics [57] and fuel properties [58]. Spray momentum (M) defined as the mass flow rate and injection pressure of fuel injection is generally represented as the force, or energy, of the spray delivered at the outlet injector hole and conserved along penetration, as seen in **Eq. 7** and **Eq. 8**.

$$\dot{M} \propto \dot{m} \cdot U_f \quad \text{Eq. 7}$$

$$U_f \propto \sqrt{P_j} \quad \text{Eq. 8}$$

Once fuel injected into the chamber, the ambient gas density will become one of the most dominating parameters as the resistance to the spray penetration. As the gas density can be reduced by increasing the ambient temperature, a longer spray penetration can be expected. The injector geometry has an effect on the cavitation and turbulence of flow inside the nozzle orifice, leading to qualitatively change of the spray characteristics [57], [59], [60] while fuel properties like the fuel viscosity and density have a slight effect on the spray penetration as presented by Dernotte et al. [50]. As seen in **Figure 12** (a), an increase of fuel viscosity from 2.3 to 7.1 mm²/s induces an increase of the spray tip penetration of 5 to 7%. The increase in fuel density by 100 kg/m³ (from 749 to 869 kg/m³) induces an increase in the spray tip penetration of 5 to 6% for injection pressures lower than 90 MPa and a low gas density (11.8 kg/m³), correlated with a slight decrease in the spray angle (see **Figure 12** (b)). From the discussion of Kook and Pickett [53], there is no significant impact of the modification of the flow characteristics induced by a change in fuel density on the spray penetration if the spray angle is unaffected. However, the fuel density is still presented in several empirical correlations or/and models to estimate the vapor spray penetration and spray angle because of providing to obtain a non-dimensional air-fuel density ratio term, ρ_a/ρ_f [29], [49], [50]. The summary of the impact of different parameters influencing the vapor spray penetration is also presented in **Table 1**.

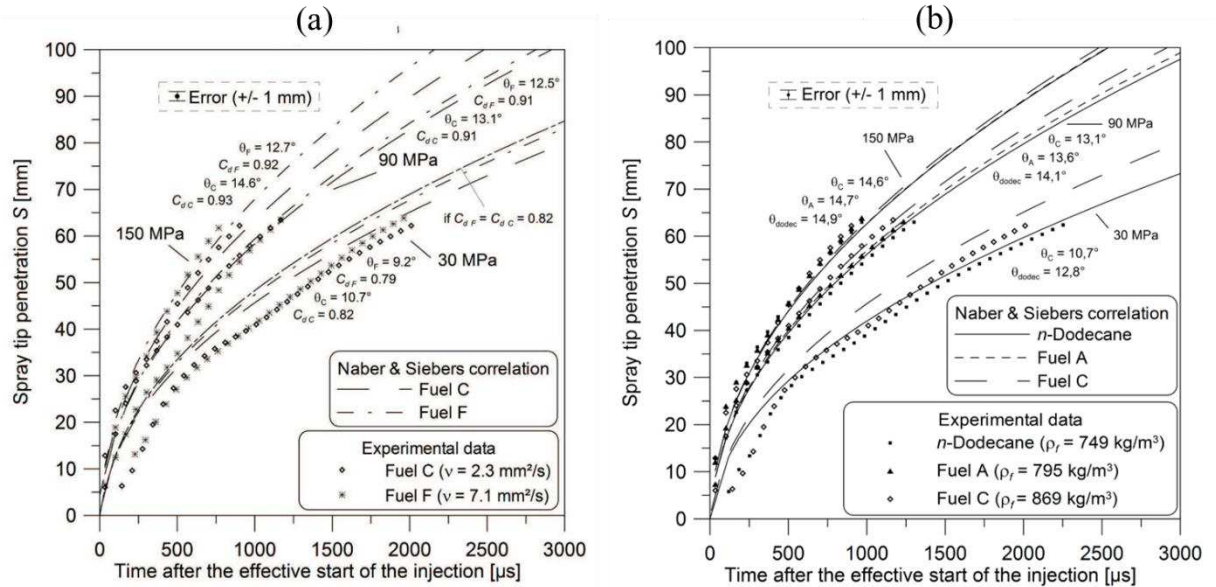


Figure 12 Effect of fuel density (a) and viscosity (b) on vapor spray penetration for three-injection pressures at 11.8 kg/m³ of ambient density [50].

Based on the experimental results, there are several correlations and models to estimate the vapor spray penetration. Hiroyasu and Arai [29] proposed the two expressions to estimate S in function of time, t , depending on the break-up time, t_b , as presented in **Eq. 9** to **Eq. 11**.

For a short time limit:
 $0 < t < t_b$;

$$S = 0.39 \sqrt{\frac{2(P_f - P_a)}{\rho_f}} \cdot t \quad \text{Eq. 9}$$

For a long time limit:
 $t > t_b$;

$$S = 2.95 \sqrt{\sqrt{\frac{(P_f - P_a)}{\rho_a}} \cdot \sqrt{D \cdot t}} \quad \text{Eq. 10}$$

where

$$t_b = 28.65 \frac{\rho_f \cdot D}{\sqrt{\rho_a(P_f - P_a)}} \quad \text{Eq. 11}$$

Lately, a well- known scaling law correlation was introduced by Naber and Siebers [49], based on the steady non-dimensional mass and momentum conservation equations for a conical control volume as seen in **Figure 13**. This model takes into account the effect of the ambient conditions (pressure and density), fuel density, spray dispersion, injection pressure as well as the injector tip configuration of the flow like a velocity coefficients (C_v) and area coefficients (C_a). In order to compare with other correlations such that from Hiroyasu and Arai, they rewrote their model, as presented in **Eq. 12** to **Eq. 14**.

For a short time limit:
 $t < t_b$;

$$S = C_v \sqrt{\frac{2(P_f - P_a)}{\rho_f}} \cdot t \quad \text{Eq. 12}$$

For a long time limit:
 $t > t_b$;

$$S = \sqrt{\frac{C_v \cdot \sqrt{2 \cdot C_a}}{a \cdot \tan(\theta/2)}} \cdot \sqrt{\sqrt{\frac{(P_f - P_a)}{\rho_a}} \cdot \sqrt{D \cdot t}} \quad \text{Eq. 13}$$

where the breakup time is

$$t_b = \frac{\sqrt{2C_a}}{C_v \cdot a \cdot \tan^2(\theta/2)} \cdot \frac{\rho_f \cdot D}{\sqrt{\rho_a(P_f - P_a)}} \quad \text{Eq. 14}$$

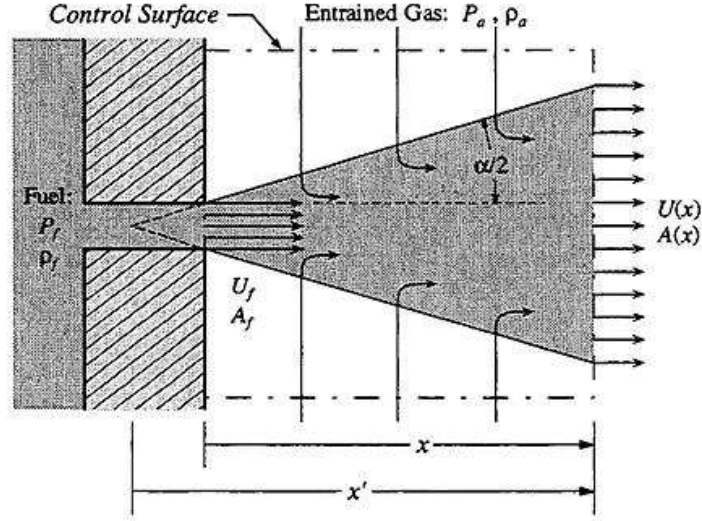


Figure 13 Scheme of the Naber and Siebers spray model for the spray penetration [49].

The main differences between **Eq. 9** and **Eq. 12**, and **Eq. 10** and **Eq. 13** are the injector tip design and the spray angle after the transition phase, by replacing arbitrary constants by physical expressions. Nevertheless, the jet velocity from Naber and Siebers correlation is considered invariant as a function of time at any axial location or in a steady jet. So their solution cannot predict the dynamics of the spray with an unsteady injection rate. In order to improve this constraint, Musculus and Kattke [61] discretized the domain in the axial direction and added the transient terms for the spray momentum and fuel mass transport equation in each discretized control as seen in **Figure 14**. This correlation is accepted by Engine Combustion Network (ECN) to compare with the experimental results, the code is available to download on the ECN website (<https://ecn.sandia.gov/download-code/>).

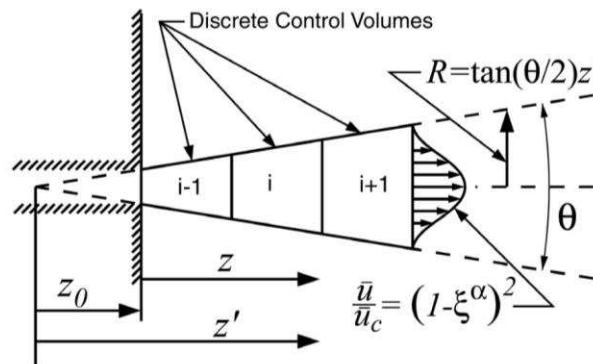


Figure 14 Scheme of one-dimensional discrete control volume transient diesel jet for Musculus and Kattke correlation [61].

1.3.4 Spray Angle

Another important parameter to indicate the spray characteristic is a spreading spray angle (θ) which represents the spray distribution in the radial direction and air entrainment [62]. This parameter has a strong relationship with the vapor spray penetration, as an increase of θ decreases the spray penetration length. As observed from experimental results, the spray angle increases with the increase of the ambient gas density [29], [49]. But it has a slight effect on the fuel properties, such as density and viscosity. As example, studied by Dernet et al. [50], an increase of fuel density by 100 kg/m³ and viscosity by 6.5 mm²/s induced a narrower spray angle up to 3 degree in quasi-stationary conditions. If injection conditions are considered, there is no significant effect of the high injection pressure (more than 75 MPa) and the effect of the injector hole diameter is not so clear. Naber and Siebers [49] suggested the geometry parameters of the injector tip would be more important than just through the unique consideration of the hole diameter. The important parameters, impacting the spray angle are also presented in **Table 1**. Both empirical correlations from Hiroyasu and Arai and Naber and Siebers are presented in **Eq. 15** and **Eq. 16**.

$$\theta = 83.5 \left(\frac{l}{D} \right)^{-0.22} \cdot \left(\frac{D}{D_o} \right)^{0.15} \cdot \left(\frac{\rho_a}{\rho_f} \right)^{0.26} \quad \text{Eq. 15}$$

$$\tan(\theta/2) = c \cdot \left[\left(\frac{\rho_a}{\rho_f} \right)^{0.19} - 0.0043 \sqrt{\left(\frac{\rho_f}{\rho_a} \right)} \right] \quad \text{Eq. 16}$$

The spray angle can be defined according to several ways as reviewed by Payri et al. [47]. The difference of 4 criteria, illustrated in **Figure 15** is briefly described by following:

- a) **Triangle criteria:** based on the creation of the angle of an isosceles triangle on the spray image. The isosceles triangle is created by the distance along the spray axis to a location where half the spray penetration ($S/2$) and the projected area of the upstream half of the

spray in an image, as presented in **Eq. 17**. This criterion was established and described by Naber and Siebers [49] and also included in the standard code of ECN.

$$\theta = \tan^{-1} \left(\frac{A_{p,S/2}}{(S/2)^2} \right) \quad \text{Eq. 17}$$

- b) **Trapezoid Criteria:** similar to the triangle criteria, but adapted for the cases when the contour of the spray is not available near the nozzle.
- c) **Fitted angle between intervals:** based on the use of two lines, fitted around the contour of the spray, starting at 12% of the penetration and ending at 60%
- d) **Fixed Origin:** the origin is fixed and then two lines are fitted using a weighted average of each point in the contour defined in polar coordinates.

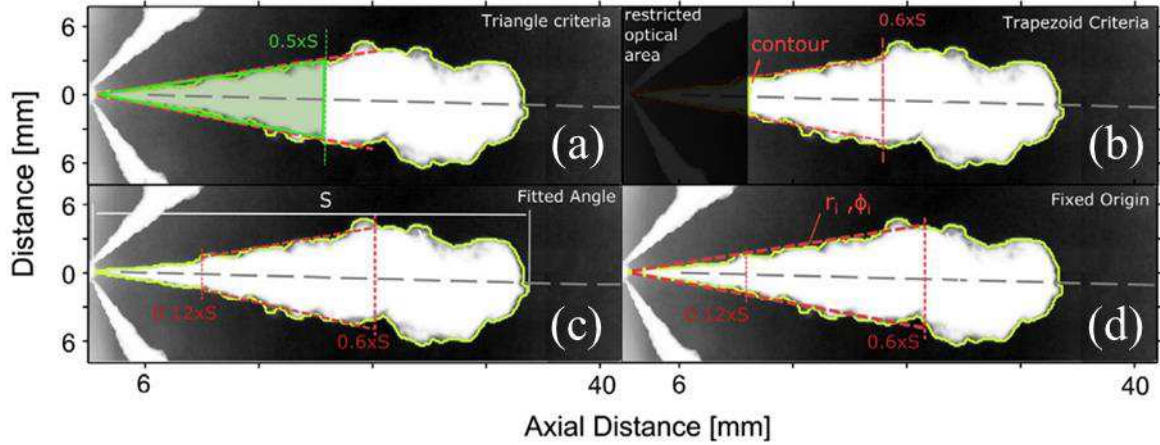


Figure 15 Different estimates of spreading spray angle [47].

1.3.5 Ignition delay

Ignition Delay (ID) is a very important parameter for diesel spray combustion, usually defined as the time between the start of injection (SOI) and the start of combustion (SOC). During the combustion process, there are two states of ignition: the first one usually called ‘cool flame’ and the second one called ‘main flame’ [63], [64], [65], [66]. The cool flame is the moment when the parent fuel molecules are broken down and raise the temperature slightly so when the first light is emitted by natural luminosity, especially by the HCHO^* and HCO^* radicals [63], [67]. After that, the entrainment of hot air and heat release from the cool flame

increase the temperature to a level where hydrogen peroxide dissociation reactions dominate the chemistry [64], producing significant heat release and rising rapidly in the cylinder pressure. The beginning of significant heat release is presented at the start of the second stage of ignition or main flame, represented as the start of combustion (SOC) of ignition delay.

ID represents the ability of fuels to auto-ignite, usually represented by the Cetane Number (CN): the highest CN corresponds to the shortest ID. The suitable value of ID depends on the combustion mode: in conventional diesel combustion, shorter ID (or higher CN) is favored for smoother running [68]. In the case of advanced combustion modes (as Low Temperature Combustion, Premixed Charge Compression Ignition or Homogeneous Charge Compression Ignition), a longer ID is required to reduce local rich mixture to reduce soot formation [61], [68]. For the impact of ambient condition on ID, an increasing of ambient temperature and the pressure promotes the chemical reaction rate, resulting in a shorter ID [69], as seen in **Figure 16** (a). Moreover, some fuel properties, i.e. latent heat vaporization and volatility also have an effect on the physical part of the ignition process [10], [70]. The oxygen concentration in fuel, $[O]_{\text{fuel}}$ seems to have a minor effect on ID as it promotes slight shorter ID only at the low ambient temperature when fuels have the same range of CN [71], as seen in **Figure 16** (b). The effect of these parameters on ID is schematized and summarized in **Table 2**.

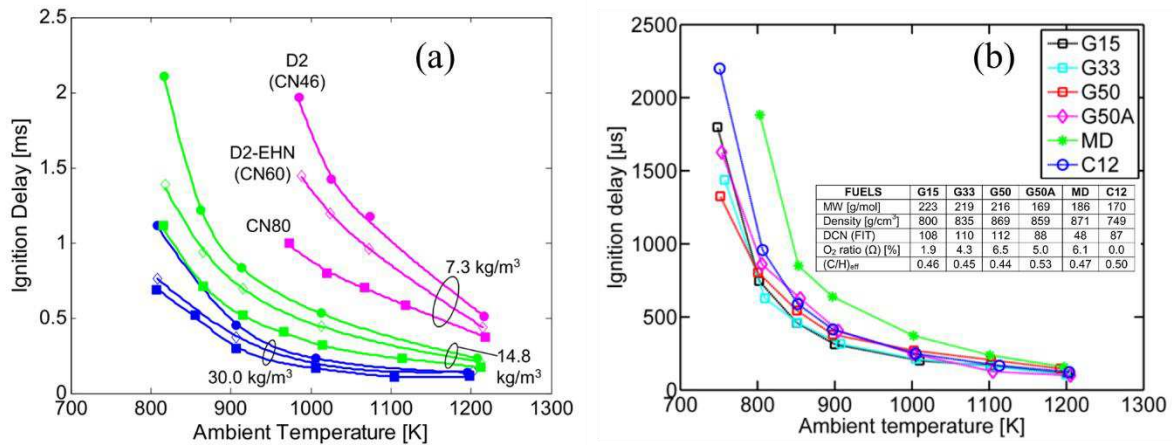


Figure 16 Effect of different parameters on ID: (a) the different ambient density and the cetane number [69] and (b) different oxygen content and the derived cetane number, i.e. DCN [71].

Table 2 Major parameters affecting on combustion characteristics.

Parameters	Ignition Delay (ID)	Lift-Off Length (LOL)
↑ Ambient density	↓ ([52], [69], [72])	↓ ([52], [69], [73])
↑ Ambient Temperature	↓ ([52], [69], [72])	↓ ([52], [69], [73])
↑ Oxygen content in Ambient condition	↓ ([69], [72], [74])	↓ ([75], [73])
↑ Injection pressure	↓ ([52], [74])	↑ ([52], [69], [73])
↑ Injection temperature	↓ Slightly ([52])	↓ Slightly ([52])
↑ Injector hole diameter	-	↑ [69]
↑ Cetane Number	↓ ([68], [71], [70])	↓ ([68], [71])
↑ Oxygen Content in Fuel	↓ ([71] at low T_{amb} for same CN)	↑ ([68], [71])

Note: ↑ = Increase; ↓ = Decrease; NE = No effect

1.3.6 Lift-off length (LOL)

After the auto-ignition occurs, a spray-driven diesel fuel jet becomes a lifted turbulent diffusion flame until the end of injection. Usually, the distance between the injector tip and the location of the stabilized flame is defined as the “lift-off length” (LOL). LOL is believed to affect diesel combustion and emission processes by allowing fuel and air to premix prior to reaching the initial combustion zone in a diesel spray [76]. As presented by literatures, LOL depends on the ambient gas condition, injection condition, injector configuration and some fuel properties. The higher ambient density (temperature) and oxygen concentration induce a shorter LOL, while the increase of injection pressure and orifice diameter increases the LOL [73], [76]. As observed in several studied, the cetane number is one of fuel property that related to the LOL, as LOL is strongly related to ID, i.e. fuels with shorter ID (high CN) generally produces the shorter LOL [61], [68], [69], [76], as seen in **Figure 17** (a). $[O]_{fuel}$ has also effect on LOL, as the increasing of oxygen in a molecule of fuel (similar CN) extends the length of the stabilized flame position [68], [71] (see **Figure 17** (b)). Furthermore, there is a strong link between the

fuel-air mixing upstream of the lift-off length and soot formation. The increase of LOL increases the amount of fuel-air premixing upstream of LOL, reducing soot incandescence [76], [77]. The effects of parameters on LOL are summarized in **Table 2**.

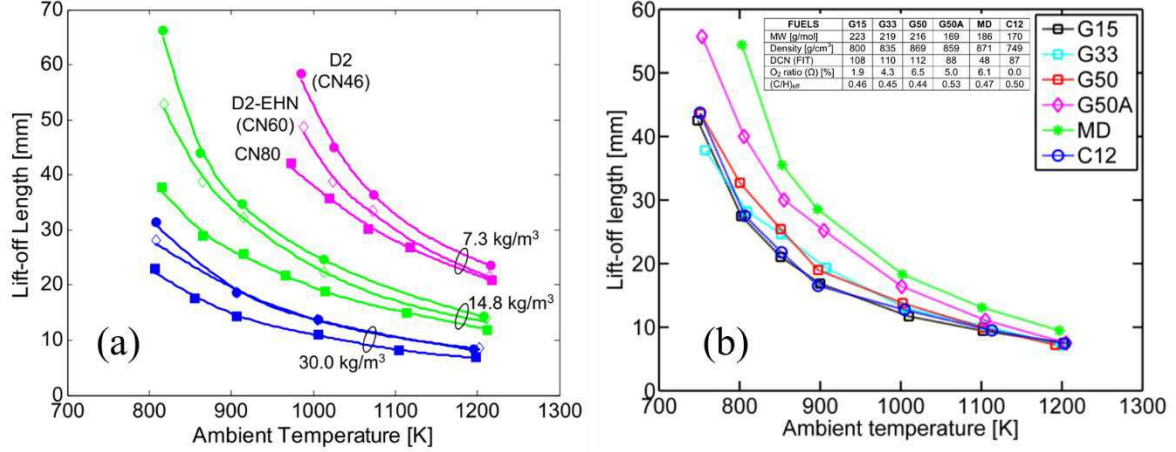


Figure 17 Effect of different parameters on LOL: (a) different ambient density and cetane number [69] and (b) different oxygen content and the derived cetane number, i.e. DCN [71].

Empirical Correlation for Reactive Condition parameters

According to the experimental results, the power-law empirical model suggested by Pickett and coworkers [69], [73], takes into account the effects of the ambient conditions, injector diameter and injection condition from wide range experimental data to estimate the LOL and the ID as in **Eq. 18** and **Eq. 19**:

$$ID = A \cdot \exp\left(\frac{E_a}{RT_a}\right) \cdot \rho_a^{-1.3} \cdot Z_{st}^{-1} \quad \text{Eq. 18}$$

$$LOL = C \cdot T_a^{-3.74} \cdot \rho_a^{-0.85} \cdot D^{0.34} \cdot U^1 \cdot Z_{st}^{-1} \quad \text{Eq. 19}$$

with T_a , ρ_a and U the ambient gas temperature, density and fuel velocity, C a proportional constant, while A , E_a and R are the pre-exponential constant, the apparent activation energy for the fuel auto-ignition process and the universal gas constant, respectively. The stoichiometric mixture fraction, Z_{st} represents the effect of oxygen concentration in the ambient gas. The Z_{st}

is increased by increasing oxygen concentration in the ambient gases, which induces the shorter of ID and LOL. It can be calculated by [78], [79]:

$$Z_{st} = \left(1 + \frac{Y_{F,0} \cdot W_O \cdot v_O}{Y_{O,0} \cdot W_F \cdot v_F} \right) \quad \text{Eq. 20}$$

where $Y_{F,0}$ and $Y_{O,0}$ represent the fuel and oxidizer mass fraction, W_F and W_O are the species molecular weights of fuel and oxidizer, and v_F and v_O are the fuel and oxygen stoichiometric coefficients, respectively.

1.4 Alcohols/Diesel Blends for CI Engine

An increasing concern of the depletion of oil resources and the global warming by greenhouse effect gases in the transportation sector, induced the research and innovation focus on alternative fuels as alcohols, biodiesel and biogas to substitute the petroleum fuels. Alcohol fuels, such as methanol, ethanol and butanol were considered as alternative fuel for compression ignition (CI) engines. However, the physical and chemical properties of butanol (see **Table 3**) indicate that butanol is suitable for CI engine, as concluded in several studies [4], [5], [6], [15], [80], [81], [82], [83]:

- Higher ability of auto-ignition: it has a higher auto-ignition temperature and Cetane Number compared to methanol and ethanol.
- Higher energy content: the lower heating value of alcohols normally rises as the carbon atom number. It is a four carbon alcohol, containing more energy than methanol and ethanol by 66% and 24%, respectively. Therefore, the fuel consumption will reduce and obtain a better mileage.
- Higher lubricity: it is also more suitable for diesel injection systems thank to its higher level of viscosity, more like diesel fuel and no water content.
- Better miscibility: it can be blended with diesel fuel at any concentration without any co-solvents addition and also does not separate when mixed at the low temperature. In comparison, methanol cannot be mixed easily with diesel fuel due to its highly polar

nature and ethanol has a limit of the blend at 25% by volume because of low viscosity and energy content.

- Oxygen content: the higher oxygen concentration in the molecule of butanol can contribute to the post-oxidation of soot during the combustion process.
- Easier distribution and storage: it has a lower water solubility than other alcohols leads to decreasing the tendency to microbial-induced corrosion in fuel storage and pipelines during transportation.
- It is more safety due to the higher flash point and lower vapor pressure.

Table 3 Comparative fuel properties between diesel and alcohol fuels [4], [5], [6].

Properties	Diesel	Methanol	Ethanol	Butanol	ABE (3:6:1)
Molecular formula	C ₁₂ -C ₂₅	CH ₃ OH	C ₂ H ₆ O	C ₄ H ₁₀ O	-
Density at 15°C [kg/m ³]	829	786.6	794.1	813.3	805
Viscosity at 40°C [mm ² /s]	1.9-4.1	0.59	1.08	2.63	-
Lower heating value [MJ/kg]	42.5	19.9	26.8	33.1	31.4
Cetane number [-]	40-55	3	8	25	-
Research octane number [-]	15-25	136	129	96	-
Auto-ignition temperature [°C]	235	463	423	397	-
Stoichiometric ratio [-]	14.3	6.49	9.02	11.21	10.5
Boiling point [°C]	180-370	64.5	78.4	117.7	-
Flash point [°C]	74	12	13	35	-
Vapor pressure at 25°C [kPa]	0.05	16.9	7.9	0.6	-
Latent heat of vaporization at 25°C [kJ/kg]	270-360	1162	918	582	595
Oxygen concentration (% by mass)	-	50	34.8	21.6	24.7
Solubility in 100 g of water	Immiscible	Miscible	Miscible	Immiscible	Miscible

Due to all advantages presented above, several studies presented the benefit of use of the butanol-diesel blends on the engine performance, combustion, and emissions, as reviewed Kumar et al. [4]. However, the brake specific fuel consumption increases with the proportion of butanol in the blend due to the decrease of heating value compared to diesel fuel [84], [85]. Therefore, to optimize pollutant emissions without significant penalty on engine performance,

the engine control parameters, such as injection pressure and strategies, and EGR dilution were investigated [85], [86]. The combined effect of butanol addition (until 40% by volume) with high level of EGR provides a longer ignition delay to reduce both local equivalence ratio and combustion temperature with as a consequence the drastic decrease of NO_x emissions without any drawback on soot, HC and CO emissions. The oxygen content in the butanol molecule enhances the soot oxidation to limit the particle matter emission in comparison with regular diesel fuel [8], [82]. By increasing butanol volume fraction (up to 40%) in diesel blend will induce longer ID and LOL, the higher resistance to auto-ignition will then lead to a better mixing rate before the start of combustion and certainly an improvement in NO_x and smoke emissions [7], [8], [9]. Last, butanol-diesel blends are also considered for advanced combustion modes of CI engines [10], [87], [88] due to its longer ignition delay, high oxygen content and high volatility. Also, to achieve higher oxygen concentration in fuel, other kinds of the oxygenated biofuel blends, such as butanol-ethanol-diesel blend were investigated to evaluate combustion and pollutant emission impacts [7], [8], [89], [90] with more benefit for PM-NO_x trade-off.

Due to its higher volatility, the spray of pure butanol is shorter and narrower in the liquid phase than for diesel fuel [15]. In the case of butanol blends, some studies [91], [92], concluded the spray tip penetration length and droplet size are reduced with the increase of butanol volumes in blending fuels (5 to 20% by volume), while spray angle remains constant for all fuels. Last, the increase in butanol increases the ignition delay.

1.5 Acetone-Butanol-Ethanol (ABE) Mixture for CI Engine

Although butanol has attractive properties for CI engine, there are some main drawbacks in which prohibited it to implement in the commercial scale as the fuel of transport vehicles, i.e., the low yield of production and high energy supply in separation process (related to cost) [12], [93], [94]. Bio-butanol can be produced from the abundant materials, such as agricultural crops i.e., sugarcane, corn, cassava and molasses (a byproduct of sugar refining) and lignocellulosic biomass, i.e., bagasse, wheat straw, corn-stover, switchgrass, etc. [12]. The Acetone-Butanol-Ethanol (ABE) fermentation is one main method to produce the first generation bio-butanol [5]. As seen in **Figure 18**, by using *Clostridium* bacteria, *Clostridium beijerinckii* or *Clostridium*

acetobutylicum, the sugars and starches from crops are fermented to produce a mixture of Acetone, Butanol and Ethanol (ABE) normally in a volume ratio of 3:6:1 [11], [12], [13], after which it is distilled and dehydrated to separate the pure butanol from the ABE mixture.

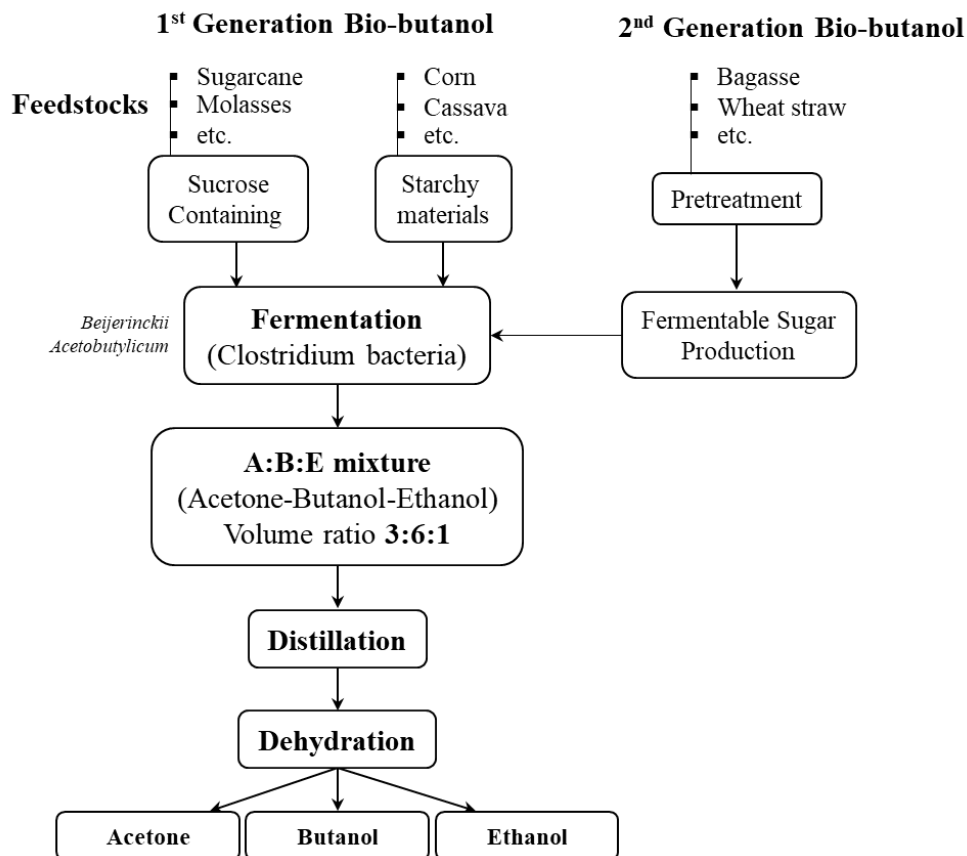


Figure 18 Schematic diagram of the bio-butanol production by ABE fermentation method (modified from [12]).

However, the drawback of this method is a low yield of butanol production due to the significant production of other byproducts, acetone and ethanol, which makes the feedstock consumption very high. For example, at least 6–7 tons of corn is needed to produce 1 ton of butanol depending on butanol ratio in total solvents, while only 3 tons of corn is used for 1 ton of ethanol [12], [93]. Therefore, as the feedstock consumption is more challenging for ABE fermentation, most of the research activities shift to the second generation bio-butanol, derived from the lignocellulosic biomass from nonfood feedstocks such as bagasse, wheat straw and other agricultural waste materials [12], as seen in **Figure 18**. Lignocellulose seems to be more

promising for the large scale of ABE fermentation as available in large quantity of low-cost materials. However, due to the high price of hydrolytic enzymes and the necessity to implement an expensive pretreatment step (see **Figure 18**) the high level of production process remains challenging [12], [87], [95]. Another drawback of the typical ABE fermentation is the high energy of production recovery to separating butanol from ABE mixture, for example in traditional direct distillation up to 18.4 MJ/kg is required in this process, which is 55% of butanol heating value [96]. For these reasons, butanol is not competitive with ethanol, as seen in **Figure 19**.

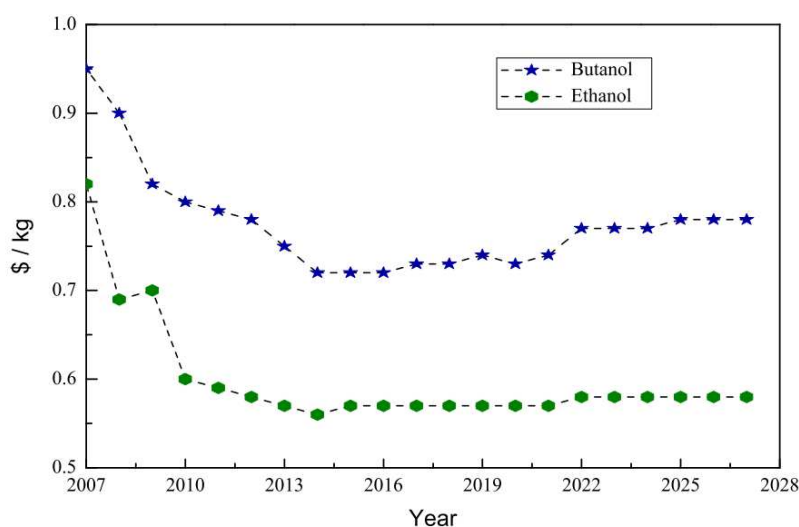


Figure 19 Projected prices of ethanol and butanol based on expected future market and historical trends [6], [97].

By concerning in these drawbacks, the intermediate of butanol production, called Acetone-Butanol-Ethanol (ABE) mixture, is recently interested as a new potential alternative fuel for CI engines. Since the main component in the ABE mixture is butanol (approximately 60%v), resulting its physical and chemical properties are similar to butanol [10], [11], as seen in **Table 3**. If the ABE mixture can be used as fuel, the cost and energy consumption of the separation process of butanol from ABE would be eliminated.

There are few studies of the ABE-diesel blend on the engine performance and emissions. Chang and co-workers [11] found that the blending of ABE in diesel up to 30%v (ABE30) can reduce the PM and no penalty on NOx [11]. By using 0.5%v of water in a 20%v ABE-diesel

blend (ABE20W0.5), PM and NO_x were respectively reduced up to 61.6% and 16.4% with an increase of the thermal efficiency up to 8.56%. In another work of this research group [14], the water-containing ABE-biodiesel-diesel blends were investigated on the engine performance and emissions. The results showed that the addition of water-containing ABE solution in biodiesel-diesel blends induced higher brake thermal efficiency than pure diesel and biodiesel blends up to 7.88%. Meanwhile, it could simultaneously reduce both PM and NO_x up to 30.7% and 63.1%, respectively.

The spray and combustion characterization of ABE diesel-blends were only investigated by Wu and co-workers [15] in a Constant Volume Preburnt Chamber. They showed that the pure ABE (3:6:1) and butanol have narrower and shorter spray feature than pure diesel due to higher volatility values, especially in the lowest ambient temperature. The ignition delay (ID) and lift-off length (LOL) of pure ABE are longer compared to pure diesel, especially at low ambient temperature. The effect of ABE composition itself (i.e. 3:6:1, 6:3:1, 0:10:0) blended at 20%v in diesel was investigated in [10], [16] and [98]. The result showed that with the highest concentration of acetone, the combustion characteristics (i.e. ID and combustion duration) are similar to pure diesel, with also lower natural flame luminosity compared to diesel, but higher than ABE20(3:6:1) and ABE20(0:10:0).

Wu et al. [13] also investigated the spray and combustion characteristics of ABE blends by varying the volume fraction of typical ABE(3:6:1) mixture in diesel blends by 20%v, 50%v and 80%v (ABE20, ABE50 and ABE80, respectively) to compared with pure diesel (D100). The lower blend, ABE20, performed a similar spray feature (spray size and LL) to D100, due to its lower amount of ABE, while in the high blend of ABE50 presented the same spray feature with ABE80. They suggested that certainly exists a critical ratio of ABE influencing spray characteristics between 20%v and 50%v. But, ABE50 provided similar combustion phase and ignition delay than those of n-D100, due to the good balance between the enhancement of atomization and spray performance, cetane number and latent heat of vaporization. In conclusion, they suggested that ABE blend with an ABE ratio between 20%v and 50%v would be the best ratio to be used in CI engine without any major modifications. The main knowledge about ABE-diesel blends from literature review is summarized in **Table 4**, experimental set-up, measurements techniques and conditions are added for future discussion.

Table 4 Summary of spray and combustion characteristics for different ABE blends.

Reference	Reference fuels & ABE blend (A:B:E ratio)	Experimental set-up and conditions	Technical Measurement	Spray characteristics of ABE blend compared to diesel	Combustion characteristics of ABE blend compared to diesel
Wu et al. [15]	D100 Bu100 ABE100(3:6:1)	- CVP chamber - 6 holes injector VCO (145 μm diameter) - Reactive Condition - T_{amb} =800-1200 K - % O_2 = 11, 16, 21 - P_j = 1300 bar - Inj. Duration = 3.5 ms	- LL: Mie-scattering, - ID: P_{cyl} (HRR) - LOL: Natural flame luminosity imaging	↓: LL ~ : Spray shape with Bu100	↑ : ID ↑: LOL ↓: Combustion Duration ↓: Natural luminosity
Wu et al. [10], [16], [98]	D100 ABE20 (6:3:1) ABE20 (3:6:1) ABE20 (0:10:1)	- CVP chamber - 6 holes injector VCO (145 μm diameter) - Reactive Condition - T_{amb} =800-1200 K - % O_2 = 11, 16, 21 - P_j = 1300 bar - Inj. Duration = 3.5 ms	- ID: P_{cyl} (HRR) - LOL: Natural flame luminosity imaging	NA	↑: ID for all ABEs ↑: LOL for all ABEs ~ : Combustion characteristics for ABE20(6:3:1), ID and LOL, closed to D100 ↓: Combustion Duration, lowest by ABE20(6:3:1) ↓: Natural luminosity, lowest by ABE20(6:3:1)
Wu et al. [13]	D100 ABE20(3:6:1) ABE50(3:6:1) ABE80(3:6:1)	- CVP chamber - 6 holes injector VCO (145 μm diameter) - Reactive Condition - T_{amb} =800-1200 K - % O_2 = 11, 16, 21 - P_j = 1300 bar - Inj. Duration = 3.5 ms	- LL: Mie-scattering, - ID: P_{cyl} (HRR) - LOL: Natural flame luminosity imaging	~ : Spray shape by ABE20 ↓: LL by increasing ABE ratio	↑: ID by increasing ABE ratio ↑: LOL by increasing ABE ratio ↓: Combustion Duration by increasing ABE ratio ↓: Natural luminosity, by increasing ABE ratio ~ : Combustion characteristics for ABE50 as ID and LOL closed to D100

Note: ↑ = Increase or Longer; ↓ = Decrease or Shorter; ~ = similarity; NA = Not Available.

According to Wu et al.'s experimental results [10], [13], [15], [16], even though the spray and combustion parameters were characterized by optical measurements, their experimental results were not so quantitative due to the low signal to noise ratio of signals. As in **Figure 20** (a), they measured LL by using the Mie-scattering technique in the reactive conditions, the luminosity light from soot incandescence could be collected in the camera and

interfered on the image. As a result, the low quality of Mie-scattering images is obtained, when the saturation in the image can be observed as in **Figure 20** (b). Moreover, they used the natural flame luminosity image to characterize LOL. But this technique was not able to identify the location of the stabilized flame, as the soot incandescence can be observed, as it can be seen in orange in **Figure 20** (c).

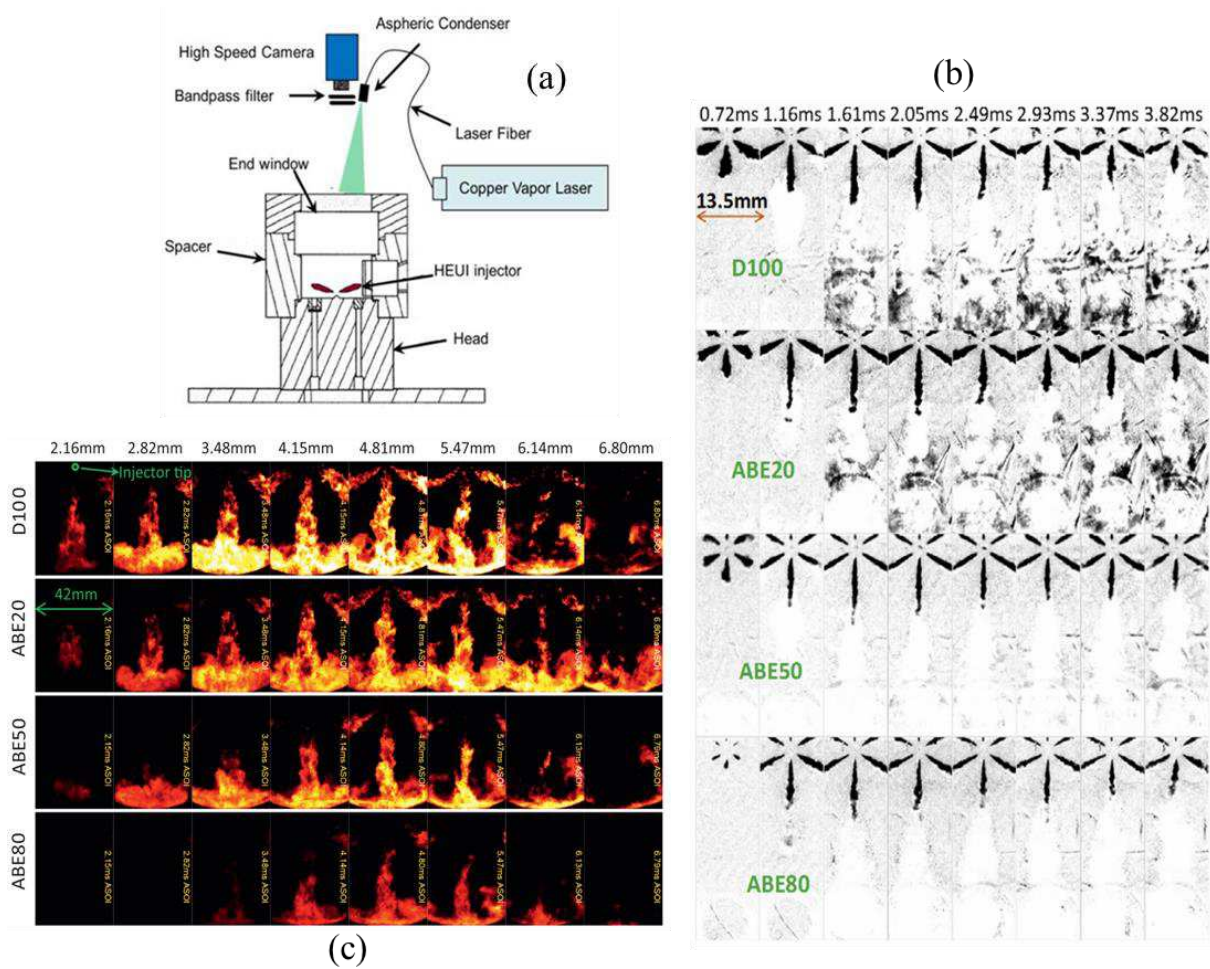


Figure 20 Experimental set-up and images from Wu et al. [13], [15]: (a) scheme of optical set-ups (b) the liquid phase length and (c) the natural luminosity imaging to determine the lift-off length and soot.

1.6 Conclusion

The spray characteristics of diesel engine are the primary parameters that control the process of mixing formation, auto-ignition, combustion and subsequently emissions. Currently, the high development of injection technologies of modern diesel engine plays a significant role to improve engine performance, combustion and also mitigate exhaust emission without the penalty of engine performance. As a result, the better understanding of the complex phenomena of spray and combustion is necessary to improve in order to develop the next step of diesel engine technology and consider the new alternative fuel.

By blending Butanol with conventional diesel fuel (up to 40%v) and optimizing EGR, the smoke and NO_x can be reduced the significant penalty on engine performance. However, the low yield of production and high energy in the separation process, related to the high production cost per unit, prohibit butanol to be implemented in the commercial scale as the fuel of transport vehicles.

The intermediate product of the fermentation process of butanol production called ABE mixture has a real potential to use directly to diesel engine as new alternative fuels due to similar its properties to butanol. Indeed, ABE20 (3:6:1) displayed similar spray characteristics to diesel, while ABE50 (3:6:1) performed the combustion characteristics close to diesel. Wu et al. suggested that an ABE ratio between 20%v and 50%v would be the most appropriate quantity to be used in CI engine with minor modification as it could be maintained combustion characteristics similar to D100.

As reviewed in the literature, the lack of research can be found and especially as:

- 1) Even if several studies present some results about the high potential of ABE and butanol diesel blends to reduce simultaneously soot and NO_x, there is not yet a complete comparative study of these fuels on spray and combustion behaviors to understand better the effect of fuel properties.
- 2) Other alcohol blends also have a high potential for CI engine as presented the low soot and NO_x emission due to high oxygen content in the molecule such as butanol-ethanol-diesel blends or ethanol-diesel blend (20%v). However, there is no research fully compare and characterize them on the spray and combustion characteristics.

- 3) There is ambiguous on the suitable blending ratio of ABE, as Wu et al. suggested that the critical ratio is between ABE20 and ABE50. It needs more research to reveal on which quantity is the most suitable.
- 4) Although the spray and combustion parameters have been characterized as presented in the literature review for several ABE ratios, the quality of experimental results has invalidated. Therefore, the use of standard conditions, measurement techniques and post-processing as determined in ECN are required in order to provide accurate quantitative experimental results.

Therefore, this study is focused on the investigation of the effect of fuel properties for different alcohols and ABE blended in n-dodecane on the spray and combustion behaviors in high-pressure and high-temperature conditions by using ECN conditions to provide accurate results to analyze and evaluate the potential of these blends.

CHAPTER 2

CONCEPTUAL DESIGN OF HIGH-PRESSURE AND HIGH-TEMPERATURE CHAMBER

2.1 Engine Combustion Network

The international Engine Combustion Network (ECN, <https://ecn.sandia.gov/>), initiated by Sandia National Lab (USA) and IFPen (France) since 2009, aims to share highly accurate experimental data in order to enhance scientific understanding of spray combustion in the conditions specific to gasoline and diesel engines to validate and improve CFD models [99], [100]. All members of the ECN group agree to setup an experiment with the same injectors and ambient conditions, thereby enabling direct comparison between different facilities. Nowadays, ECN is an important network which represents many researchers and companies around the world interested in this topic as seen in **Figure 21**.

In France, IFPen has initiated and led an ECN France project (sponsored by ANR) to trigger the participation of French engine combustion community laboratories in ECN such as IFPen, PPRIME, CORIA and PRISME. They have developed in different kinds of the combustion chamber and the advanced optical diagnostics for engine combustion analysis, as shown in **Table 5**. IFPen has taken part in ECN since the creation of the network, its experience in standardization is used as the reference for the project. All of the injection devices such as the injector and common rail were characterized by IFPen to ensure that all the experiments are carried out in similar conditions, and also the spray and combustion parameters to compare experimental results.

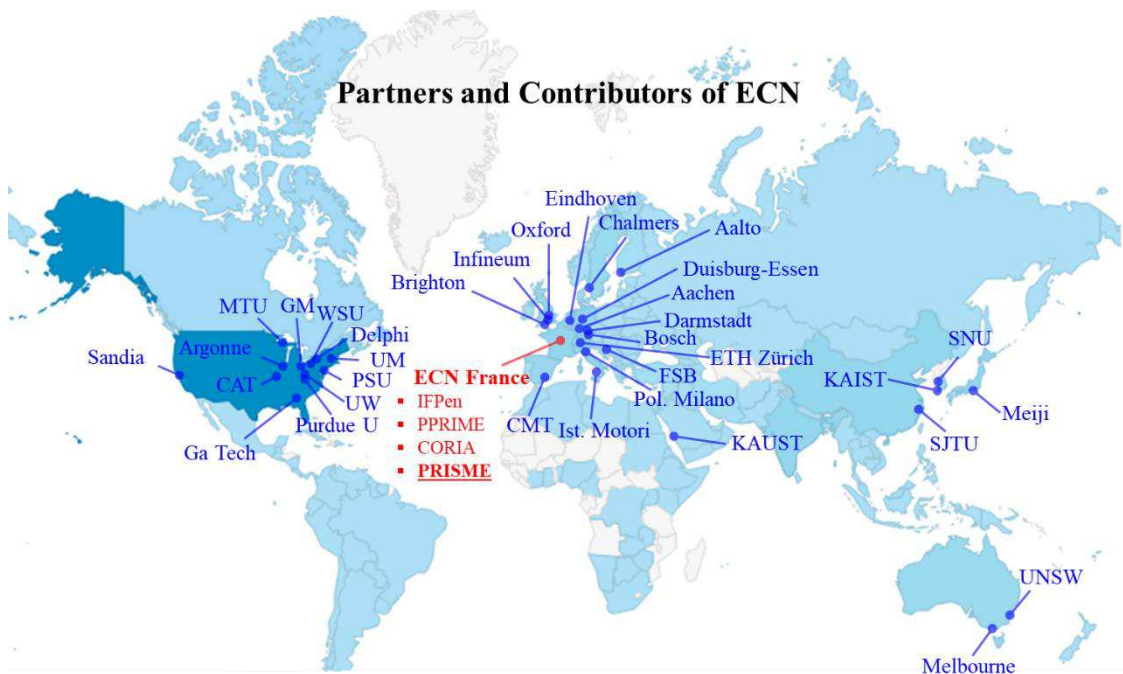


Figure 21 Partners and contributors of Engine Combustion Network in 2018.

(<https://ecn.sandia.gov/>)

Table 5 Participate institutes and kind of combustion chamber in ECN France.

Laboratories	Kind of combustion chambers
IFPen Institut Français du Pétrole énergies nouvelles – Paris	Constant-Volume Preburnt (CVP)
PPRIME Institute PPRIME - Université de Poitiers	Rapid Compression Machine (RCM)
CORIA Complexe de Recherche Interprofessionnel en Aérothermochimie - Université de Rouen	Constant-Pressure Flow (CPF)
PRISME Institut Pluridisciplinaire de Recherche en Ingénierie des Systèmes, Mécanique et Energétique - Université d'Orléans	New Rapid Cycling Machine (RCYM) called New One Shot Engine (NOSE)

2.2 Spray-A Operating Condition of ECN

The “**Spray-A**” of ECN was established as one of the standard operating condition for the diesel spray and combustion, defined as the low-temperature diesel engine combustion conditions relating to engines with a moderate rate of exhaust-gas recirculation (EGR) [100]. The main parameters for Spray-A conditions are given in **Table 6**. The ambient temperature is varied by 800, 850 and 900 K at the start of injection timing. The ambient density is maintained at 22.8 kg/m³ for all ambient temperatures by adjusting the cylinder pressure around 60 bar. The experiments can be done in both of non-reactive conditions with pure N₂ and reactive conditions with 15% of O₂. To evaluate how the experimental sets-up reach the conditions of Spray A, the fuel considered as a reference is the single-component Diesel surrogate fuel, n-dodecane, as also the complete knowledge of the chemical and physical properties [99].

Table 6 Main specifications for Spray-A ambient conditions of ECN

Parameter	Value
Ambient gas temperature	800, 850, 900 K
Ambient gas pressure	near 60 bar
Ambient gas density	22.8 kg/m ³
Ambient gas oxygen	Pure N ₂ 15% O ₂ and 85% N ₂
Non-reactive condition	
Reactive condition	
Ambient gas velocity	Near-quiescent, less than 1 m/s
Injection Pressure	1500 bar
Injection Duration	1.5 ms
Fuel	n-Dodecane
Fuel temperature	363 K

2.3 High Pressure-High Temperature (HPHT) Chamber

In the last 20 years, to comply with increasingly drastic emission standards, many studies have focused on spray and combustion for Internal Combustion Engines (ICE) in order to improve efficiency and reduce pollutant emissions. The development of Computational Fluid Dynamics (CFD) simulation has been made to compute a wide variety of chamber geometries

and operating conditions to optimize at a substantially lower cost than with experimental methods [45]. However, the predictability of CFD depends on the degree of understanding of the physical phenomena of spray and combustion in the chamber. Thank to optical techniques revealing this complexity in the last two decades [45], [63], the several combustion chambers were developed to reach High Pressure-High Temperature (HPHT) thermodynamic conditions, representing current common-rail diesel engine operating modes. For example, Constant-Volume Preburn (CVP) chamber, Constant-Pressure Flow (CPF) chamber, Rapid Cycling Machine (RCYM) [45], [100], [101], [102], are frequently used to investigate basic phenomena of diesel spray and combustion by using optical set-ups.

2.3.1 Constant-Volume Preburn (CVP) Chamber

In the CVP chamber, premixed combustion is used to rapidly generate HPHT conditions by varying a combustible-gas mixture [45], [99], [101], [103]. Then, the ambient gas pressure and the temperature slowly cool down due to heat losses to obtain the desired target ambient conditions in which the injection is generated to perform the spray and combustion measurements. This chamber is equipped with wide optical accesses enabling the application of advanced optical diagnostics. **Figure 22** illustrates the example of CVP operation and for more details of the operating conditions were extensively described in several studies [99], [100], [101], [104].

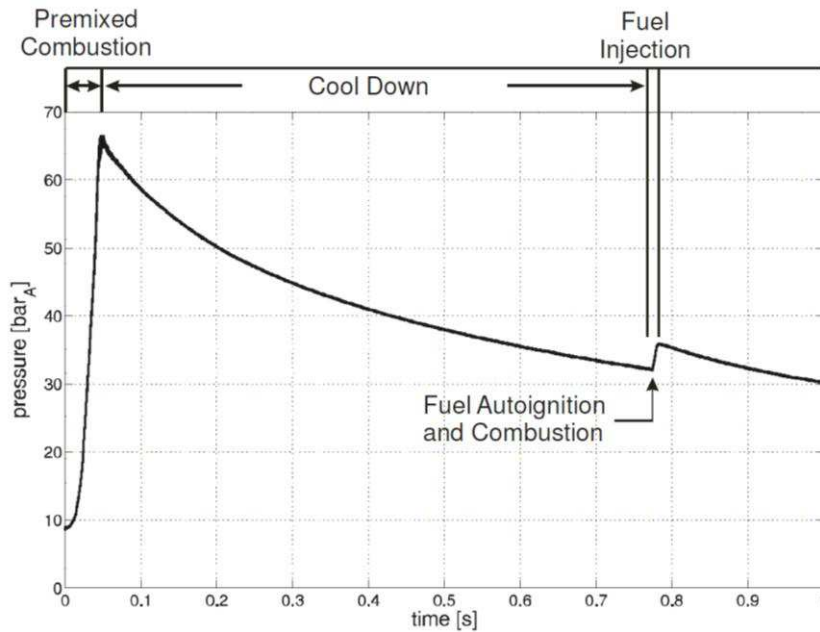


Figure 22 Principle of the Constant-Volume Preburn [101].

During pre-burn combustion, the major combustion products (CO_2 , H_2O , Ar, N_2 and O_2) and minor species (NO, NO_2 and OH) are generated and can be presented at the injection timing of the testing [100]. These products can affect the ignition delay, the lift-off length, the soot production, oxidation, as presented in several studies [105], [106], [107]. Nesbitt et al. [105], investigated the effect of the production of minor species (NO, NO_2 and OH) on auto-ignition delay during the premixed burn and cool-down period in the CVP. They found that both major (CO_2 , H_2O , O_2) and minor species (NO, NO_2 and OH) influenced the ignition delay. The changes in ignition delay resulting from minor species were small relative to those from major species. Even though these species can be reduced by varying the pre-burn composition, they remain present [108]. Another drawback of this chamber is the long time needed to reach the target condition after the pre-burn event. As a result, the fuel-air mixing and the charge temperature distributions can differ from those in a real engine combustion chamber [45], [101]. However, many institutes, such as IFPen, Sandia, TU/e, MTU, etc., use this chamber [100], [101], [108], [109], due to its advantages related to the large optical window size which enables the long free spray penetration distance to be investigated. It is also possible to control a wide range of ambient temperatures and pressures and to switch rapidly between ambient temperature

levels for different conditions. The low cost of developing this facility is a further advantage for the study of combustion processes. Some examples of pictures of this chamber are shown in **Figure 23**.

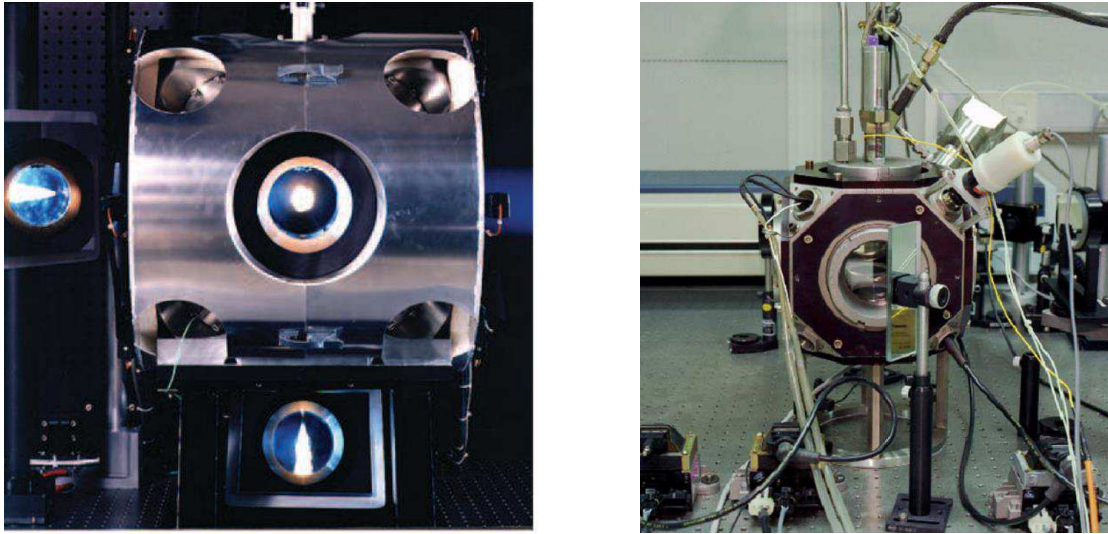


Figure 23 Constant-Volume Preburnt (CVP) of Sandia (left) and IFPen (right) [99].

2.3.2 Constant-Pressure Flow (CPF) Chamber

In the CPF chamber, the facility is composed of four parts: gas compressors, gas heaters, test vessel, control system [110]. The gases are compressed by a volumetric compressor in a high-pressure tank and flow continuously through the electrical resistances to reach the target temperature before entering the test chamber. After finish the spray and/or combustion test, the hot gas flow scavenges the injection fuel and/or combustion products to maintain the ambient condition. A control system provides the desired testing condition by measuring temperature and pressure to continuously adjust the power of the heater and gas flow to supply the upstream of the chamber. The operating conditions of this chamber have been described in detail by Payri et al. [45], [52], [100], [110]. Generally, this chamber is similar to a large pipe as seen in **Figure 24**. The spray and combustion evolution can be observed from a distance through the multiple large windows (127 mm in diameter), positioned at an angle of 90° around the circumference

of the chamber. Due to the continuous flow, a high number of tests can be realized, but the need for highly compressed clean air and a continuous gas flow [102] induces large, heavy and expensive facility.



Figure 24 Constant-Pressure Flow (CPF) chamber of CMT [110].

2.3.3 Comparison and Discussion between CVP and CPF Chamber

The boundary conditions, spray development and combustion parameters of CVP and CPF have been extensively compared in the papers of engine combustion network (ECN) [45], [99], [100], [106]. Both chambers show a high ability to control the standard Spray-A ambient conditions (i.e., 900 K, 60 bar and 22.8 kg/m³). In the CPF, the gas temperature remains steady inside the chamber along the test section with only 8 K of deviations, while in the CVP deviations were 11-14 K [45]. However, both chambers require a cooling system to control the fuel temperature at the injector tip at 90 °C as high sensitivity on spray and combustion parameters [45], [105]. For the ambient gas chemical compositions, as expected, there are no combustion products present in the CPF, because only O₂ and N₂ are used to reach Spray-A conditions. While the CVP presented major and minor species from the pre-burn reaction, as mentioned above. The major and minor species of pre-burn combustion do not affect the spray development [100], [106], but the ignition delay is sensitive to the major pre-burn species (CO₂ and H₂O) and also minor species as OH [111].

2.3.4 Rapid Cycling Machine (RCYM)

The RCYM [101], [102], [112], [113] seems to be an interesting option to study the diesel spray and combustion in HPHT conditions, due to the absence of combustion products unlike in the CVP and the possibility of covering a full range of diesel engine working conditions (up to 100 bar). The use of a 2-stroke engine allows the gases to flow and be exchanged through side-port-scavenging [101]. The original cylinder head is modified to enable optical measurements from different sides of the combustion chamber. The engine speed is usually regulated at 500 rpm to compress the gases inside the cylinder to reach HPHT conditions around Top Dead Center (TDC), where the fuel is injected into the chamber. **Figure 25** illustrates some examples of RCYM.

As it operates continuously and scavenges the injected fuel and combustion products every cycle, the number of tests is not limited, and the ambient gases are only due to the well-known intake gases themselves. However, the main drawbacks of this device are the need to use a very large displacement engine as well as the high vibration and noise levels produced during operation. Lastly, because of side-port-scavenging, high-velocity fields inside the chamber can be generated, affecting spray and combustion processes [114].

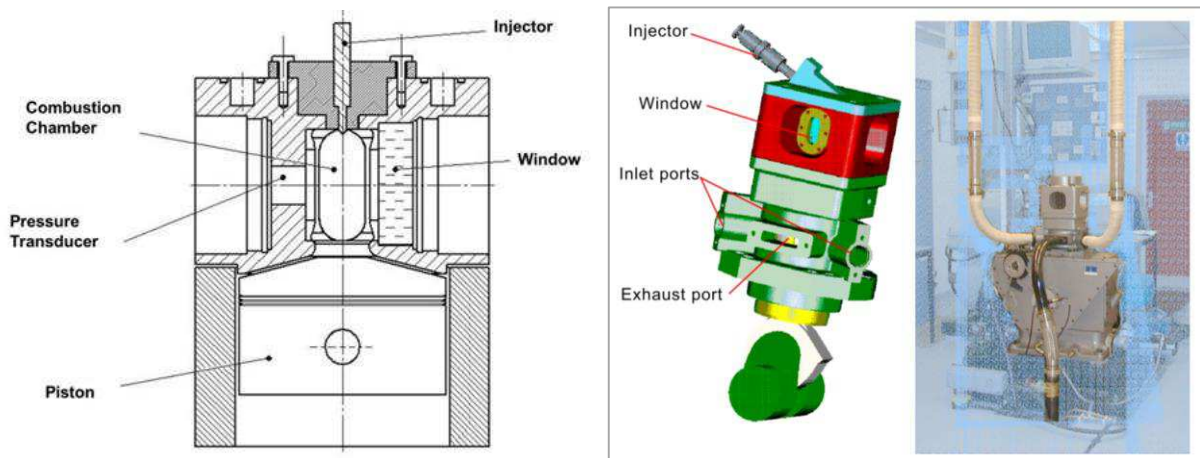


Figure 25 Examples of Rapid Cycling Machine (RCYM) from CMT (left) [114] and from University of Brighton (right) [113].

2.4 Conceptual Design of the New One Shot Engine (NOSE)

To participate in ECN community, PRISME Laboratory of Université d'Orléans has designed and developed a new chamber able to reach the HPHT thermodynamic conditions of current common-rail diesel engines, called “New One Shot Engine” (NOSE). The design optimized the advantages and limited the drawbacks of the different HPHT chambers reviewed above and summarized in **Table 7**, compared to the CVP chamber. NOSE is based on the concept of RCYM to prevent the generation of pre-burn combustion species as in the CVP and uses a low energy and gas supply, unlike a continuous gas flow test rig. A 4-stroke low-speed diesel engine was used to avoid the effect of velocity fluctuation from the gas flowing and exchanged through the side-port-scavenging of a 2-stroke engine, as in the RCYM. The original cylinder head was replaced by a dedicated chamber to provide a sufficient field of view. Moreover, the piston head angle and the gap distance were optimized to eliminate squish and reduce gas velocity inside the chamber to obtain a near-quiescent gas condition, less than 1 m/s, following the ECN Spray-A requirement. The general idea is to drive the engine with a high power electric DC motor with a highly accurate velocity feedback controller to control the speed of piston movement during the compression stroke and to stop the piston smoothly in the expansion stroke in order to avoid noise and vibration.

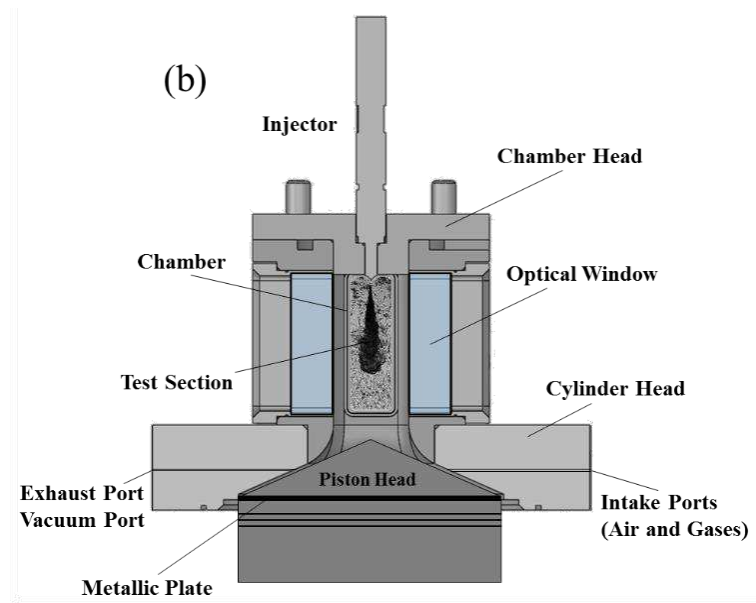
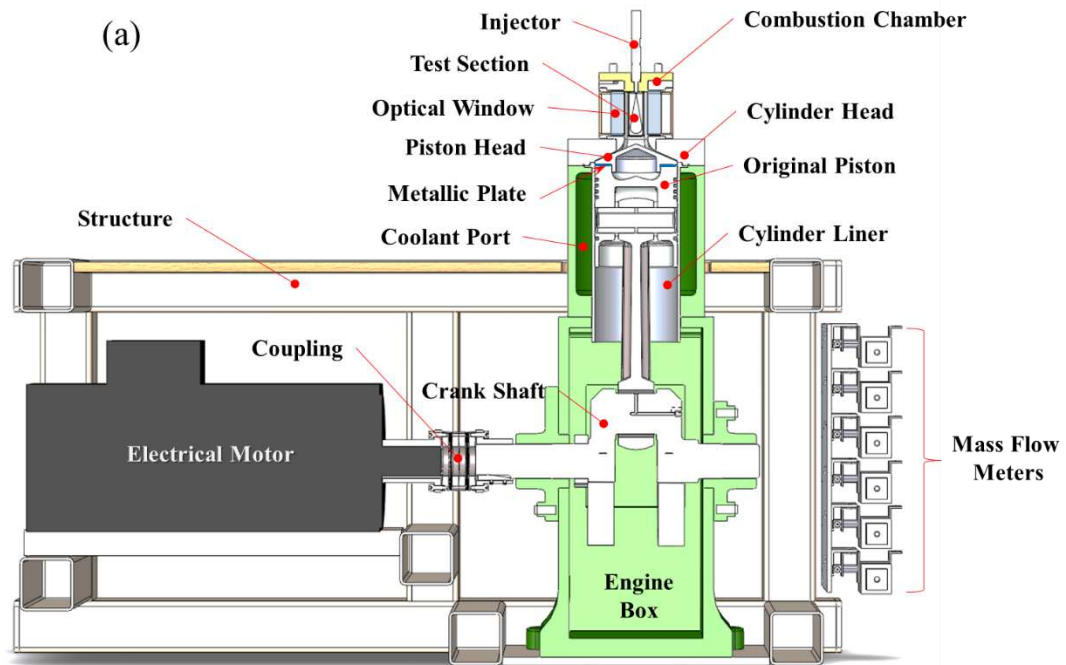
Table 7 Comparison of the strengths and weaknesses of the different kinds of HPHT chamber based on the previous review of Baert et al., [101]. The relative quality is compared with CVP as a reference; “0” = neutral, “+” = better and “-” = worse.

Information	Chamber		
	CVP	CPF	RCYM
Optical accessibility	+	++	++
Similarity to the real engine situation	0	0	0
Free spray penetration distance	++	++	-
Control ambient condition (P and T)	++	++	+
Combustion production effect	--	0	0
Flow field impact on spray and combustion	-	0	-
Number and price of facility	++	0	0
Noise and vibration	0	0	--

Information	Chamber		
	CVP	CPF	RCYM
Time to switch between operating condition (i.e. T)	++	0	0
Time between tests [s]	600	1-3	1

To reach the HPHT conditions of the standardized Spray-A of ECN, a single-cylinder 18 horsepower low-speed diesel engine at 750 rpm was used, as shown in **Figure 26** (a). The swept volume is 3600 cm³ with a 155 mm bore, 177.8 mm stroke and an initial compression ratio of 15:1 as detailed in **Table 8**. The original cylinder head was modified and replaced by a dedicated chamber. This chamber is optimized to provide a sufficient field of view to study the spray development and to enable optical measurements from four quartz windows (25 mm thick, 25 mm wide and 80 mm long). **Figure 26** (b) presents the cross-section view of the middle plane of the chamber. The injector is mounted at the center of the chamber head. The four optical windows are fastened to the main chamber structure on each side. The chamber shape in top-view is a square 44 x 44 mm and 90 mm long, connected to the piston head at downstream as presented in **Figure 26** (c) and (d). The total volume of the combustion chamber is around 240 cm³. The piston roof angle was designed to obtain near-quiescent gas conditions and avoid the squish effect inside the chamber [115].

To control the fuel injection temperature at the injector sac, four heaters are embedded, one at each corner of the chamber structure as shown in **Figure 26** (c)-(d). Thus, there is no need for an injector cooling system as presented in the CVP and CPF. The inlet gases and air are connected to the chamber via gas and air intake ports and are precisely controlled the number of gases by the mass flow meter as seen in **Figure 26** (a). On the opposite side to the intake ports, the exhaust port is also connected to the chamber to release all the gases after finishing the operation, while the vacuum port is used to clean and create a vacuum inside the chamber for the next operation. Finally, the real pictures of the NOSE set-up are presented in **Figure 27**. For more details about the engineering drawings and photographs of the combustion chamber are presented in **Appendix A.1**.



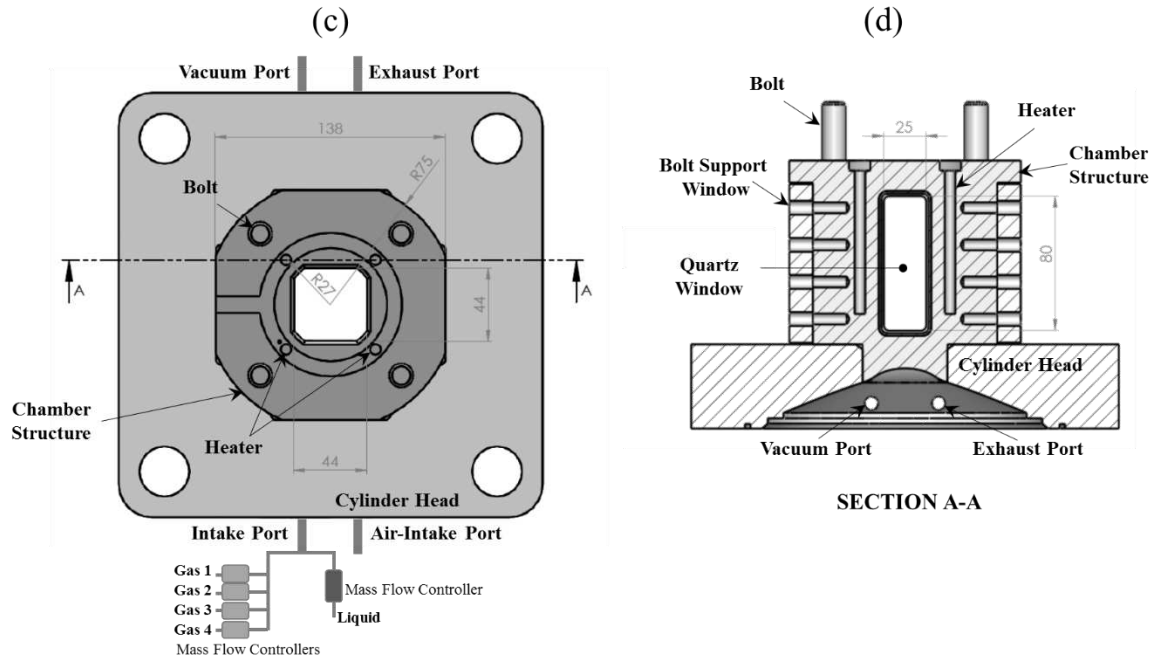


Figure 26 The NOSE chamber: (a) overview set-up, (b) cross-section view in the middle plane of the chamber [115], (c) top-view without the chamber head and (d) cross-section view A-A without the chamber head.

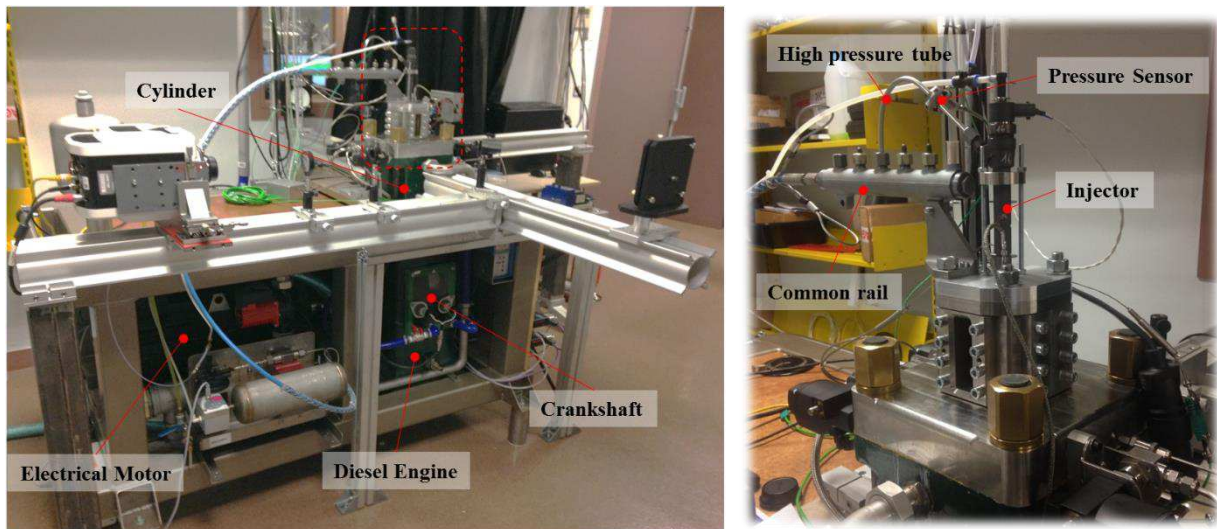


Figure 27 Views of NOSE: (a) overview set-up, (b) zoom of the combustion chamber.

Table 8 Main specifications of NOSE [115].

Specifications	Value
Sweep volume	3600 cm ³
Bore x Stroke	155 x 177.8 mm
Compression ratio	15:1
Number of optical windows	4
Window size	25 x 80 mm
Intake gas (able to switch)	Gaseous species (N ₂ , O ₂ , Air, CO ₂ ,) and liquid species and fuel (H ₂ O, Silica oil)
Cooling system of Engine	Water
Engine speed (at TDC)	~100 rpm

As NOSE is based on the principle of adiabatic compression process, the initial conditions such as initial pressure and temperature must be defined before starting operation at Bottom Dead Center (BDC) to achieve the target conditions of pressure and temperature near Top Dead Center (TDC). The piston of NOSE is driven by a brushless DC motor (PHASE Automation U31340) coupled with a high-performance electric driver motor (PHASE Automation AxM300-400) through an in-house LabView 8.1 interface, which is able to reach 1100 Nm of maximum torque and 1500 rpm of maximum speed (Furthermore details of motor and driver specifications are presented in **Appendix A.2**). The driving force of the piston depends on many parameters such as the driving torque, velocity and friction between the piston ring and liner, dominated by the temperature and oil film. These parameters can be responsible for a high cycle-to-cycle variation of ambient conditions. Therefore, a highly accurate closed-loop velocity feedback function was developed for NOSE in order to control the piston speed during the compression stroke for high repetition rate tests to obtain stable thermodynamic ambient conditions and also to prevent noise and vibration at the end of the operation by stopping the piston smoothly in the expansion stroke. The details of the operating conditions are explained in the following section.

The intake system of NOSE was designed to be able to supply many kinds of gases and to control the volume of gas intake into the chamber before starting each operating condition at BDC to reach the initial condition. The quantity of inlet gases is controlled by the BROOKS®

model 5860S gas flow meters, coupled with the BROOKS® model 5850S mass flow rate controller to ensure a highly accurate gas flow rate ($\pm 0.7\%$ of rate). **Figure 26** (c) presents the four mass flow meters installed at the intake port to control the volume of inlet gases such as N₂, O₂, NO, CO₂, etc. Moreover, this system was designed to supply liquid additive in order to perform measurements for different purposes, such as silicon oil seeding particles for PIV measurement, water to study its influence on combustion parameters, etc.

During the operation, a high response piezo-electric pressure sensor (KISTLER Type 7001) is set up at the chamber head and coupled with a charge amplifier (KISTLER Type 5011). The cylinder pressure and temperature inside the vessel, the injector driving current and crank angle are recorded as a function of time with a National Instrument Compact RIO at 250 kHz. To release gases after the operation, the exhaust port is opened and then dry air of 7 bar is injected from the air-intake port into the chamber to purge all residuals from the spray and combustion products during around 10 seconds. After that, the vacuum port is opened and connected to the vacuum pump to remove all the gases inside the chamber before refilling with gases for the next operation.

2.5 NOSE Operation for ECN Spray-A

The initial temperature is specified by setting the point of cooling temperature in the LabView program. The cooling substance is circulated by a centrifugal pump and an adaptive heater is installed at the discharge port of the pump to control the set point of the cooling temperature. The chamber is heated thanks to 4 heaters, one at each corner. For example, for Spray-A conditions at 900 K (60 bar and 22.8 kg/m³), the piston is initially positioned at Bottom Dead Center (BDC) with a cooling temperature set at 83 °C. The chamber is heated up to 100 °C to achieve 90 °C inside the injector sac. The chamber is then filled with pure Nitrogen (N₂) until an initial pressure of 1.8 bar is reached (see **Figure 28** (a)). The first mode of engine operation is started by driving the piston up in the reverse direction (anticlockwise) from the starting position at BDC, i.e. 180 CAD before TDC, to “the initial position” of the velocity feedback control at 280 CAD before TDC (see **Figure 28** (b)). This method was chosen to

reduce static friction at the initial BDC position and ensure smooth piston movement. (If the piston was directly driven from BTD to TDC, the maximum pressure is only around 40 bar.)

After that, the control system is immediately switched to the velocity feedback control mode. In this mode, the controller tracks the optimized velocity profile, by comparing with the feedback velocity obtained from the crank angle position versus time as presented in **Figure 29**. From its starting position, the piston starts to move down quickly by speeding up to 1000 rpm. Then it passes the BDC at 40 ms (see **Figure 28** (c) and **Figure 29**) to compress gases inside the chamber until a minimum of piston speed at TDC, around 100 rpm to avoid high friction (see **Figure 28** (d)). Finally, at 120 ms (70 CAD after TDC), the piston is automatically braked by the electric motor to stop the engine smoothly and prevent vibration and noise after the operation. As this new device compresses ambient gases only one cycle from BDC to TDC, it is called a “New One Shot Engine.”

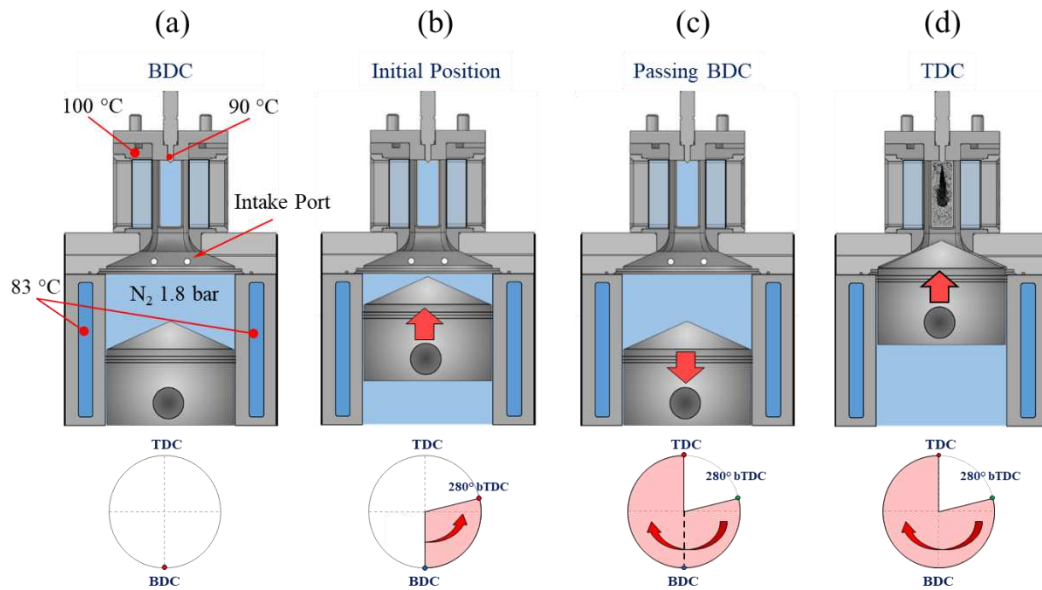


Figure 28 Scheme of NOSE operating conditions: (a) position for setting initial condition at BDC, (b) initial position of the velocity feedback control mode at 280 CAD before TDC, (c) piston moves passing BDC and (d) target condition around TDC for Spray-A condition (60 bar, 900 K and 22.8 kg/m^3).

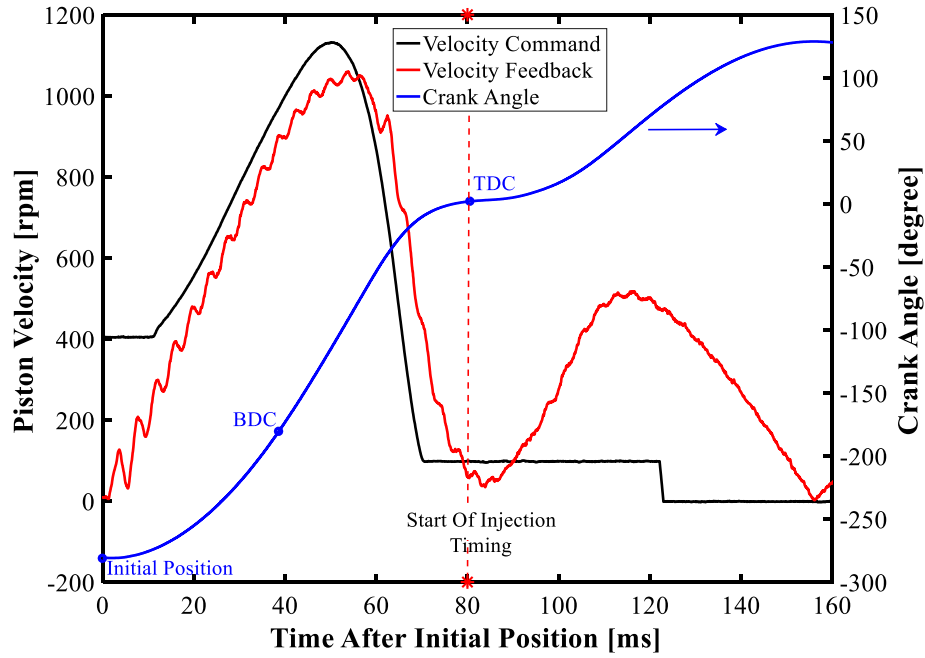


Figure 29 NOSE operating conditions: the feedback control command to control the piston movement as a function of time after the initial position (280 CAD before TDC).

As plotted in **Figure 30** (a), the cylinder pressure reaches the value of 60 bar, the ambient temperature 900 K and the density, 22.8 kg/m^3 near the TDC as standard Spray-A condition requirements. **Figure 30** (b) shows the very good accuracy ($> 99\%$) of these values around TDC for 10 repetitive tests, certifying that the thermodynamic ambient conditions are well controlled with NOSE and that injection can be done in the TDC period. These results confirm that NOSE can provide the wide range of standard Spray-A conditions and ensure stable ambient conditions.

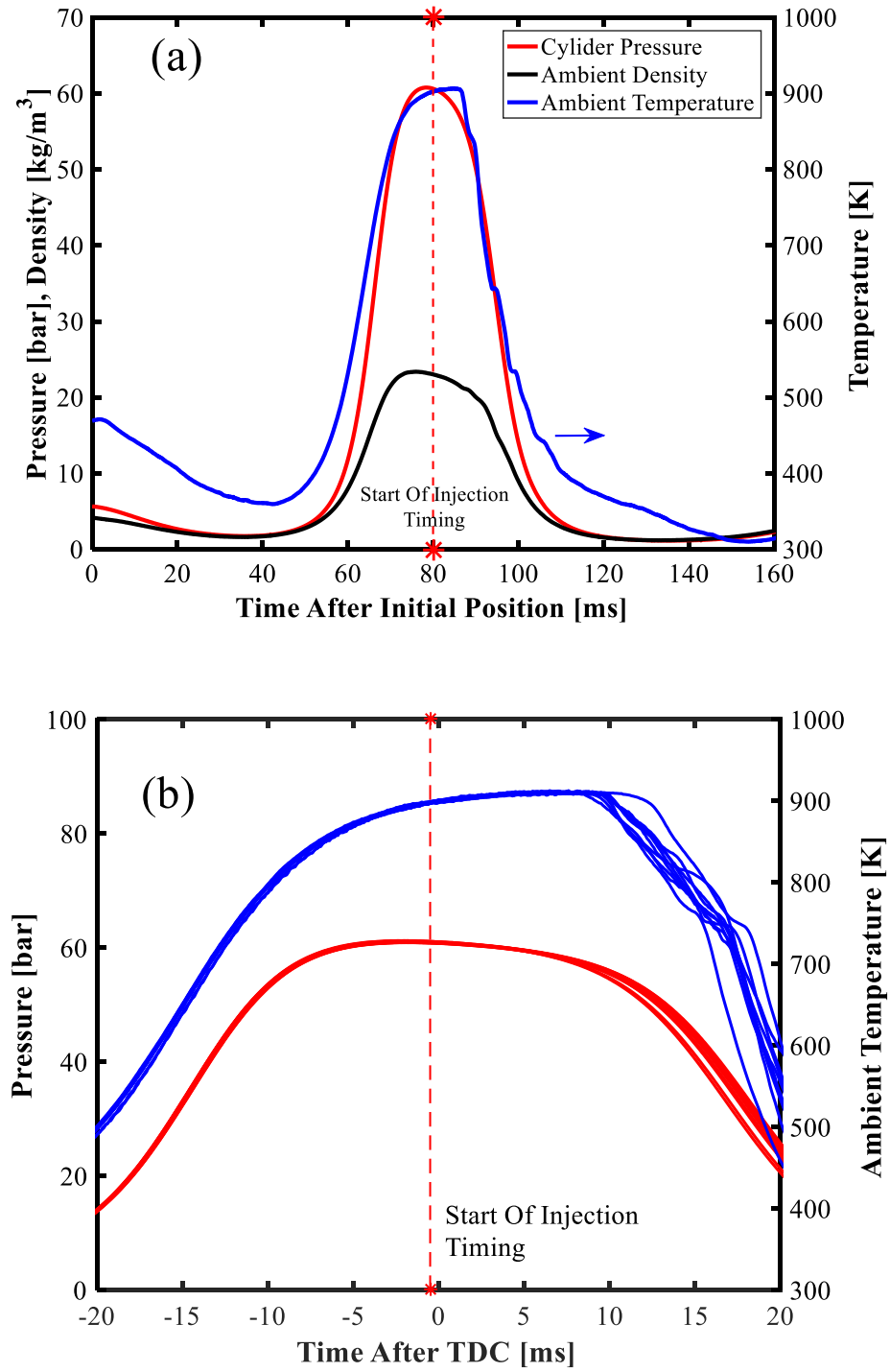


Figure 30 Thermodynamic conditions of NOSE: (a) an example of pressure, temperature and temporal density evolution (b) pressure and temperature evolutions from -20 to 20 ms after TDC for 10 repetitive tests.

2.6 Ambient Gas Characterization for ECN Spray-A

2.6.1 Ambient Temperature Characterization

To confirm the quality of the thermodynamics conditions obtained by NOSE, the ambient gas temperature around TDC was characterized by a fine wire thermocouple. This temperature represents the local ambient temperature which can affect either the macroscopic spray development or combustion parameters [35]. Although the fine wire thermocouple has a fast temporal response, heat transfer between the bead thermocouple, hot gases and cylinder walls affect the accuracy of the measured gas temperature. The gas temperature (T_{ms}) has therefore to be corrected by applying the energy balance equation at the location of the bead thermocouple and also Dupont's correlation [67] as described in **Eq. 21**.

$$T_{cor} = T_{ms} + \left(\frac{\rho_w \cdot C_w \cdot d_b^2 [1 + 0.5(d_w^2/d_b^2)]}{6Nu_b \cdot k} \right) \frac{dT_{ms}}{dt} + \frac{\epsilon\sigma}{h} (T_{ms}^4 - T_w^4) \quad \text{Eq. 21}$$

where T_w is the wall or cooling temperature [K], ϵ the emissivity of the bead thermocouple [-], σ the Stefan-Boltzmann constant, 5.6703×10^{-8} [W.m⁻².K⁻⁴] and h the heat transfer coefficient [W.m⁻².K⁻¹]. For the thermocouples, subscript w denotes the wire thermocouple, b the bead thermocouple, ρ the density of the thermocouple [kg.m⁻³], C_w the specific heat density of the thermocouple [J.kg⁻¹.K⁻¹], d the diameter of the wire and bead thermocouple [m], Nu the Nusselt number of the thermocouple (a spherical shape is assumed) [-] and k the thermal conductivity of gas [W.m⁻¹.K⁻¹]. For more details of description and derivation of **Eq. 21** is found in **Appendix B**.

The second term in **Eq. 21** presents the convective heat transfer between the thermocouple bead and hot gases inside the chamber, including the time constant of the thermocouple as shown in brackets. The time constant of thermocouple is the response time of the thermocouple to changes in temperature, which is calculated by the properties of the thermocouple bead and hot gases around the bead. In this work, Dupont's correlation was applied to determine the time constant as the bead shape is spherical. The last term presents the radiation heat transfer between the thermocouple bead and the surface of the chamber walls.

The conduction heat transfer of the wire can be neglected in this equation due to the small diameter of the thermocouple wire (wire diameter 13 μm). The temperature gradient throughout the wire is thus assumed to be uniform.

Four K-type fine-wire thermocouples (with wire and bead diameters of 13 μm and 39 μm , respectively) were implemented to measure the gas temperature at different spatial locations as schematized in **Figure 31**. The origin coordinate (0,0) represents the position of the injector tip. First, the four thermocouples were characterized in the centerline of the chamber along the spray axis, i.e., X-axis = 0 mm at different locations along the Y-axis (9.5, 29.5, 49.5 and 69.5 mm) for thermocouples No. 1, 2, 3 and 4, respectively, as shown in **Figure 31** (a). After that, to characterize other radial positions, all the thermocouples were moved in 5 mm steps along the X-axis to the last position at 15 mm. **Figure 31** (b) presents the real picture of temperature measurement at the centerline of the chamber, corresponding to the diagram in **Figure 31** (a). The 25 μm thermocouple was used as a reference to compare the effect of the thermocouple size on temperature measurement.

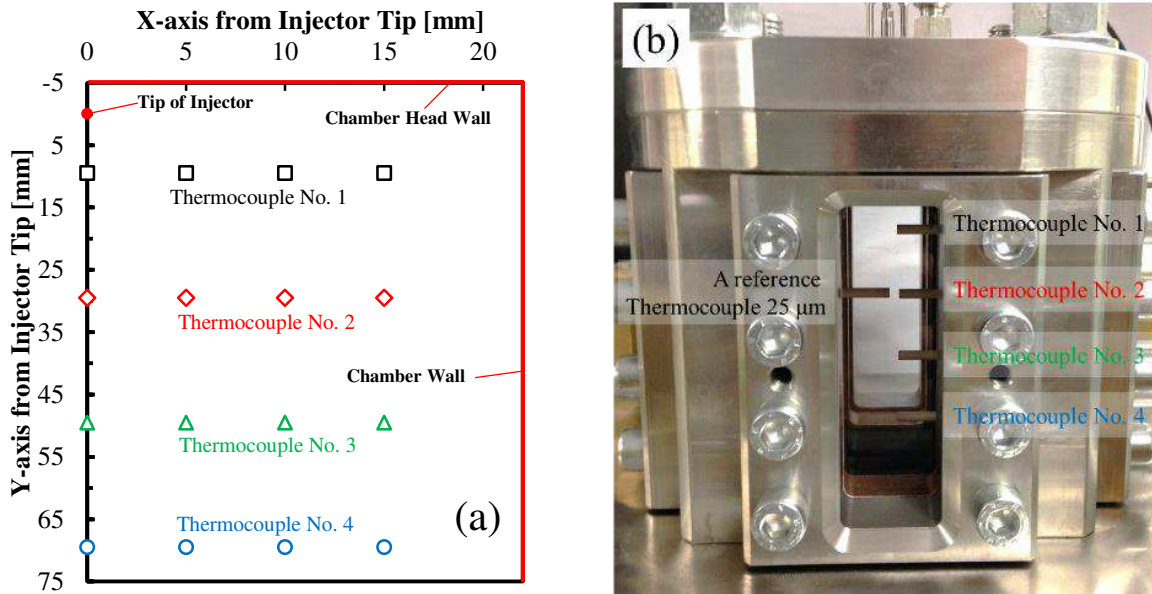


Figure 31 Spatial local positions of temperature measurement from four 13 μm fine-wire thermocouples: (a) schematic position of measurement and (b) the picture of measurement at the centerline of the chamber along the spray axis (X-axis = 0 mm).

In **Figure 32** (a), an example of ambient temperature evolution from Thermocouple No. 2 is plotted around TDC. The significant difference between the measured temperature (T_{ms}) and the corrected gas temperature (T_{cor}) can be explained as follows:

- Before TDC, T_{cor} is dominated by the convective heat transfer from hot gases to the bead of the thermocouple due to the strong temperature gradient.
- Around TDC, the piston velocity is lower, allowing sufficient time for sensitive thermocouple measurements, while the radiation between hot gas and bead dominates rather than convection. As a result, the temperature difference between T_{ms} and T_{cor} around 3-5 K can be observed.
- After TDC, convective heat transfer dominates again but from the bead thermocouple to gases so T_{cor} is lower than T_{ms} .

In **Figure 32** (b), the average evolution of the ambient temperature near TDC obtained from 10 tests is plotted with the standard deviation represented by the shaded-error bars. The low disparity confirms how ambient conditions can be controlled with the NOSE set-up:

- The pressure decreases slightly from 59.8 bar at TDC to 59.3 at 10 ms after TDC with 0.1% of variation.
- The measured temperature increases slightly from 885 to 900 K during 0-4 ms and remains at 900 K till 5 ms with 0.5% of variation. Then, it decreases slightly to 890 K at 10 ms with 1% of variation.
- The ambient gas density varies from 22.8 kg/m³ to 21.7 kg/m³ at 10 ms after TDC with 1.3% of variation.

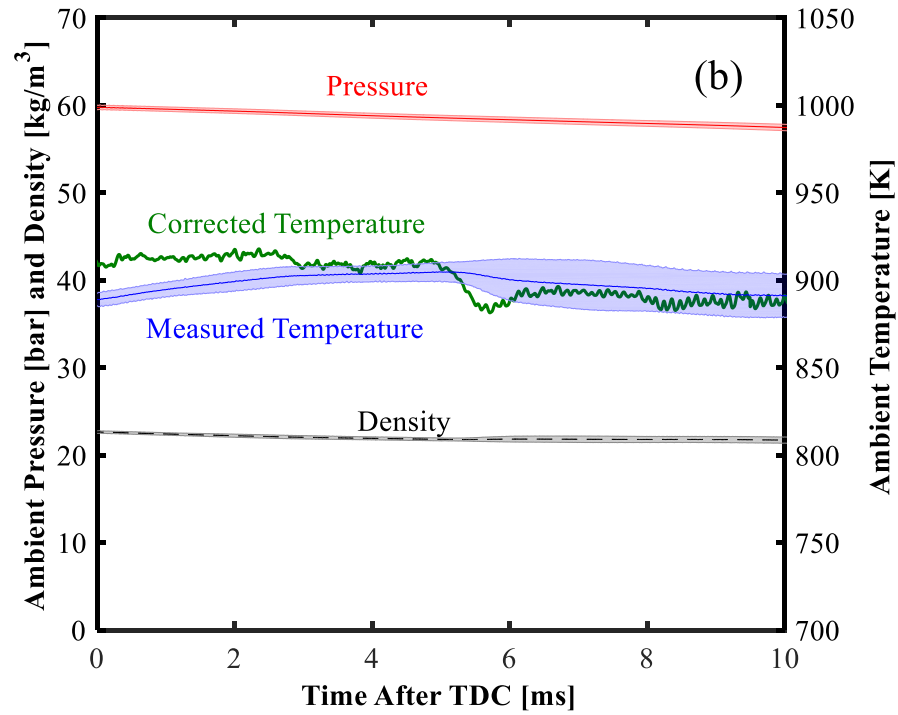
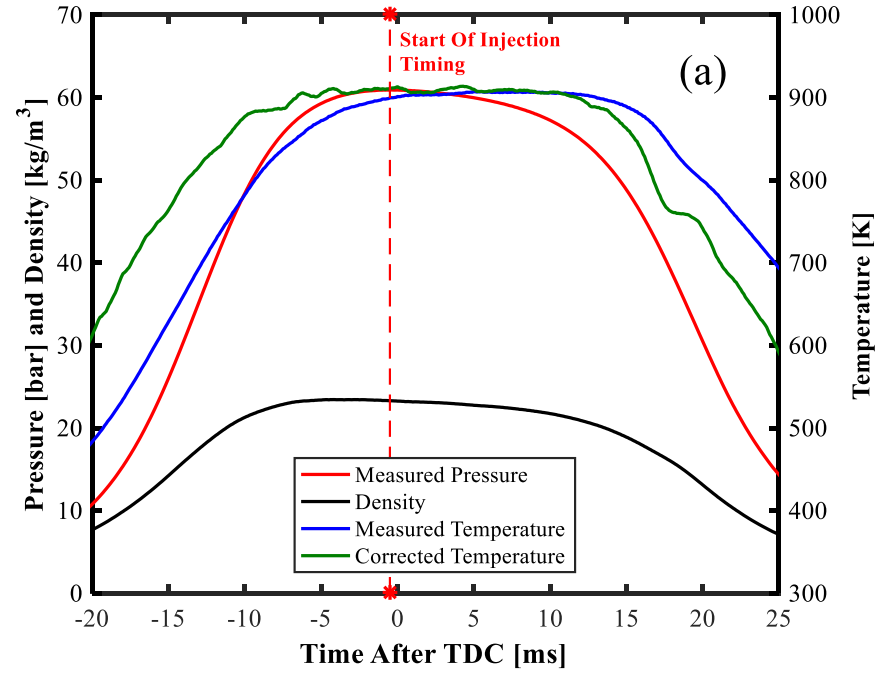


Figure 32 Characterizations of ambient conditions: (a) example of evolution of thermodynamic conditions around TDC, (b) average evolution of ambient conditions of the reactive condition at 900 K. The shaded-error bars represent the standard deviation of 10 measurements.

These results confirm that the NOSE set-up can be reached the standard condition for Spray-A during 10 ms after TDC. In **Figure 33**, the measurement of ambient gas temperature from the 4 thermocouples is plotted as a function of the X location (see diagram in **Figure 31** (a)), averaged over 5 ms after TDC. The temperature from the Thermocouple No. 1 is the highest due to its location closest to the top of the chamber wall, leading to higher heat transfer, while the lowest temperature is obtained downstream by Thermocouple No. 4. As presented by the mean temperature of 4 thermocouples (black line), the mean temperature slightly decreases along the radial location by 13 K. However, the average temperature over the spatial positions is 895 K with 0.8% of variation (7 K of STD).

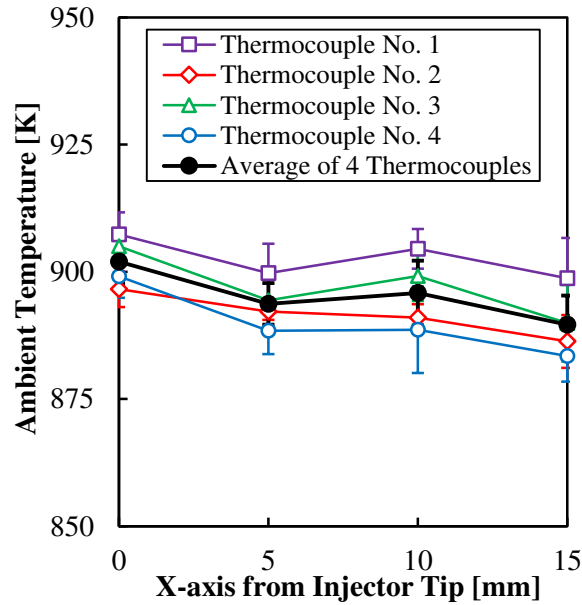


Figure 33 Evolution of average ambient temperature at different axial and radial locations for a TDC temperature of 900 K, 5 ms after TDC.

To reach the different target temperatures of 800 K and 850 K of the original Compression Ratio (CR) 15.0, the initial temperature must be adjusted from 83 °C to 33 °C and 55 °C for 800 K and 850 K, respectively, while the initial pressure is kept at around 1.8 bar for both temperatures. The temperature measurements of 800 K and 850 K for CR 15.0 are plotted as a function of distance from the injector tip to downstream (Y-axis on **Figure 31** (a)) in **Figure 34** (solid line with closed symbols). It can be seen that the two ambient temperatures are

inhomogeneous as the local high temperature at the position close to the injector tip (9.5 mm) is around 832 K for 800 K and 862 K for 850 K. This can be explained by the high temperature gradient between the initial temperature in the cylinder at BDC (33 and 55 °C for 800 and 850 K) and the heating chamber temperature (controlled at 100 °C), leading to gas inhomogeneity during the compression stroke because it has short residual to transform and distribute the lower temperature to the higher temperature inside the chamber, especially at the chamber head close to the injector tip.

As the system is based on an adiabatic compression process, to obtain a homogeneous ambient temperature of 800 K and 850 K, the CR has to be adjusted as well as the initial conditions (pressure and temperature) following **Eq. 22**:

$$T_{TDC} = T_{BDC} \left(\frac{V_{BDC}}{V_{TDC}} \right)^{\gamma-1} = T_{BDC} CR^{\gamma-1} \quad \text{Eq. 22}$$

where T , V and γ are the temperature, volume and ratio of specific heat capacities. The subscript TDC is the top-dead center, representing the target condition, while BDC is the bottom-dead center which represents the initial condition. By adjusting the thickness of the metallic plate at the piston base (see **Figure 26** (b) and more details in an **Appendix B.4**), CR is modified due to changing the volumetric ratio of compression (V_{BDC}/V_{TDC}) as seen in **Eq. 22**. The original thickness of the metallic plate was reduced from 4 mm to 3.0, 2.5, 2.0, 1.5 and 1.0 mm, CRs of 14.0, 13.5, 13.0, 12.7 and 12.3, can be obtained respectively. Therefore, to obtain a homogeneous ambient temperature of 800 K and 850 K, the metallic plates were installed in NOSE and a fine-wire thermocouples were used to characterize the ambient temperature at the chamber centerline along the Y-axis (Thermocouple No.2, as seen in **Figure 31**). It was found that the suitable CR for 800 K and 850 K were 12.3 and 13.5, respectively. **Table 9** summarizes the initial conditions at BDC and the CR, related to the ambient temperature condition required at the end of the compression stroke and the ambient density 22.8 kg/m³. In **Figure 34**, the measured (solid line with open symbols) and the corrected (dot-line with open symbols) ambient temperature evolutions obtained for 800 K, 850 K and 900 K as target conditions are plotted in the case of CRs of 12.3 and 13.5 for 800 K and 850 K, respectively. Adjusting the CR allows a better homogeneity of the ambient temperature due to the increase in the initial gas temperature in the cylinder at TDC (59 and 70 °C for 800 K and 850 K). Therefore, the gradient temperature

between the initial and heating chamber temperature are reduced. As a result, the measured and the corrected (**Eq. 21**) temperatures are around the target value with a low distribution. For this reason, it can be confirmed that the NOSE set up can reach the target conditions with a good spatial homogeneity of the ambient temperature for 800 and 850 K, following ECN requirements.

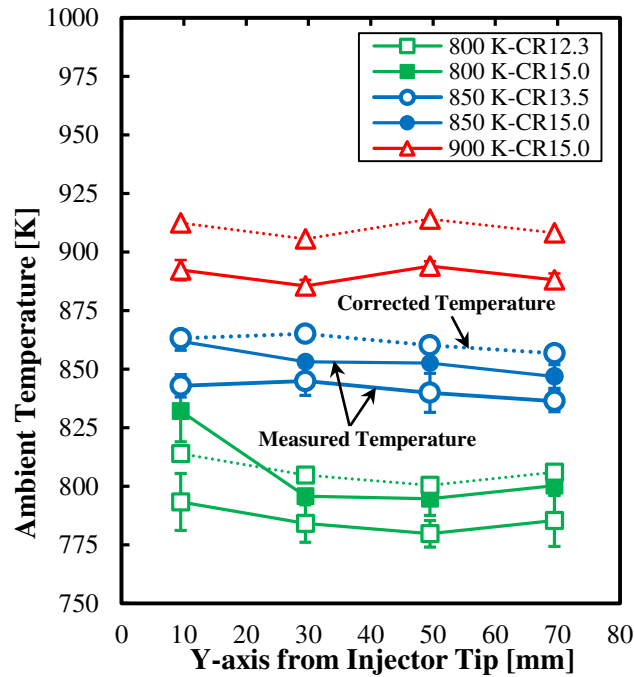


Figure 34 Measured and corrected ambient temperature at TDC for 3 target temperature conditions. The error bar presents the standard deviation of 10 repetitive tests.

Table 9 Ambient conditions required to reach target ambient temperature conditions 800, 850 and 900 K.

Ambient Condition	CR [-]	Initial Condition at BDC		Target ambient Condition at TDC		
		Pressure [bar]	Temperature [K]	Pressure [bar]	Temperature [K]	Density [kg/m ³]
Non-Reactive (Pure N ₂)	12.3	2.1	59	54.2	800	22.8
	13.5	2.0	70	59.0	850	22.8
	15.0	1.8	83	60.9	900	22.8
Reactive (15%v O ₂ and 85%v N ₂)	12.3	1.98	59	52.5	800	22.8
	13.5	1.84	70	55.9	850	22.8
	15.0	1.81	83	59.2	900	22.8

2.6.2 Ambient Gas Velocity Characterization

The original geometry of the piston head and the combustion chamber were simulated using the open-source CFD library OpenFOAM, thanks to a collaboration with Vrije University in Brussels [115]. A 2D wall-resolved axisymmetric highly-refined mesh was developed (218,000 cells at BDC and 112,000 cells at TDC). An analytical piston trajectory deduced from the real stroke was considered. The RANS equations were solved using the $k-\omega$ -SST turbulence model. The results indicate that the original piston geometry induced a squish motion at the corner of the chamber, leading to a high local average velocity as shown in **Figure 35** (a). Some alternatives to overcome this limitation were studied such as varying the angle of the piston head and/or gap distance. But even if reducing the piston head angle and increasing the gap distance can eliminate squish and hence reduce the gas velocity itself inside the chamber, they both affect the volume of the chamber and therefore the cylinder pressure and compression ratio. The simulation predicted that a piston head angle of 23° with the original gap distance could provide satisfactory conditions, i.e., an ambient gas velocity below 1 m/s while maintaining cylinder pressure as shown in **Figure 35** (b).

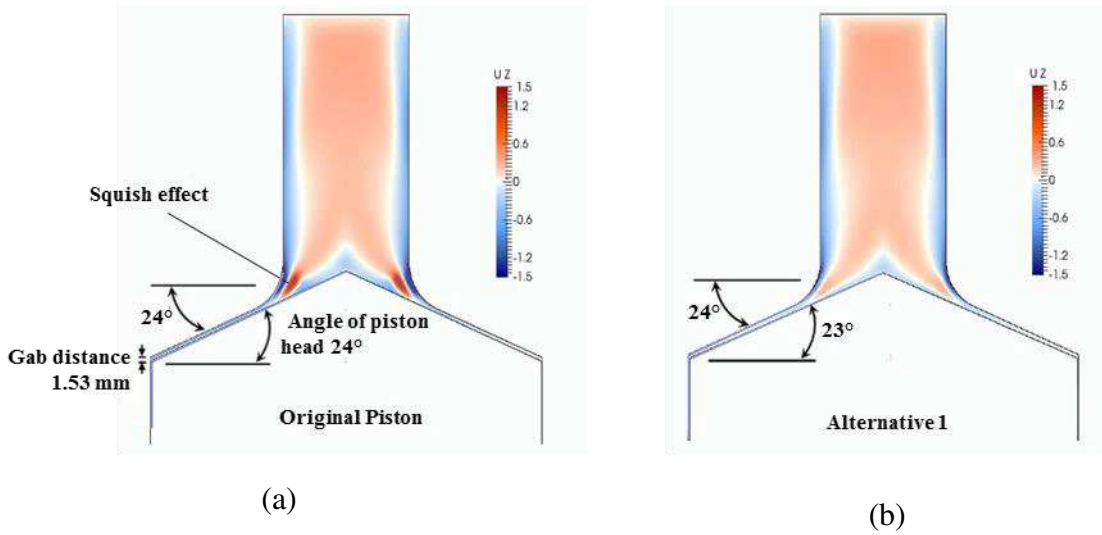
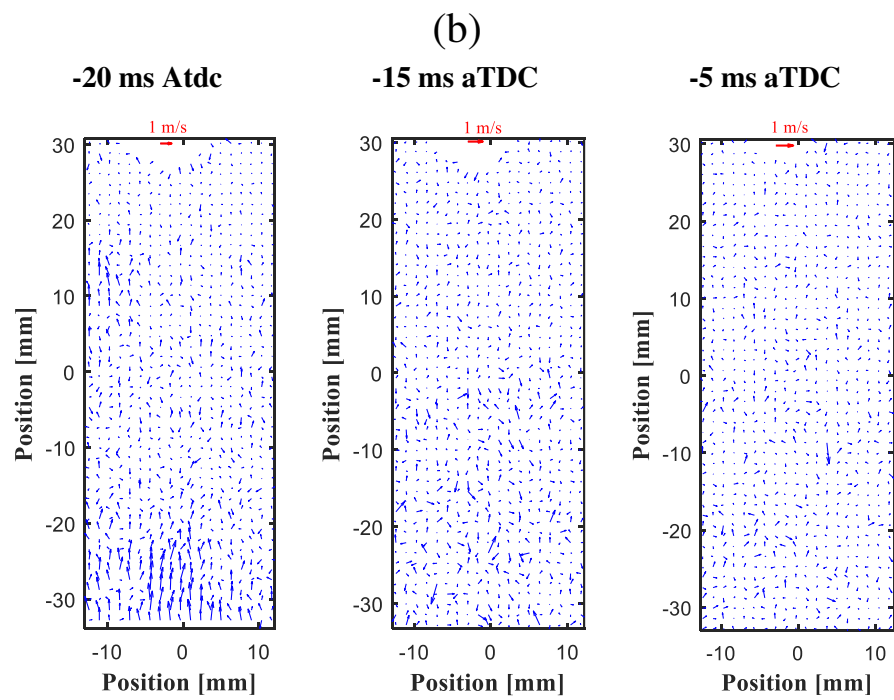
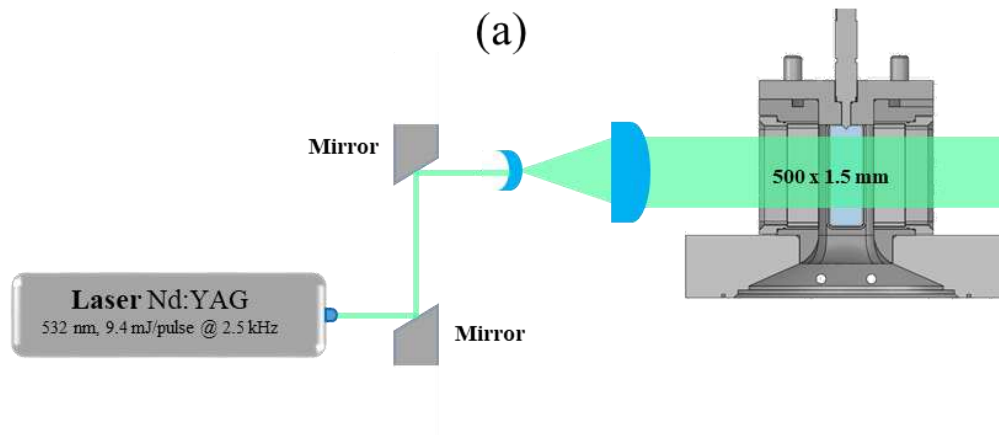


Figure 35 Velocity field from simulation with piston head angles of (a) 24° and (b) 23° .

To verify whether, with the NOSE set-up, the aerodynamics inside the combustion chamber was very low, High Speed PIV was installed by implementing a laser sheet from Dual Hawk HP (9.4 mJ/pulse, 532 nm at 2.5 kHz) and recording scattering images of silicon oil seeding (Phantom, resolution of 896×800 pix²), with an area of interest 24×70 mm², as presented in **Figure 36** (a). The velocity fields were calculated using DAVIS software. A masking technique and image correction of post-processing image was used to avoid light reflections on the metallic and glass parts.

Figure 36 (b) presents examples of the instantaneous velocity fields obtained at different crank angle degrees from -20 to 15 ms around TDC at 800 K. They confirm the absence of convection motion in the area of interest. Indeed, during the compression stroke, due to the compression of the gases by the piston, the vectors are oriented from downstream to upstream (especially at 20 ms before TDC). At the end of the compression stroke, around TDC, the gas velocity clearly reaches its lowest value and the small energy content is totally dissipated. During the expansion stroke, the piston moves down to BDC and the vector fields start to be oriented to downstream from 15 ms after TDC. **Figure 36** (c) presents the average evolution of the gas velocity vector around TDC, in the field of view. It can be seen that the average gas velocity around TDC is lower than before the compression and after the expansion stroke and remains below 0.1 m/s for all ambient temperatures. In the case of 800 K, the average velocity is higher before and after TDC due to the piston speed difference. These measurements confirmed that NOSE achieves the requirement of meets ECN conditions: the ambient gas is in a near-quiescent condition, less than 0.2 m/s during -0.5 to 0.5 ms around TDC. So, the 0.5 ms (or 0.5 CAD) before TDC will be considered to be the start of injection (SOI) timing for all experiments in this study.



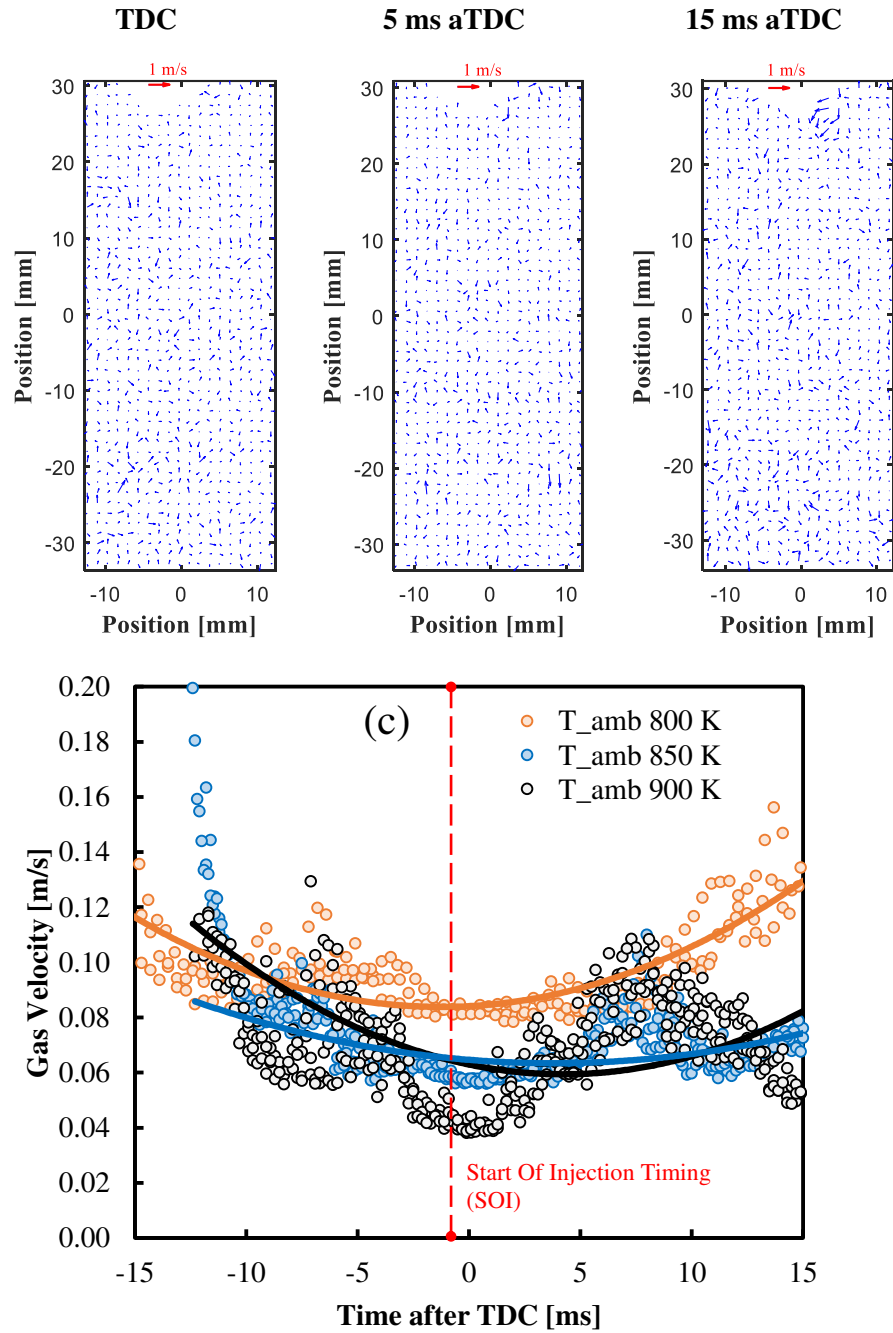


Figure 36 PIV results: (a) PIV set-up, (b) instantaneous gas velocity fields at ambient temperature 800 K. The white semicircle at the top of the image represents the position of the injector tip, masked to avoid light reflections in post-processing. (c) temporal evolution of average gas velocity around TDC for 3 ambient temperatures. The thick line represents the polynomial curve fitting of the data.

2.7 Injection System

The entire fuel injection system comprising the common-rail, the injector and the high-pressure tube was provided by IFPen, to validate ECN Spray-A requirements. The common-rail volume is 22 cm³ with a total length of 28 cm, the distance from the injector inlet to the common-rail is set to 24 cm. The fuel pressure sensor is located 7 cm from the injector inlet (or 24 cm from the nozzle), as seen in **Table 10**. The injection pressure is measured by a high response piezo-electric pressure sensor (KISTLER Type 6533A11) with a charge amplifier (KISTLER Type 4618A2). A high-pressure pneumatic pump (MAXIMATOR M189 DVE-HD), driven with compressed air at 7 bar maintained the pressure around 1500 bar (± 20 bar) before the start of injection (SOI), as seen in **Figure 37**.

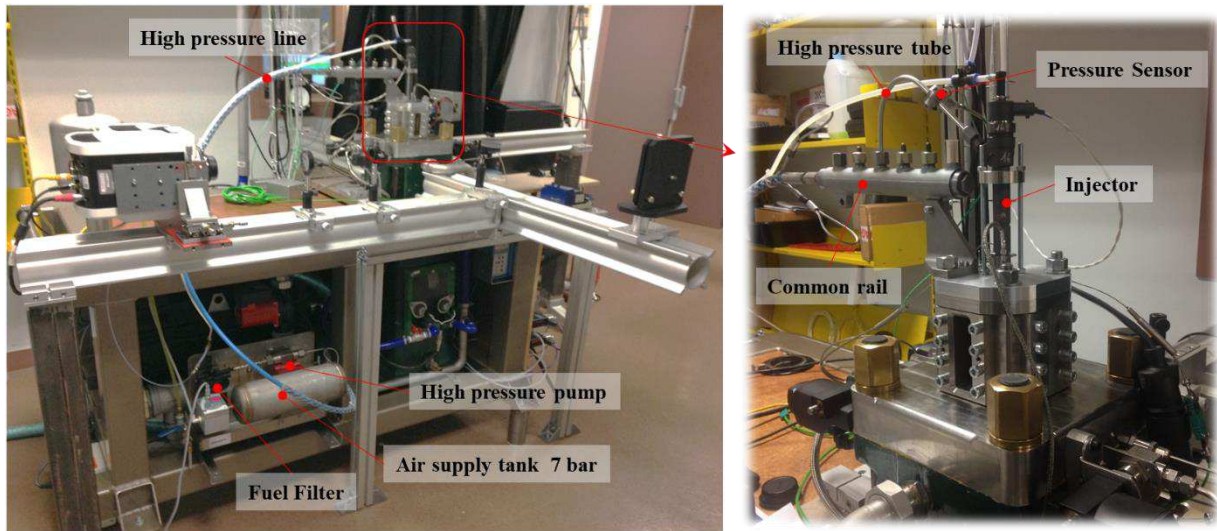


Figure 37 Details of injection system set-up for NOSE: an overview picture (left) and a zoom of NOSE chamber (right).

The injector is located at the center of the chamber head and connected to the common-rail by a high-pressure tube, as in **Figure 37** (right). By calibrating with a dummy injector, in which a thermocouple is placed inside the injector sac, the chamber casing was heated by four-heaters up to 100 °C to achieve 90 °C inside the injector sac. Two K-type thermocouples were placed inside the chamber to measure the gas temperature and in the metal structure near the

injector itself to know the fuel injection temperature as seen in **Figure 38**. It should be noted that this gas temperature is measured by the low sensitivity K-type thermocouple in order to check the initial ambient gas temperature in each test. For more details, other schemes and pictures of the combustion chamber are in **Appendix A.1**.

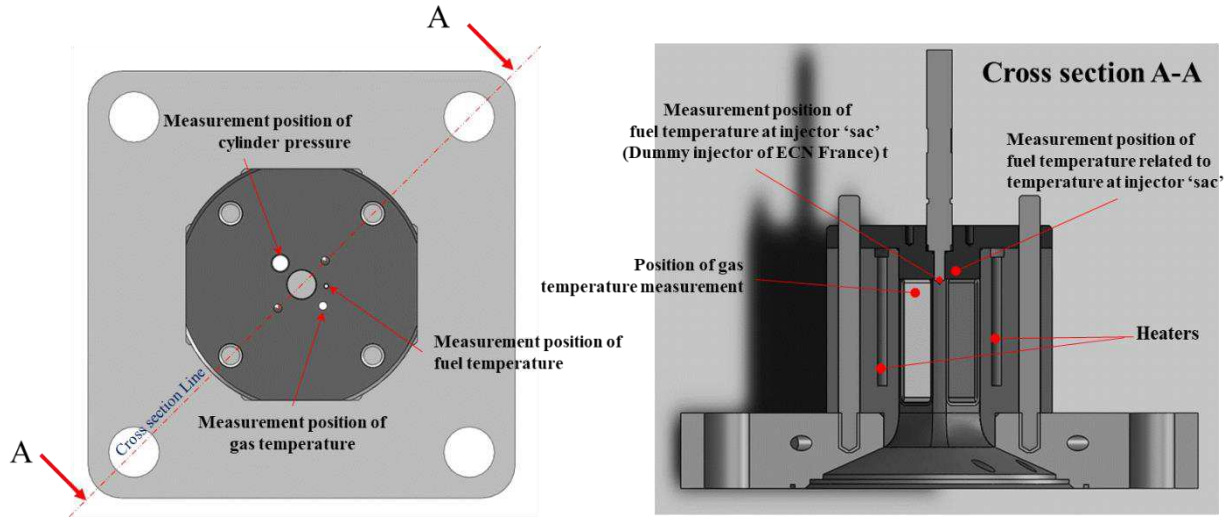


Figure 38 The local positions of thermocouples for the ambient gas and fuel temperatures measurements: (a) top-view of NOSE chamber, (b) cross-section A-A.

Three different injectors with the same nominal orifice outlet diameter were used in this work to validate NOSE: the main difference is that injectors A and B were ‘less’ pre-used than injector C and studied during ECN France project by IFPen before. The injector characteristics are presented in **Table 10**.

Table 10 Specifications of injectors [108].

Specifications	Details
Injector body type	Bosch CR 2.16 for A and B
Nozzle type	Single hole, axially oriented
Nozzle outlet diameter	90 μm (nominal)
Measured outlet diameter:	
Injector A	89.7 μm
Injector B	88.5 μm
Injector C (pre-used longer)	90.2 μm
Nozzle shaping	Hydro-eroded

Specifications	Details
Nozzle k-factor	1.5
Mini-sac volume	0.2 mm ³
Discharge coefficient (Cd)	0.86

The outlet diameter of injectors A and B, is slightly different from the nominal value (0.3%). The diameter of injector B is closer to the nominal value even if it had been previously more used in different vessels, especially in the pre-burn combustion chamber and also with other fuels (such as alcohol fuels, n-heptane, gasoline and n-dodecane mixed with Cerium) as reported in [116], [117], [118], [119], [120]. **Figure 39** presents the Scanning Electronic Microscopy of the injectors. Injector C is higher rough, larger hole size and shape due to corrosive of longer pre-used.

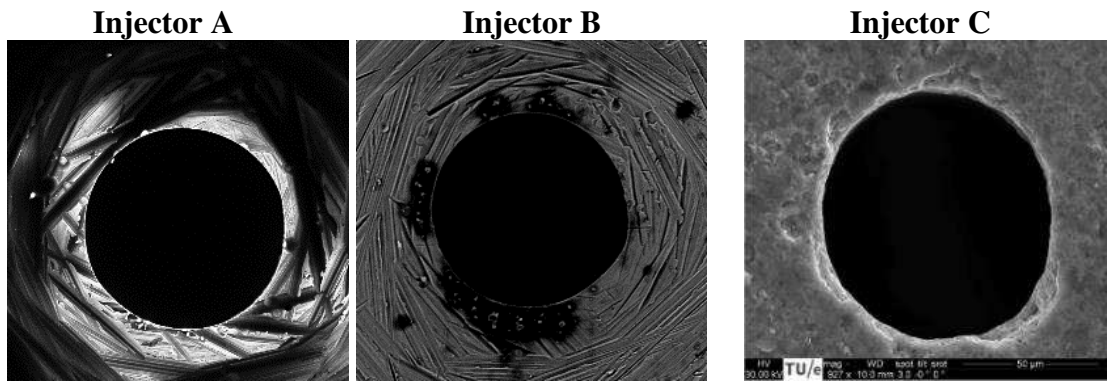


Figure 39 Scanning Electron Microscope (SEM) images of injectors A and B before testing in NOSE (*Courtesy of IFPen*) and of injector C after extended pre-use (*Courtesy of TU/e*).

2.8 Conclusion

A new experimental set-up was designed and set-up in order to provide Spray-A conditions defined by ECN. The results of thermodynamic measurement and characterization are summarized below:

- 1) The measurements of ambient thermodynamic conditions (pressure and temperature) demonstrate that NOSE can reach the standard Spray-A condition of ECN (near 60

bar, 900 K and 22.8 kg/m³) with a homogeneous ambient temperature field as indicated by the spatial distribution of temperature measurements.

- 2) By adapting the compression ratio of the NOSE, the homogeneity of the ambient temperature can be obtained for different values (800 K, 850 K and 900 K).
- 3) The reduction of the piston head angle and the increase in the gap distance can eliminate squish and reduce the gas velocity inside the chamber. The simulated results and PIV measurements confirm that the ambient gas velocity is below 1 m/s as required by ECN Spray-A specifications.

CHAPTER 3

VALIDATION OF THE NEW ONE SHOT ENGINE (NOSE) ON ECN SPRAY-A

3.1 Introduction

In the previous chapter, the details of the NOSE set-up and operating conditions to meet the ECN Spray-A standard conditions were fully described. In this chapter, the spray and combustion characteristics of the three injectors (A, B and C) are investigated in NOSE at HPHT conditions defined as standard Spray-A operating conditions of ECN, as reminded in **Table 11**. The optical techniques, post-processing and criteria to determine different characteristic parameters recommended by ECN network are set-up: the liquid and vapor spray parameters are characterized by Diffused-Back Illumination and Schlieren techniques in non-reactive condition and the lift-off length and ignition delay by OH* chemiluminescence in reactive condition. All the experimental results are presented and compared to the IFPen results and ECN database.

The experimental set-ups described in this chapter are not only used to validate the experimental results of three injectors with ECN database but also to study the effect of fuel properties from different alcohols and ABE blends on spray and combustion parameters in **Chapter 4** and **Chapter 5**.

Table 11 Main specifications for Spray-A ambient conditions of ECN (<https://ecn.sandia.gov/>).

Parameter	Value
Ambient gas temperature	800, 850, 900 K
Ambient gas pressure	near 60 bar
Ambient gas density	22.8 kg/m ³
Ambient gas oxygen	Pure N ₂ 15% O ₂ and 85% N ₂
Non-reactive condition	
Reactive condition	

Parameter	Value
Ambient gas velocity	Near-quiescent, less than 1 m/s
Injection Pressure	1500 bar
Injection Duration	1.5 ms
Fuel	n-Dodecane
Fuel temperature	363 K

To investigate the effect of the homogeneity of the ambient temperature on the spray and combustion parameters, these three injectors were tested but not for all cases. Each configuration and measurement associated to each injector are summarized in **Table 12** for different average ambient temperatures (800, 850 and 900 K), obtained as described previously (**Chapter 2**) by adapting the compression ratio (12.3, 13.5 and 15, respectively). Identical conditions were also used for injectors A and C in order to compare them. Moreover, the results for injectors A and B are compared to those obtained by IFPen, in the Pre-combustion Chamber. It should be noted that only the injector C was used to study the effect of fuel properties of alcohol and ABE blends on spray and combustion parameters in **Chapter 4** and **Chapter 5**.

Table 12 Different conditions used to characterize each injector (MFR=mass flow rate, LL=liquid penetration length, S= vapor penetration length, ID = ignition delay, LOL=lift-off length).

Injector	CR	Ambient Condition	Data	IFPen Data
Injector A	12.3, 13.5 and 15 (for 800, 850 and 900 K)	Homogeneous temperature	▪ MFR ▪ LL, S ▪ ID, LOL	Available
Injector B	15.0	Homogeneous at 900 K Inhomogeneous at 800 and 850 K	▪ MFR ▪ LL, S ▪ ID, LOL	Available
Injector C	12.3, 13.5 and 15 (for 800, 850 and 900 K)	Homogeneous for all conditions	▪ MFR ▪ LL, S ▪ ID, LOL	Unavailable

3.2 Mass Flow Rate Measurement

The measurement of fuel MFR provides the information about the injection rate profile, the total mass injection, the start and end hydraulic delay of injection and discharge coefficient (Cd). Generally, there are two basic principles for the mass flow rate measurement, i.e. Zuech and Bosh method. The Zuech method is based on the measurement of the increasing pressure a constant volume chamber after fuel injected into the constant chamber due to increasing of mass fuel inside the chamber. Therefore, the buck modulus of fuel (K) and the derivative of the constant volume chamber pressure ($\frac{dP_f}{dt}$) produced the rate of injection. The governing equation for Zuech method is presented in **Eq. 23**.

$$\dot{m} = \frac{dm}{dt} = \rho_f \cdot \frac{V}{K} \cdot \frac{dP_f}{dt} \quad \text{Eq. 23}$$

where V is a chamber volume and ρ_f is a fuel density.

For Bosch method, the mass flow rate is measured from the pressure wave, produced by an injector when it injects into a length of compressible fuel [39]. The determination is based on the relationship between pressure and velocity of a transient in one-dimensional fluid flow in **Eq. 24**, combined with the mass flow rate equation by **Eq. 25**. Finally, the mass flow rate of the Bosch method can be obtained in **Eq. 26** [121]:

$$P_f = v \cdot \rho_f \cdot U \quad \text{Eq. 24}$$

$$\dot{m} = \rho_f \cdot A_c \cdot U \quad \text{Eq. 25}$$

$$\dot{m} = \frac{A_c}{v} \cdot P_f \quad \text{Eq. 26}$$

where P_f , v , ρ_f and U are a pressure, speed of sound in fluid, fuel density and flow velocity, respectively. A_c is the cross sectional area of the tube.

In this study, an IAV GmbH® Injection Rate Analyzer (model K-025-50) was used, based on the Bosch method [39]. As presented in **Figure 40**, a piezoelectric sensor installed downstream of the injector nozzle detects the dynamic pressure wave (P_f), proportional to the

injection rate as shown by **Eq. 26**. The fuel back-pressure (P_b) is generated by nitrogen supply acting on a piston and adjusted by a constant-pressure valve. A throttling orifice adjusts the amplitude of the pressure wave reflections at the end of the duct [58]. The mass flow was measured with a temporal resolution of 10 μ s with a measurement accuracy of ± 0.2 mg/stroke or approximately $\pm 1\%$ (at 20 mg/stroke). The fuel injection pressure (P_{inj}) is generated by a high-pressure pump, driven with the compressor air at 1 bar (Maximator M189 Dve-Hd) and controlled by using LabView program to maintain it around 1500 bar (± 20 bar). The feedback injection pressure is measured by a piezo-electric pressure sensor (Kistler Type 6533A11) with a Kistler (Type 4618A2) charge amplifier. According to the ECN Spray-A conditions, the backpressure of 60 bar and the duration of injection command of 1.5 ms were set for all experiments to measure the MFR for n-Dodecane and all blends. The testing conditions to measure MFR are summarized in **Table 13**.

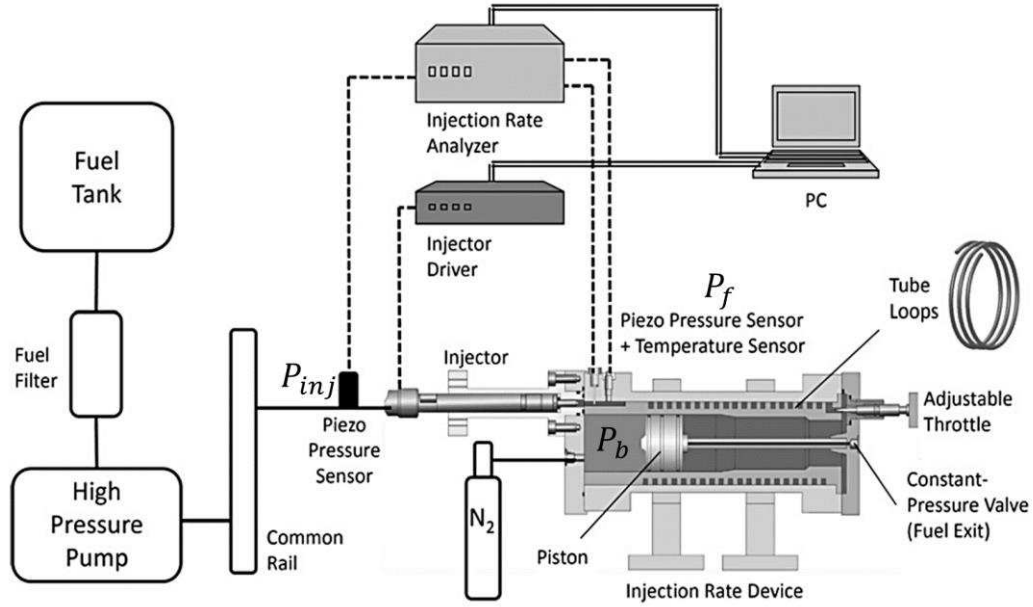


Figure 40 Mass Flow Rate experimental setup (from IAV GmbH® technical specification) [58].

Table 13 Testing condition of the mass flow rate.

Parameter	Value
Injection pressure	1500 bar (± 20 bar)
Back-pressure	60 bar

Parameter	Value
Injection temperature	20 °C (± 2 °C)
Injection duration (Command)	1.5 ms
Number of tests	3 tests/fuel
Number of injections	20 injections/test
Fuel type	n-Do100 (reference fuel) Bu20, Bu40, Bu20Eth20, Eth20 ABE20, ABE40

Figure 41 presents the average MFR evolution as a function of time. First, the initial hydraulic delay is determined from this plot, as the time between the beginning of the injection current command and the first positive MFR value, while the end of hydraulic delay is defined as the end of the injector command to the time corresponding to 0 g/s of MFR. To avoid the transient period of the start and the end of injection, the mean of MFR between 2 and 3 ms (indicated by a green rectangle in **Figure 41**) is estimated as the best representation of a kind of ‘absolute value’ of MFR. The theoretical mass flow rate, $\dot{m}_{th}$ and the discharge coefficient, C_d are calculated from **Eq. 3** to **Eq. 4** in **Chapter 1**.

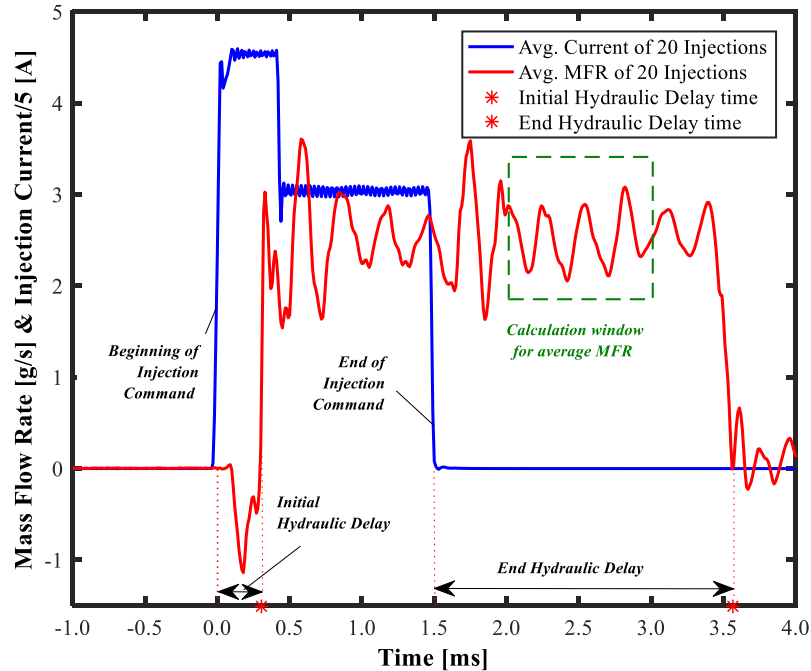


Figure 41 The temporal evolution of the mass flow rate averaged from 20 repetitive injections of n-dodecane.

3.3 Optical Set-Ups for Non-Reactive Condition

To obtain the simultaneous data between liquid and vapor spray penetrations in non-reactive condition, the Diffused Back-Illumination (DBI) and the high-speed Schlieren are set up in a cross direction, as presented in **Figure 42**. The details of each optical set-up are summarized in **Table 14**.

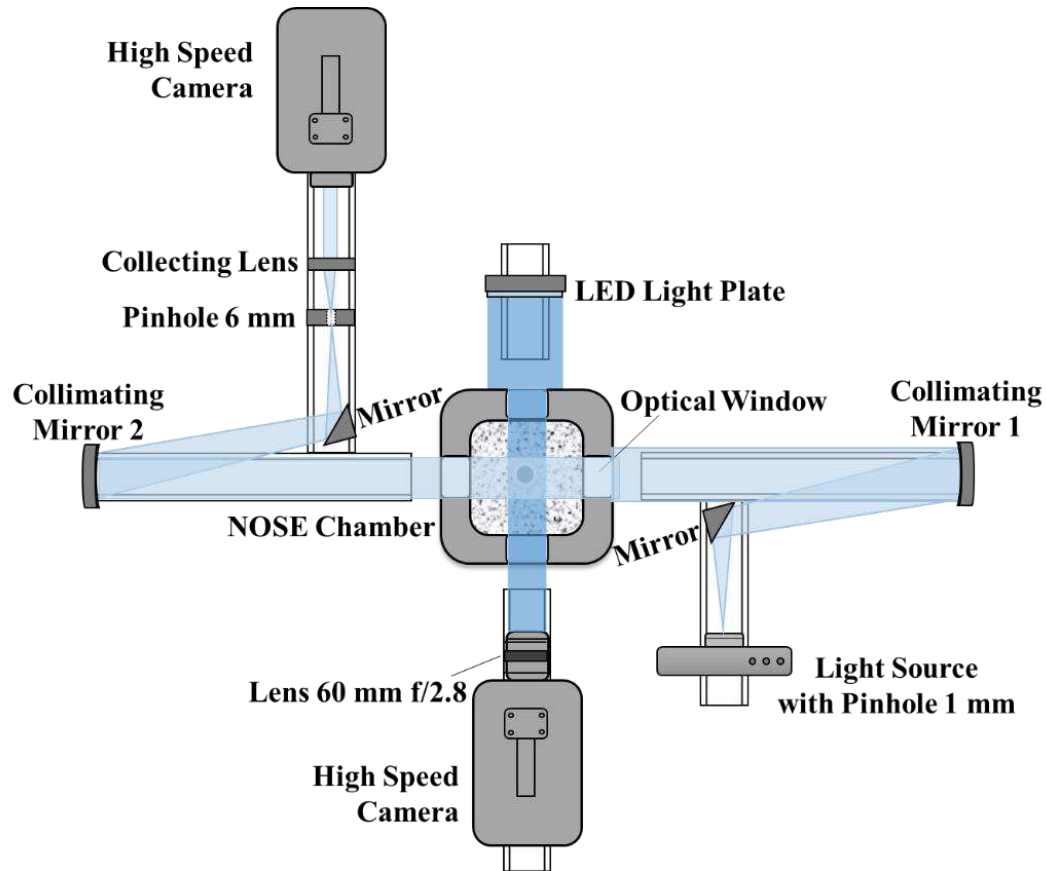


Figure 42 The scheme of optical techniques set-up for the non-reactive condition.

Table 14 Different optical set-ups used for non-reactive conditions and their details.

Optical Technique	Diffused Back-Illumination	Schlieren
Parameters	Liquid Penetration Length (LL)	Vapor Spray Penetration (S)
Light source	LED array (white) 100x100 mm	LED (white) 1 mm pinhole

Optical Technique	Diffused Back-Illumination	Schlieren
Mirrors	-	2 Parabolic Mirrors
Detector	Phantom-V1611	Phantom-V1611
Lens	60 mm f/2.8	Collecting lens: 30 cm of focal length with 6 mm pinhole
Filter	-	-
Frame speed	49 kHz	39 kHz
Exposure time	3 μ s	5 μ s
Image size (pix ²)	512 x 384	1024 x 400
Magnification	12 pix/mm	12.3 pix/mm

3.3.1 Diffused Back-Illumination for Liquid Length

To measure LL, the classical Mie scattering technique was widely used to characterize the liquid phase of diesel spray thanks to its simple implantation, as it needs only a light source to illuminate fuel droplets and a camera to capture the scattered light [46]. However, the direction of the light source, the calibration and the post-processing induce strong uncertainties on experimental results. The comparison between different measurements obtained from this technique inside four different chambers was intensively discussed by ECN [45]. One important conclusion is that even though same optical technique and post-processing criteria were used (see **Figure 43** (a)), the LL results are significantly different (see **Figure 43** (b)) mainly due to the importance of the illumination set-up on the scattering distribution. This result was also confirmed by Pickett et al. [122], as they investigated the same spray configuration with different illumination directions to assess set-up induced variations in Mie-scattering images.

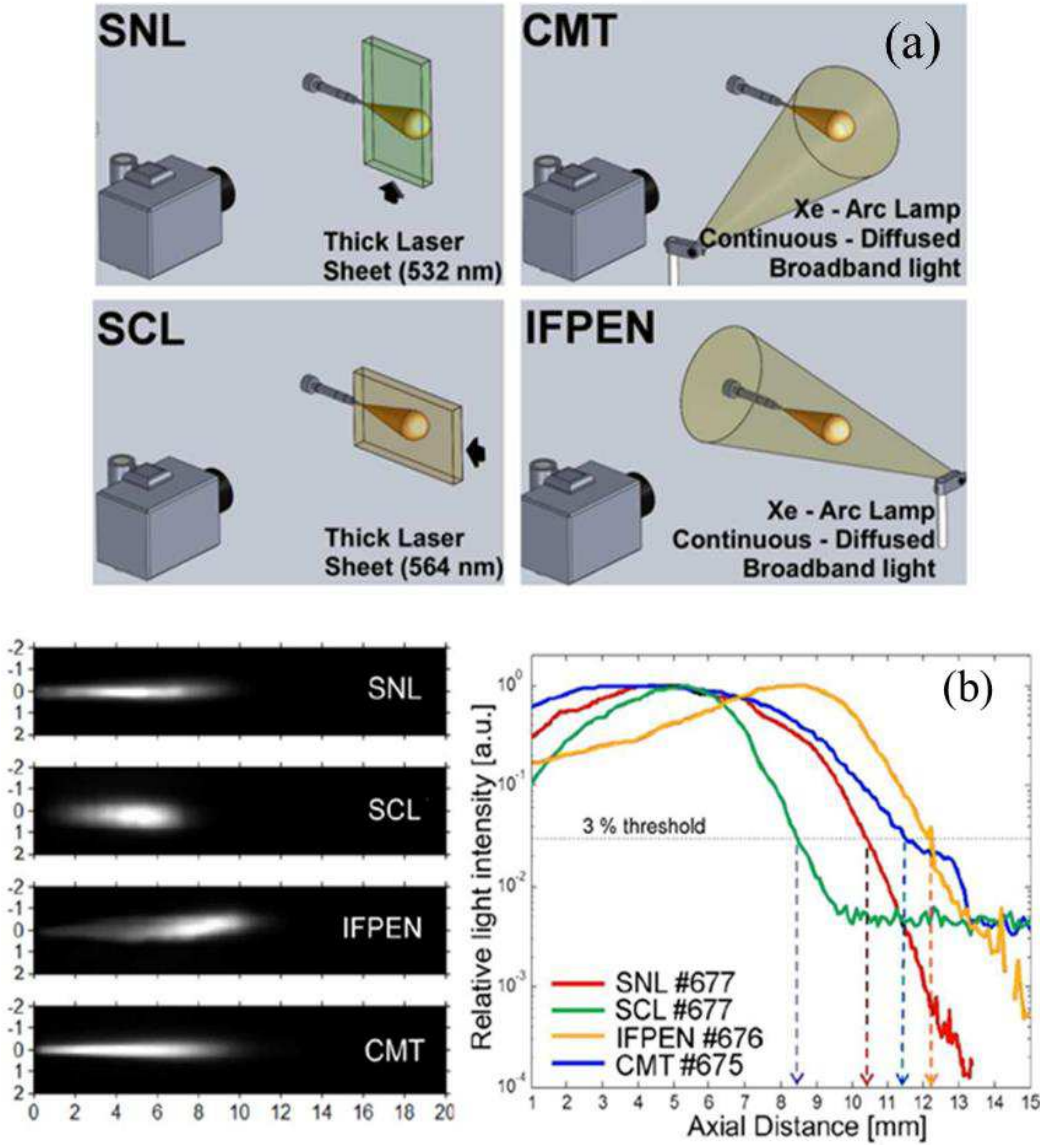


Figure 43 Effect of Mie scattering set-up on LL result: (a) scheme of the different set-ups, (b) examples of Mie scattering images and impact with the same criterion on the LL value [45].

Therefore, Diffused Back-Illumination (DBI) has been recommended by Engine Combustion Network (ECN) as the standard technique to measure LL [123]. The advantage of this technique is the use of an intensity reference from the incident illumination without the spray to determine the global extinction due to the liquid spray propagation. Moreover, DBI is cheaper as it consists of only a light source, like a LED and a camera, installed in the opposite side of the chamber, which favors facility-to-facility comparison [67], [122], [108]. However,

the main disadvantage of this technique is the possible effect of the beam steering near the liquid spray tip due to the refractive index gradient created by the vaporized fuel, as seen in **Figure 44** (a). Nevertheless, this effect can be mitigated by using the linear fit on the slope of decay of the light extinction profile along the spray axis, the distance where the linear fit line crosses the X-axis is determined as the LL of spray as seen the dashed line in as seen in **Figure 44** (b)-bottom [108], [124].

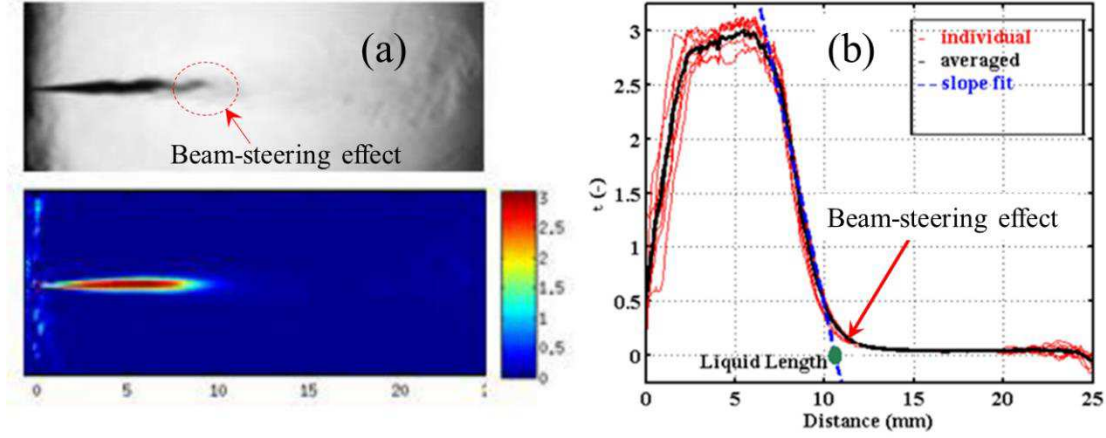


Figure 44 Determination of LL from DBI image: (a) single shot image (top) and normalized intensity of averaged image (bottom), (b) post-processing method to determine LL [124].

To validate our experimental results with ECN database, the DBI was implemented by using a continuous white-LED light of MORITEX model CV-FL-100X100W2 as the light source, as seen in **Figure 45**. It is operated at a constant voltage of 24 volts which is controlled by the LED controller model MORITEX CV-APS-DD-30-2. The LED is a square plate 100x100 mm² in size sufficiently large to cover the NOSE optical window. The homogeneous light was generated by an array of LED placed behind a diffuser plate. It was installed as close as possible to the chamber to be homogeneous and reduce the effect of beam steering on the resulting image [108]. But, a distance of 10 mm from the cylinder head was needed to avoid the heat transfer from the cylinder head (83 °C) and chamber (100 °C) as seen in **Figure 45** (bottom). The light intensity through the optical windows was collected by a high-speed camera (Phantom V1611), equipped with a NIKON 60 mm f/2.8 lens. The frame rate of 49 kHz, with an exposure time of

3 μ s and an image resolution of 512x512 μ m² present the most suitable values to capture high-quality images at a high-frequency rate.

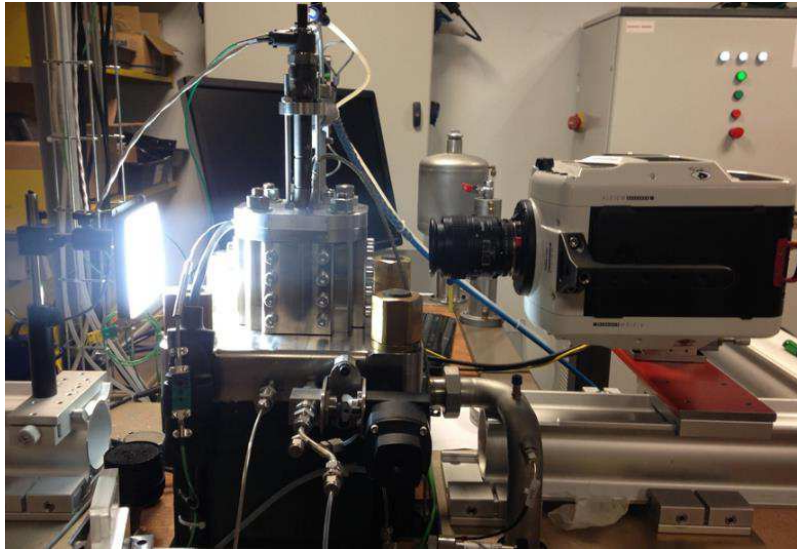
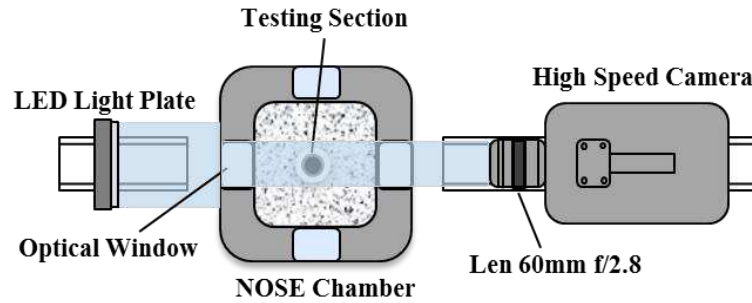


Figure 45 DBI set-up: Scheme (top) and real picture (bottom).

The DBI post-processing was based on the recommendation of the ECN. The average image light intensity, I_{avg} during the steady-state of injection (from 1.0 to 2.0 ms after SOI) was averaged to avoid the transient phases due to the start and end of injection (see **Figure 46** (a)-bottom). It is normalized by the background images, I_{bg} , obtained from the average of images before Start of Injection (SOI), as seen in **Figure 46** (a)-top. Then, the light extinction factor, τ , along the spray core was calculated using **Eq. 27** and presented in **Figure 46** (b)-top. To avoid the effect of the beam steering phenomenon, the distance where the linear fit line crosses the X-axis was determined as the LL of spray as shown in **Figure 46** (b)-bottom.

$$\tau(x, y) = -\log \left(\frac{I_{avg}(x, y)}{I_{bg}(x, y)} \right) \quad \text{Eq. 27}$$

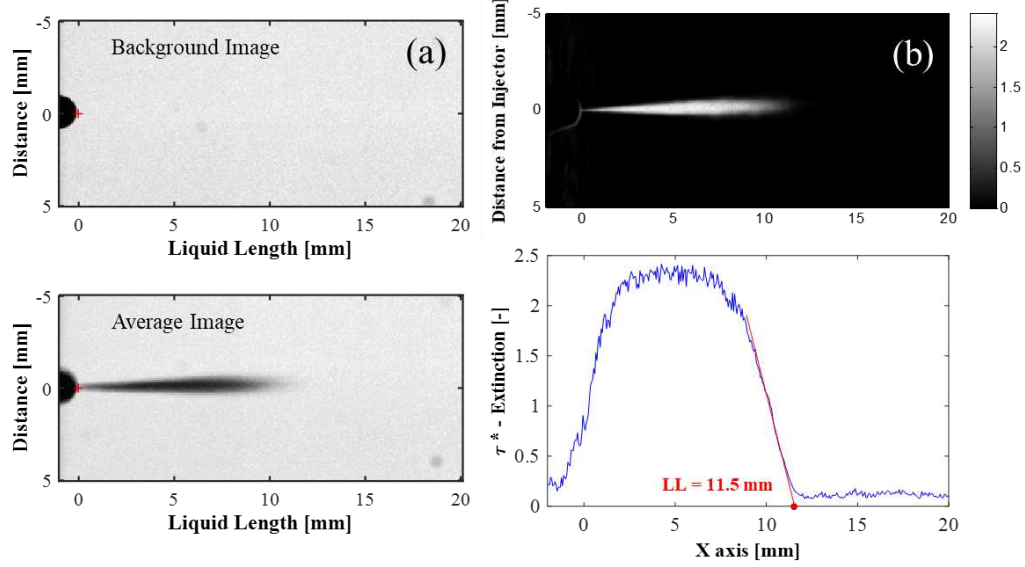


Figure 46 Image post-processing of DBI image: (a) example of background (top) and average images for ABE20 at 900 K, (b) light extinction image (top) and LL determination criterion.

3.3.2 Schlieren technique for Vapor Spray Penetration and Spray Angle

The Schlieren technique has been successfully used in many studies to identify refractive index gradients in transparent media [125], [126], [127]. The Gladstone-Dale relationship between refractive index, n and gas density, ρ is reminded in **Eq. 28**:

$$n - 1 = k_d \rho \quad \text{Eq. 28}$$

where the Gladstone-Dale coefficient, k_d , is a function of the phase, the molecular content and the organization of the component and the wavelength [125], [128]. This relation indicates that the light rays are changed in the direction when ambient gas conditions are changed, i.e., pressure and temperature, relating to gas density as presented by the simple perfect-gas state equation. The rays of a collimated light source are refracted proportionally to the gradients of refractive index that they are going through, as presented in **Eq. 29**:

$$\varepsilon_y = \frac{L}{n_0} \frac{\partial n}{\partial y} \quad \text{Eq. 29}$$

where ε the refractive angle in y-axis, L the path length, n_0 the surrounding refractive index [128]. Pastor et. al [128] presented the concept of the fundamental of Schlieren imaging for diesel spray environment as illustrated in **Figure 47**. For vapor diesel sprays, the Schlieren imaging is able to capture the line-of-sight boundary between fuel vapor and ambient gases, due to an appreciable difference in refractive indices between them [63], [129], [130]. This scheme presents the light ray deflection and their projection on a screen as a function of the density gradients of a diesel spray. At the standard air condition represented as the reference (blue line), its reflective index is around 1.0003, while it can increase to 1.005 for 22.8 kg/m³ of Spray-A condition of ECN, as presented in a purple line. When the fuel is injected into the chamber, the liquid phase fuel attenuates the light rays by absorption and scattering, therefore, rays hardly achieve to the cross section as represented in the red-dashed line. At the downstream of the liquid phase, the fuel evaporates and creates the dense vapor region, the variation of the reflective index is expected to be an order of magnitude higher than the reflective index of the dense air, enhancing greatly ray deflection as presented in yellow line. Further in downstream of the chamber, the spray continues to develop and mix with ambient gases, hence, the refractive index of the fuel-air mixture decreases asymptotically down to ambient gas values, reducing the refraction angle accordingly.

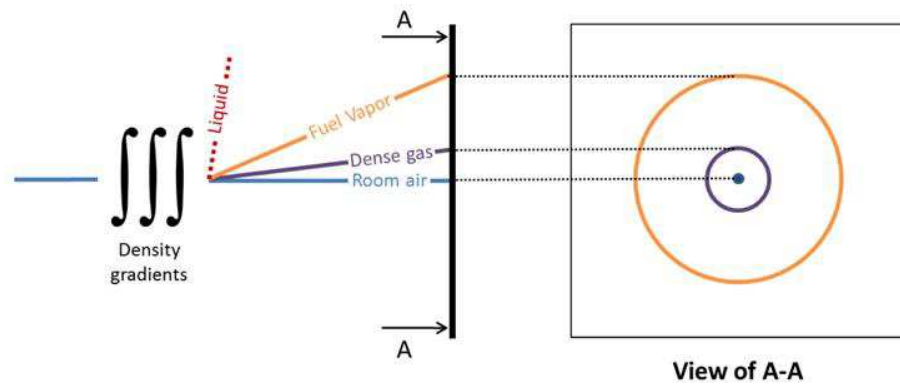


Figure 47 Schematic representation of the ray deflection caused by refractive index gradients existing in a diesel spray [128].

Pastor et al. [128] also compared different Schlieren experimental set-ups to reveal the relationship between reflective angle, the filtering and the Schlieren image resulting from the convolution. In the first case, all the reflected rays can be collected by combining lenses, excepting the liquid phase in the red line and focus them back on the image sensor of a camera. The image output obtained by this set-up is similar to DBI as seen in **Figure 48** (a). In the second set-up (**Figure 48** (b)), this set-up is often referred to as Shadowgraphy due to no mechanical cutoff light in the Fourier plane. However, the most refracted rays are not collected by this set-up, because the collection lens is placed too far from the spray, or the camera lens is placed too far from the Fourier plane. This set-up is called “uncontrolled Schlieren” because the high-pass filtering is determined to the size and the position of the optical element forming the collection system. In the last set-up (**Figure 48** (c)), it is similar to the set-up in case “b,” but all the refracted rays are collected and filtered in the Fourier plane by a mechanical cut-off (diaphragm). As it can fully control the filtering, this set-up was considered to characterize the vapor spray in this study.

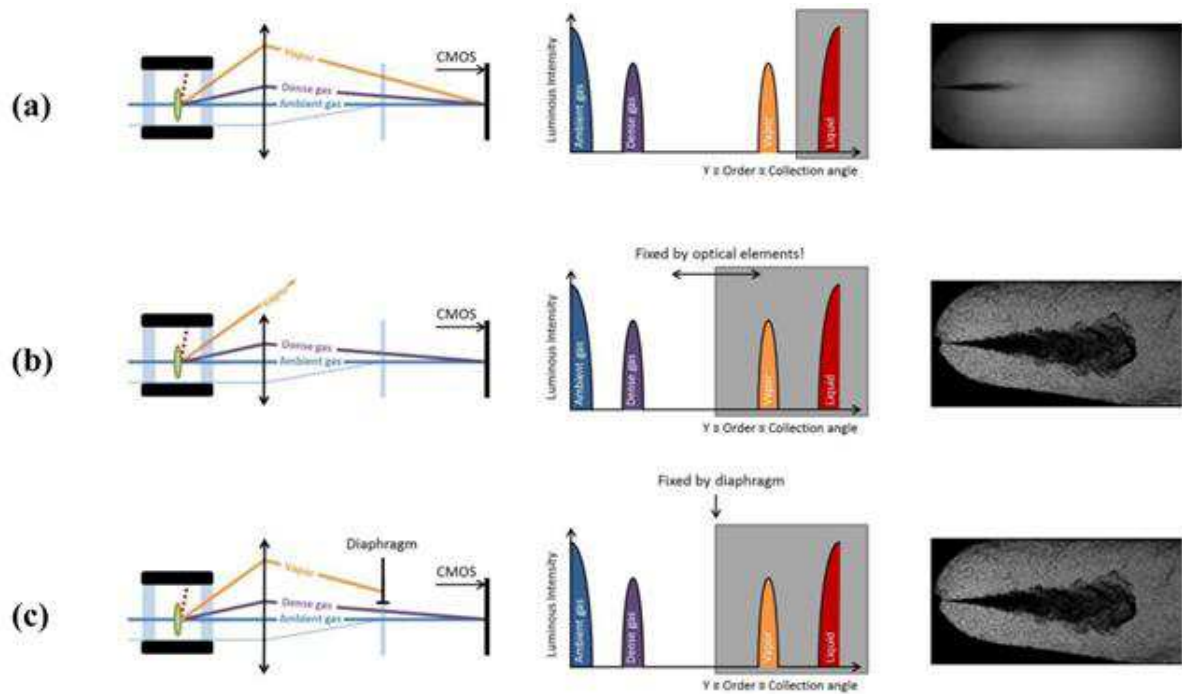


Figure 48 Schematic representation of the relationship between ray refraction, filtering at the plane of Fourier and resulting image [128].

In this work, the Schlieren set-up in Z configuration related to the set-up of case “c” is composed of the continuous white LED with a 1 mm pinhole, to provide one point-light source, as presented in **Figure 49** (a). Two parabolic mirrors (108 mm in diameter, 837 mm focal length) were used one to create the collimating light from the light source through the chamber and one to focus on a pinhole. This 6 mm pinhole was set up at the focus point to filter and control the reflected rays in order to obtain good contrast between backgrounds (gray) and spray boundary (black) as seen **Figure 49** (b)-top. To image the Schlieren deviation after the test section, the high-speed camera (Phantom V1611) was set after a collecting lens 30 mm in focal length. The image resolution was 1024x400 pix² for the highest frame rate set at 39 kHz with 5 μ s of exposure time and 0.083 mm/pix of magnification.

The image processing to determine the vapor spray penetration and spray angle was based on the standardized post-processing code from ECN to reduce uncertainties and compare the data obtained in this study with other available data [108]. The ECN code is based on the use of successive calculation of two standard deviation images in order to detect the boundary of the spray [129], [128]. A temporal standard deviation image is created by considering each image together with the two previous ones in the time sequence. Pixel-to-pixel standard deviation is calculated and highlights the pixels with a strong “activity” throughout these three instants. The high-speed frame rate of 39 kHz minimizes background changes that can happen between two consecutive images. The resulting image is processed with connectivity algorithms and the penetration length is quantified following the procedure of Naber and Siebers [49].

In **Figure 49** (b), examples of a Schlieren image and the spray boundary (red line) determined from the processed image are given. The vapor penetration length (S) is determined at the crossing point between the limit of the vertical spray front limit and the spray axis from the injector tip (blue line); while the angle between two yellow lines is presented the spreading spray angle (θ).

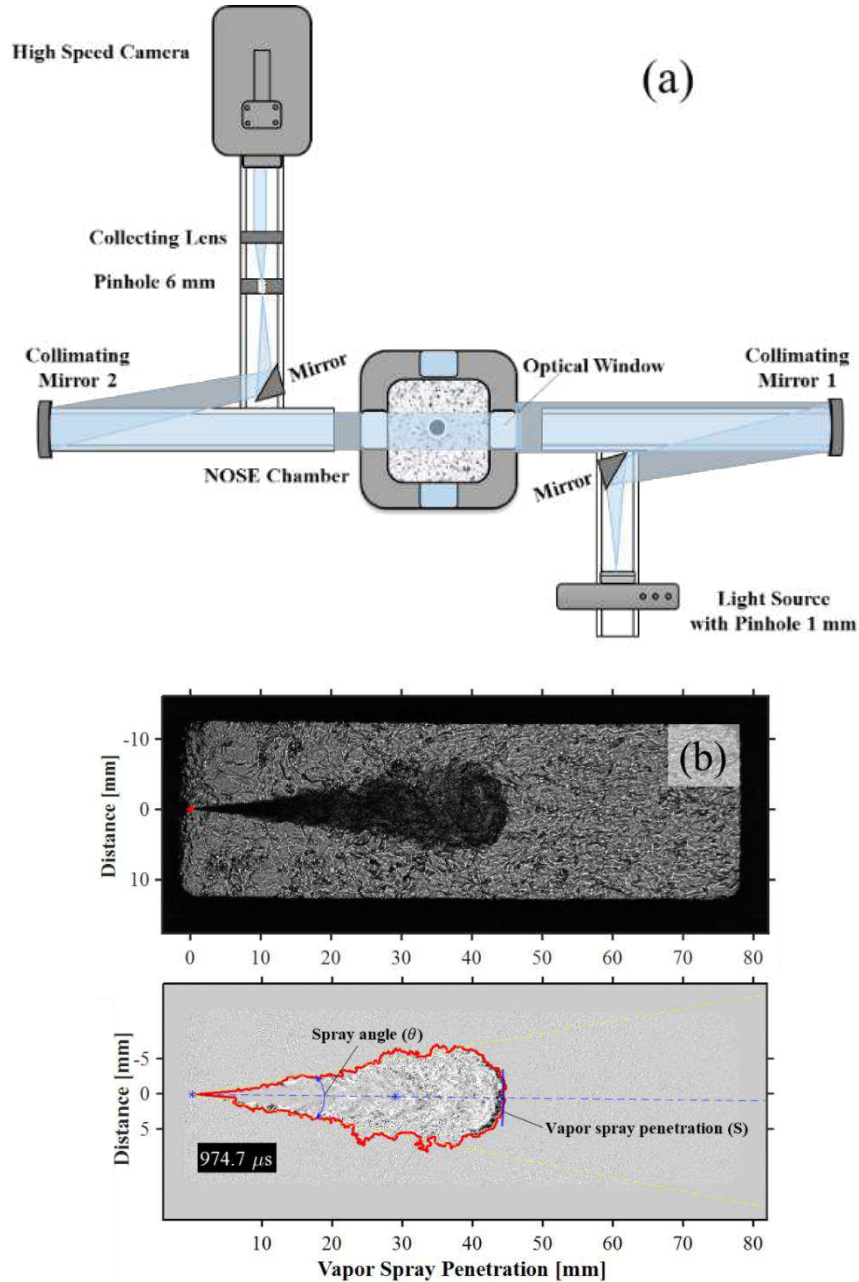


Figure 49 (a) scheme of Schlieren set-up, (b) example of Schlieren image (top) and of processed image with the identification of spray boundary (bottom).

3.4 Optical Set-Up for Reactive Condition

To obtain the absolute ignition delay, a Photomultiplier was employed to detect the OH^* chemiluminescence to determine the start of combustion (SOC) timing, while a high-speed

Schlieren imaging was simultaneously measured and installed in a different cross direction to detect the hydraulic day of injection, as seen in **Figure 50**. For lift-off length (LOL) measurement, the intensified CMOS camera was installed to simultaneously measure the length of stabilized flame. All technical details of the optical set-ups for the reactive condition are summarized in **Table 15**.

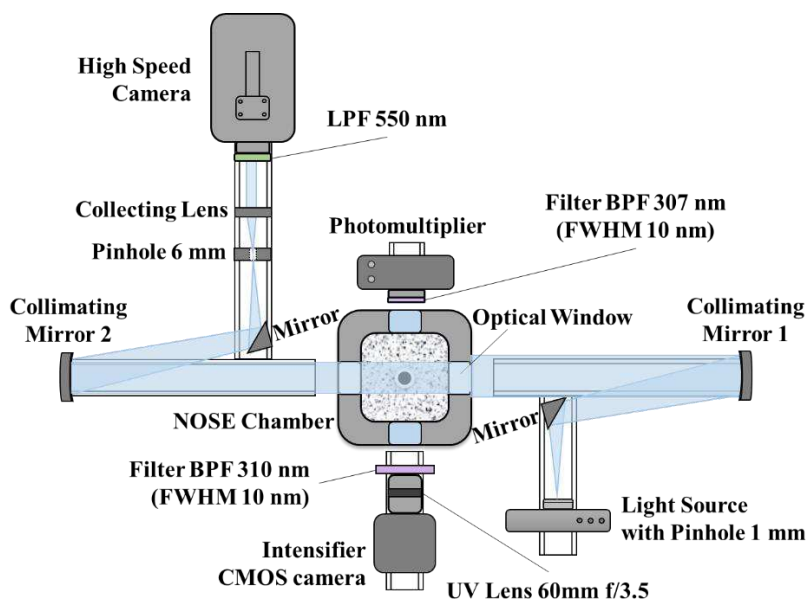


Figure 50 The schematic diagrams of physical arrangement for the reactive condition.

Table 15 Technical details of different optical setups for non-reactive and reactive conditions.

Optical Technique	OH* Chemiluminescence	Schlieren	OH* Chemiluminescence
Parameters	Lift-Off Length (LOL)	Ignition Delay (ID)	Ignition Delay (ID)
Light source	-	LED (white) 1 mm pinhole	-
Mirrors	-	2 Parabolic Mirrors	-
Detector	Photron - APX-I2	Phantom-V1611	Photomultiplier Newport PM 70680
Lens	UV 60 mm f/3.5	Collecting lens: 30 cm of focal length with 6 mm pinhole	-
Filter	BPF 310 nm FWHM 10 nm	LPF $\leq$ 550 nm	BPF 307 nm FWHM 10 nm

Optical Technique	OH* Chemiluminescence	Schlieren	OH* Chemiluminescence
Frame speed / Data Recording	2 kHz	39 kHz	250 kHz
Exposure time	499 μ s	5 μ s	-
Image size (pix ²)	512 x 1024	1024 x 400	-
Magnification	18.2 pix/mm	12.3 pix/mm	-

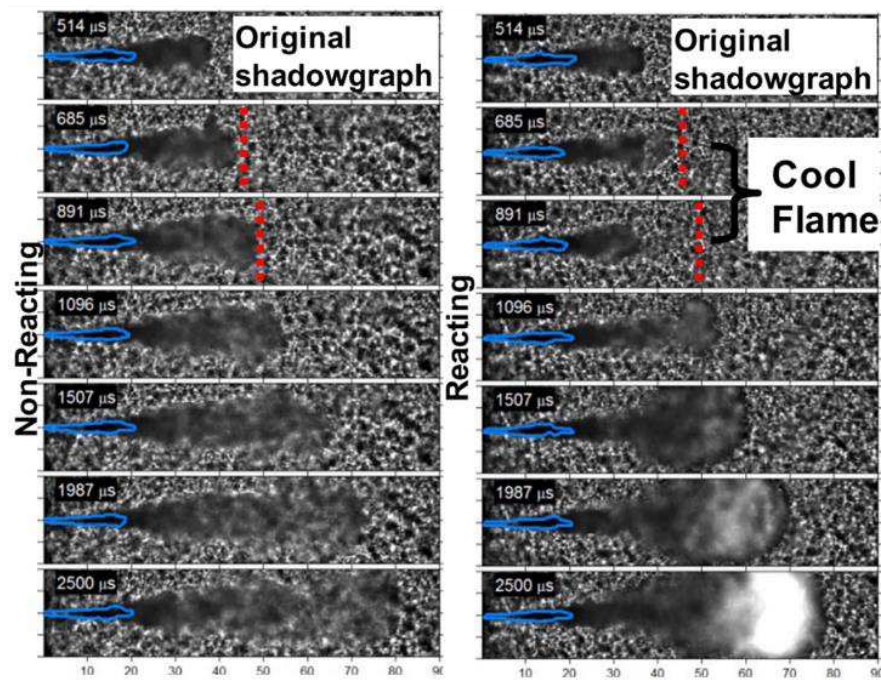
3.4.1 OH* Chemiluminescence for Ignition Delay

As a function of fuel and thermodynamic conditions, two ignition phases can be identified during the combustion process: the first one corresponds to the cool flame, i.e., low-temperature combustion and the second one to the main flame, i.e., ‘hot flame’ [45]. The cool flame corresponds to the moment when the parent fuel molecules are broken down, which slightly increases the ambient temperature. Due to this slight change in ambient temperature, an increase in cylinder pressure cannot be detected. To detect the first state ignition delay period (cool flame), the intensified camera coupled with a pass filter 450 nm can be used to detect the HCHO* and HCO* emissions as effectively transmitting wavelengths from approximately 380-450 nm [63], [131]. Another method is the Schlieren (or Shadowgraph) imaging technique. The slight increase in temperature of cool flame changes the refractive index of the spray to match the refractive index of the ambient gases, leading to more transparent images than the original Schlieren images [74]. Therefore, the cool flame can be detected at the extinction region in the reactive Schlieren images, as seen in **Figure 51** (a).

For the hot flame of ignition delay, generally, there are two principles to identify, i.e., pressure-based and light-based [123]. Based on the cylinder pressure, the piezoelectric pressure sensor is employed to acquire the cylinder pressure data. The ID can be determined from the time where the change in slope of pressure or the heat release reaches a significant amount [67], [63], [132]. When the main flame occurs and rapidly increases the combustion temperature, the chemiluminescence from excited-state OH* dominates [63], [69], [74], [133]. Therefore, by using an intensified camera or photomultiplier coupled with a 310 nm bandpass filter (10 nm FWHM), the OH* emission can be captured and used to identify the main flame or the start of combustion (SOC) timing [63], [64], as seen in **Figure 51** (b).

As ID is important for the diesel combustion process, the understanding of ignition delay process will help the development of diesel engine and investigation of the advanced new alternative fuel, fuel additive for diesel and advanced combustion modes.

(a)



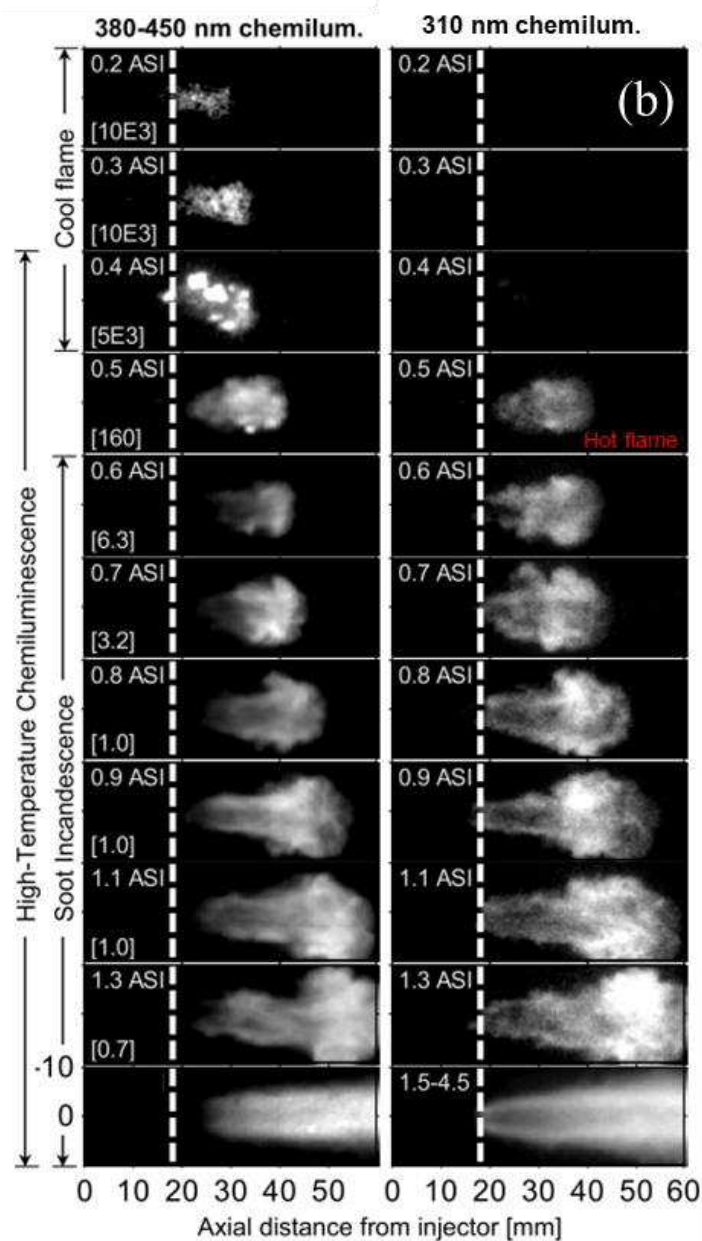


Figure 51 Different imaging methods to determine cool flame and hot flame ID measurement (a) the cool flame detection by Shadowgraphy images in reactive condition (900 K, 12% O₂) compared to Shadowgraph in non-reactive condition (modified from [63]), (b) the cool flame and hot flame detection by image pairs of chemiluminescence from 380-450 nm (left) and 310 nm (right) are shown at various time after the start of injection [69].

In this study, only the main combustion phase (i.e. ‘hot flame’) was considered, therefore the ignition delay was defined as the time between the start of injection (SOI) and the beginning of the start of combustion (SOC). A Newport Oriel Photomultiplier tube, with a PMT 70705 high voltage power supply and a band-pass filter of 307 nm (FWHM 10 nm) were used to record temporal the OH* chemiluminescence signal to determine the Ignition Delay of the main combustion phase, during 4 μ s thanks to an in-house LabView data acquisition system.

As previously mentioned, the SOI timing related to the hydraulic delay of injection was determined and used to correct the data and to compare the results with ECN databases. The high-speed Schlieren technique was set similar to the non-reactive condition, but with a 550 nm low-pass filter, added to limit emissions of soot radiation as shown in **Figure 50**. The real SOI timing for each test was defined as the first image where the injection of fuel inside the chamber appears on the Schlieren images, as seen in **Figure 52**. Therefore, the ignition delay is defined as the time from the SOI to the start of combustion (SOC) when the first peak of the OH* signal reaches the maximum, corrected by the hydraulic delay to provide ‘absolute’ ID.

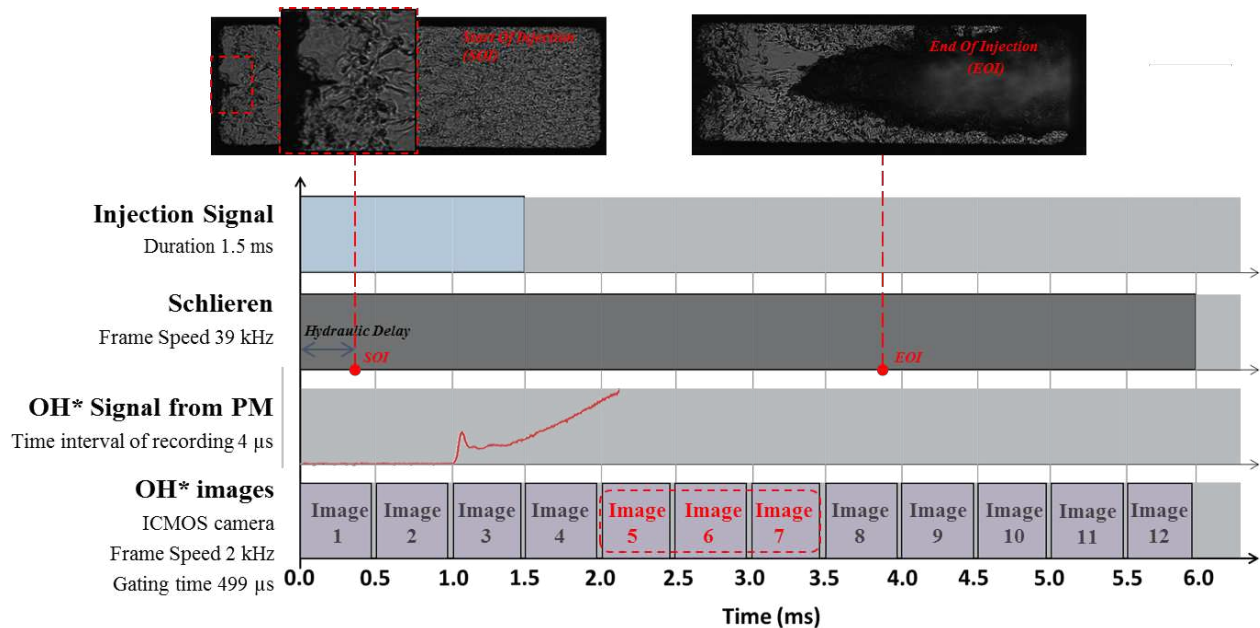


Figure 52 The schematic synchronization of the optical set-up for the reactive condition.

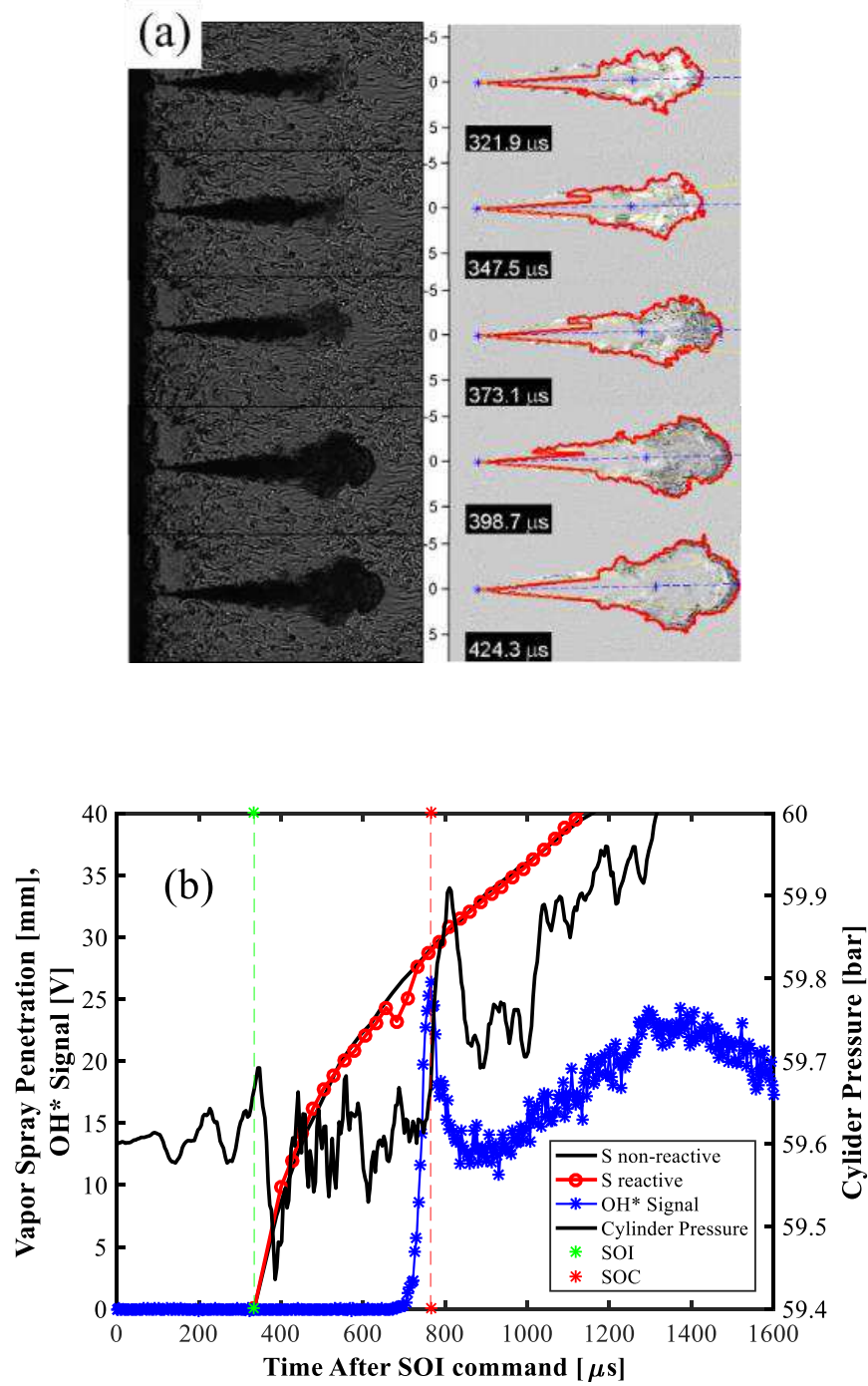


Figure 53 (a) example of Schlieren and post-processed images during cool and hot flames, (b) OH* chemiluminescence evolution in comparison to in-cylinder pressure and vapor penetration in non or reactive conditions. - 900 K, n-dodecane, Injector A.

As mentioned above, the hot flame appears after the cool flame. The cool flame can be detected at the extinction region in the reactive Schlieren images during this period, the slight increase in temperature changes the refractive index of the spray to match the refractive index of the ambient gas, leading to more transparent images than the original Schlieren images [74]. **Figure 53** (a) shows some cool flame images obtained with the Schlieren technique and their associated post-processed ones. The vapor spray length obtained in reactive conditions is shorter than in non-reactive ones, respectively $312.9\ \mu\text{s}$ and $373\ \mu\text{s}$, as shown in **Figure 53** (b). After that, the spray head reappears and the evolution of the vapor spray penetrations again becomes similar to the non-reactive trend. The light intensity from the Photomultiplier is also plotted (blue stars) to determine the start of combustion of the main flame as the time when the first maximum occurs (red dotted line), which corresponds to the second Schlieren image after the return to the normal trend. It should be noted that Schlieren imaging is unable to detect the timing of the main flame SOC directly. Even though Benajes et al. [134] determined the ID from Schlieren image processing as the local maximum of the total intensity curve, the greatest differences between chemiluminescence and Schlieren ID were observed at low ambient temperatures, low oxygen concentration and low ambient density. This is due to the fact that Schlieren images cannot detect the main combustion ID but are limited to the cool flame ID.

The evolution of in-cylinder pressure is also plotted as a function of time after the SOI command in **Figure 53** (b). The green dotted line shows the hydraulic delay from the Schlieren image around $335\ \mu\text{s}$, corresponding to the hydraulic delay from the MFR measurement. After that, the cylinder pressure immediately decreases because of spray atomization and vaporization. Then around $760\ \mu\text{s}$, it increases due to the main combustion event, corresponding to the maximum peak of OH^* signal at $765\ \mu\text{s}$. Even if the cylinder pressure data can be used to detect the SOC of the main flame, but the criterion to determine SOC was interrupted by fluctuation pressure. Therefore, OH^* chemiluminescence is considered to determine the main flame ID accurately.

3.4.2 OH^* Chemiluminescence for Lift-Off Length

Lift-off length (LOL) represents the distance at which the entrained air, premixed with vaporized fuel is transported to the initial combustion zone downstream, i.e., the distance from

the injector tip to the reaction zone where the flame is stabilized [76], [108]. During the main flame phase, high-temperature reactions produce OH radicals; therefore OH* chemiluminescence, centered at 310 nm is a good indicator to determine the LOL [76], [123]. Generally, the 310 nm band-pass filter (10 nm FWHM) positioned front of an intensified camera coupled with UV lens is used to capture the line-of-sight chemiluminescence image, as illustrated in **Figure 54** (a). The long gating time of intensifier is recommended by ECN to avoid the turbulent fluctuations in LOL and obtain the quasi-steady LOL [123]. The lift-off length is determined by finding the distances between the injector tip and the first axial locations above (blue dashed line) and below (green dashed line) the spray centerline with an intensity greater than approximately 50% of the leveling-off value, as shown in **Figure 54** (b). The average of these two axial distances is defined as the lift-off length.

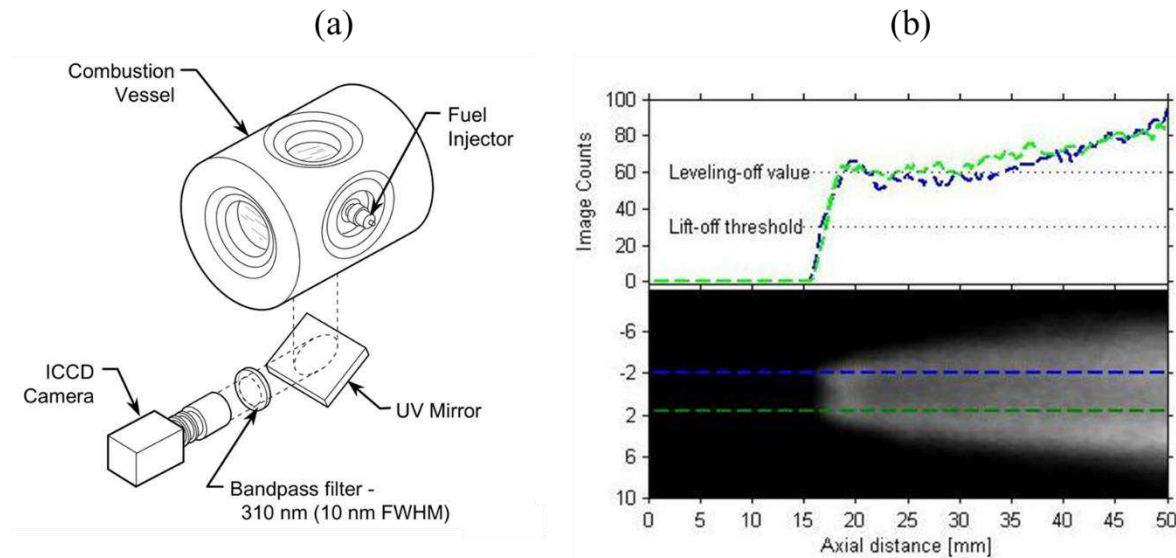


Figure 54 Scheme of the optical set up used to acquire images OH* chemiluminescence at 310 nm (a) and (b) an example image OH* chemiluminescence at ambient conditions (1000 K, 14.8 kg/m³, 21% O₂) and the criterion used to determine LOL [76].

In this study, an intensifier CMOS camera, Photron Fastcam APX I2, was used with a 60 mm f/3.5 UV lens, equipped with a 310 nm (FWHM 10nm) band-pass filter (BPF), as illustrated in **Figure 55** (a). A long constant gating time of 449 μ s was chosen to average LOL during a quasi-steady phase after SOI [68]. Ten images were recorded, but only the 5th to 7th images (2.0

ms after SOI) were used to calculate the LOL, as shown in **Figure 52** (b). **Figure 55** shows an example of OH* images and the post-processing criterion chosen: the intensities along the red and blue profiles around the spray centerline are considered to define LOL. LOL is defined as the average of the distances between the injector tip and the distance corresponding to 50% of the maximum intensity, following the ECN method [69].

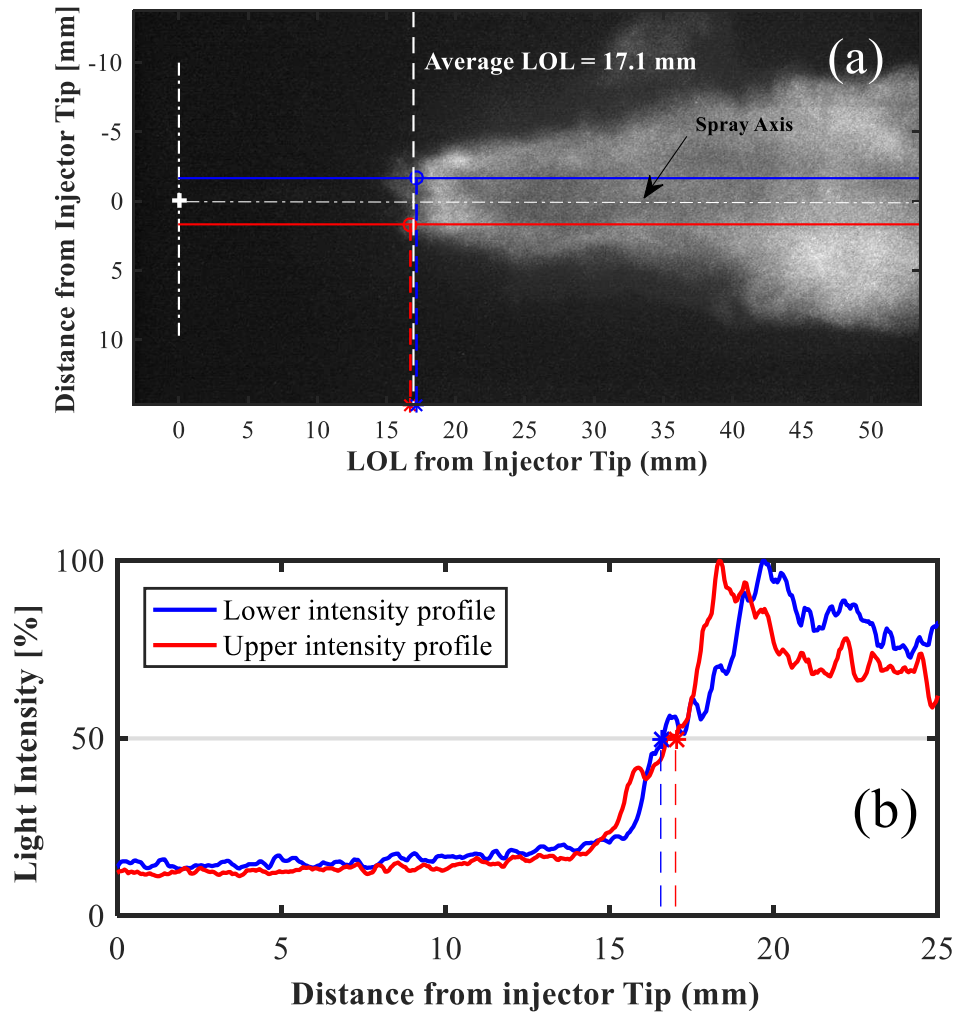


Figure 55 LOL definition: (a) an example of OH* image and LOL estimate for 850 K, (b) evolution of OH* intensity along the upper (blue) and lower (red) profile around the spray axis. Star symbols represent 50% of the maximum intensity of each profile.

3.5 Experimental Result and Validating with ECN Data Base

3.5.1 Mass Flow Rate (MFR)

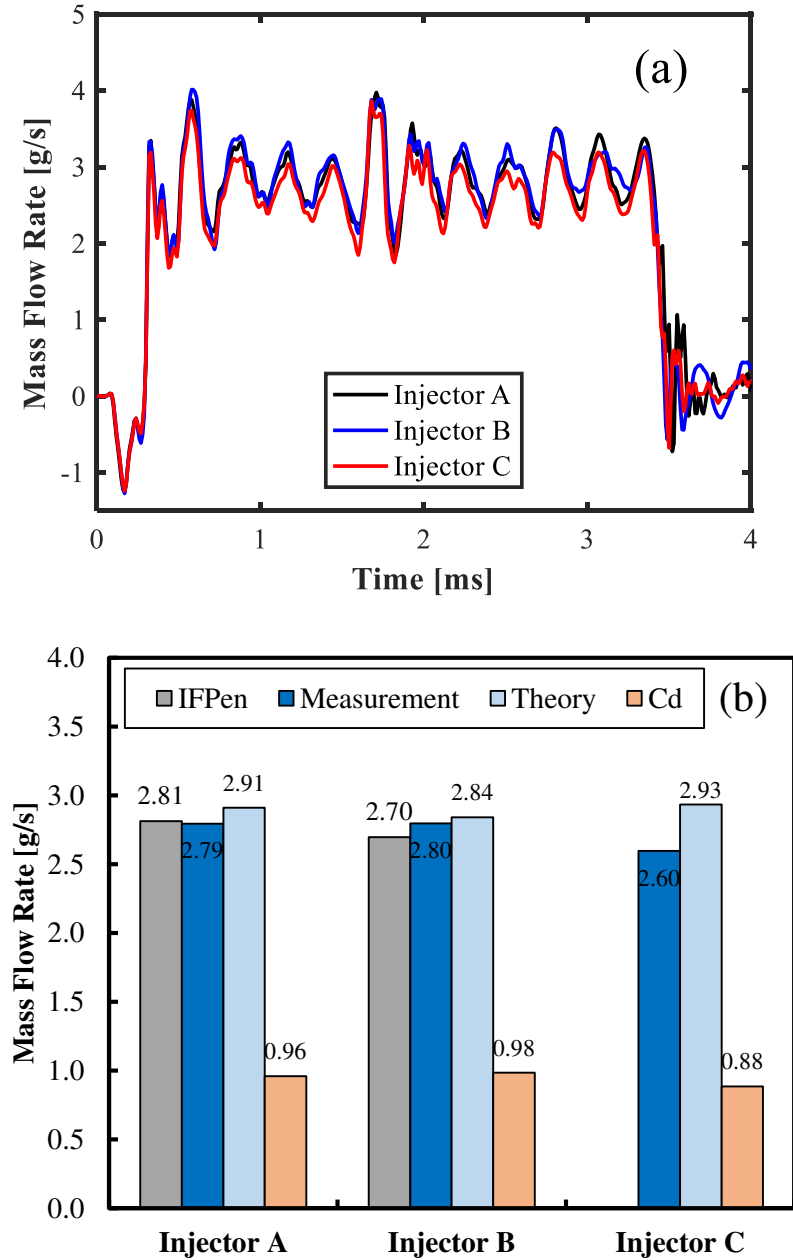


Figure 56 Mass flow rate result: (a) the evolution of mass flow rate of n-dodecane as a function of time for three injectors, (b) comparison between the mean value of MFR of three injectors, theoretical MFR and the Cd ratio. The data obtained from IFPen are also provided for comparison.

Figure 56 (a) presents the evolution of average MFR as a function of time for the 3 injectors. It can be seen that the pattern is globally the same and the onset and end of hydraulic delay are around 300 μs and 2010 μs , respectively. A slight difference in the acoustic waves can be observed, with the highest value for injector A and the lowest for injector C. The mean MFR was defined in the previous section, as presented in **Figure 41**. Injector A and B provide the same value of 2.8 g/s (less than 0.5% of difference). This difference is mainly due to the slight difference in the hole diameter, which leads to 2.4% of difference with the theoretical MFR and 2% in the Cd. The data provided by IFPen are in the same order (a difference below 4% for both injectors). For the pre-used injector C, the mean measured MFR is about 7% lower than for the others. This is mainly due to the larger outlet diameter and changing shape as a function of pre-used time, as seen in **Figure 39**. Therefore, the discharge coefficient is the smallest (0.88).

3.5.2 Liquid Length (LL)

LL provides information on the mixing field near the injector tip. **Figure 57** shows the quasi-steady liquid phase penetration results of injectors A and B as a function of ambient temperature compared to IFPen results. First, LL for both injectors decreases on increasing the ambient temperature due to higher energy entrainment at higher ambient temperature. The increase in temperature increases mass and heat transfers between the spray and ambient gases, leading to an increase in the vaporization rate.

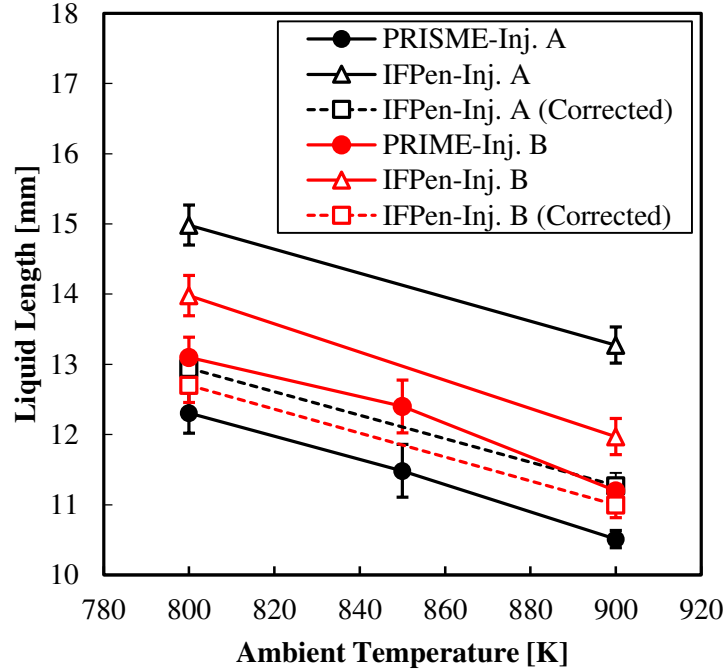


Figure 57 LL results for the non-reactive condition of 3 ambient temperatures and comparison of LL results of Injector A and B with IFPen results [108].

The experimental LL of injector A and B is lower than IFPen by up to 2.7 and 2.8 mm for 800 and 900 K. However, it should be noted that the experimental results of IFPen (solid lines and open-symbols) were obtained, when the injector had never been used before. Therefore, to compare their results with the ECN database, the measurements performed with the injectors that had undergone a high number of tests were corrected. The correction consisted in taking into account the influence of ‘injector age,’ defined as the number of pre-burn events that each injector has been exposed to because the hot gases formed during the pre-burn event were considered potentially aggressive for the injector hole and could be linked to modifications at the orifice [15]. As a result of the higher number of tests in the CVP chamber, the shorter LL can be obtained [108], and the experimental results of IFPen were corrected to 300 pre-burn events, as plotted in **Figure 57** (dotted line). Therefore, the age-corrected results of IFPen were used to compare with the experimental result of the present work. As seen in the figure, the data from this work and the corrected results of IFPen are in a good agreement with a slight difference or less than 1 mm for all ambient conditions and both injectors. The similar result is also found

in injector B which was tested in the the inhomogeneous condition at 800 and 850 K. This result indicates that the quality of the homogeneity of the ambient temperature field has a little effect on the development of the liquid part of the spray.

Table 16 The estimation results of LL compared to different ECN data provided by different institutes at 900 K [49].

Injector Name	Institute	Liquid Length [mm]
Injector A	PRISME	10.5
Injector A	IFPen	11.3
Injector B	PRISME	11.2
Injector B	IFPen	11.0
Injector C	PRISME	10.4
SN210677	Sandia	10.0
SN210675	CMT	10.6
SN210678	IFPen	11.0
SN210679	TU/e	10.3
Average LL [mm]	10.7	
STD LL [mm]	0.4	

Table 16 gives all the LL data available on the ECN website, determined by different research groups in the Spray-A condition, non-reactive condition at 900 K, obtained in different experimental set-ups. Globally all the results are in the same range, with an average of 10.7 mm and a standard deviation of 0.4 mm, i.e., less than 4% of variation. In order to investigate the statistical significance of difference of our results with ECN database, the “Student-t test distribution” were used to verify the mean value. The student-t results of injector A from 12 tests compared to the results of other laboratories are presented in **Table 17**. The null hypothesis of the test defines as mean of all injector is equal to mean of injector A. This hypothesis can be rejected, if probability $P < 0.05$. As the results, probability of student-t test (P-value) is higher than 0.05, which confirms that there is no significant difference of LL at 900 K between PRISME result and ECN database.

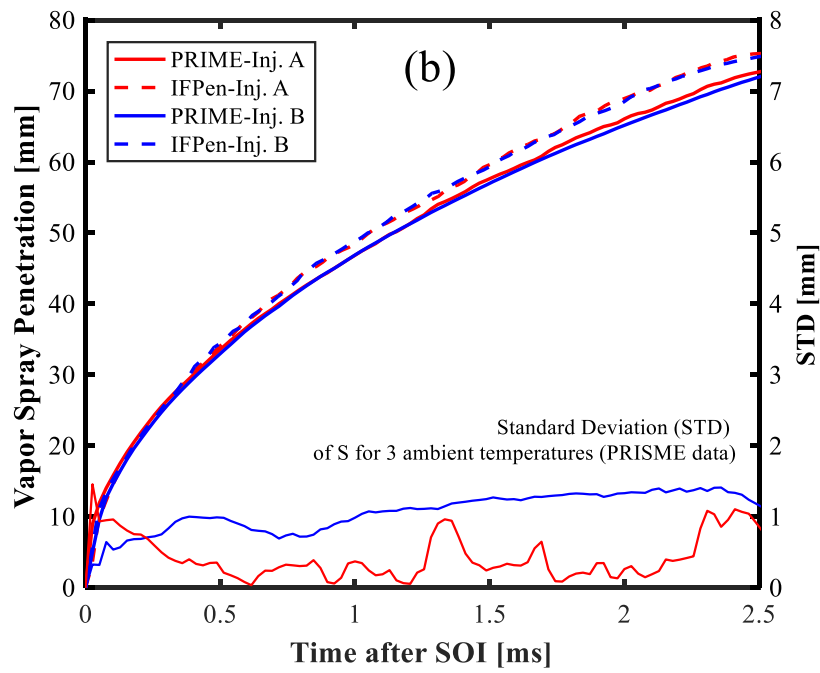
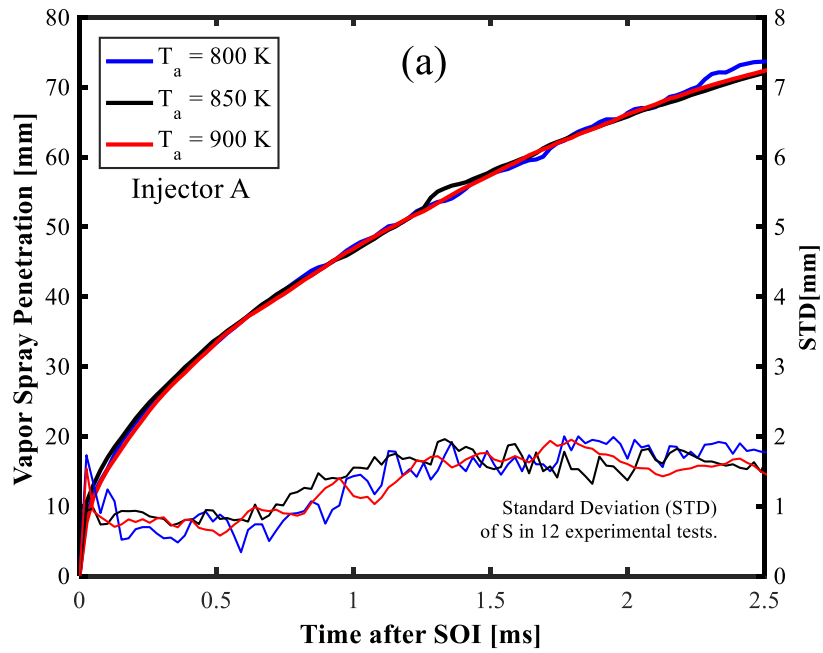
Table 17 The Student-t test result of LL for all injectors at 900 K.

Name	Test Number	Mean [mm]	STD [mm]	t-value	Probability (P-value)
LL of all Injectors	38	10.8	0.5	1.88	0.07
LL of Injector A	12	10.5	0.1		

Null hypothesis (H0) : Mean of LL from all injectors = Mean of LL from injector A. Reject the null hypothesis, if $P < 0.05$

3.5.3 Vapor Spray Penetration (S)

In **Figure 58** (a), the average evolution of S is plotted as a function of time after SOI, for injector A and three ambient temperatures. The variation between 12 repetitive tests is less than 2 mm or 3% of the average as indicated in the standard deviation. The S evolution is very similar for 3 ambient temperatures, because S mainly dominated by the spray momentum, controlled by the injection pressure and ambient density (related to pressure) [67]. As indicated in **Figure 58** (a), to maintain an ambient density of 22.8 kg/m^3 , the ambient pressure was slightly adapted which affects the pressure drop at the injector tip, generating a slight difference in spray momentum. Therefore, a mean S was determined as the mean of the average S from the 3 temperatures and is presented in **Figure 58** (b) for injectors A and B, with a standard deviation below 2.5%, 1 ms after SOI. The results from IFPen are similar until 0.5 ms after SOI for both injectors but are slightly higher, with less than 5% of difference with the results of this work, due to the different temperatures and aerodynamic fields inside the chamber. However, in comparison with the results of ECN database at 900 K, as seen in **Figure 58** (c), it can be seen that the results of this work ('PRISME') from injectors A and B are globally in the same order of magnitude. For the injector C, the S values are appreciably lower due to its lower MFR as described above and the effect of the larger diameter of the injector hole on the spray angle and the spray momentum [108].



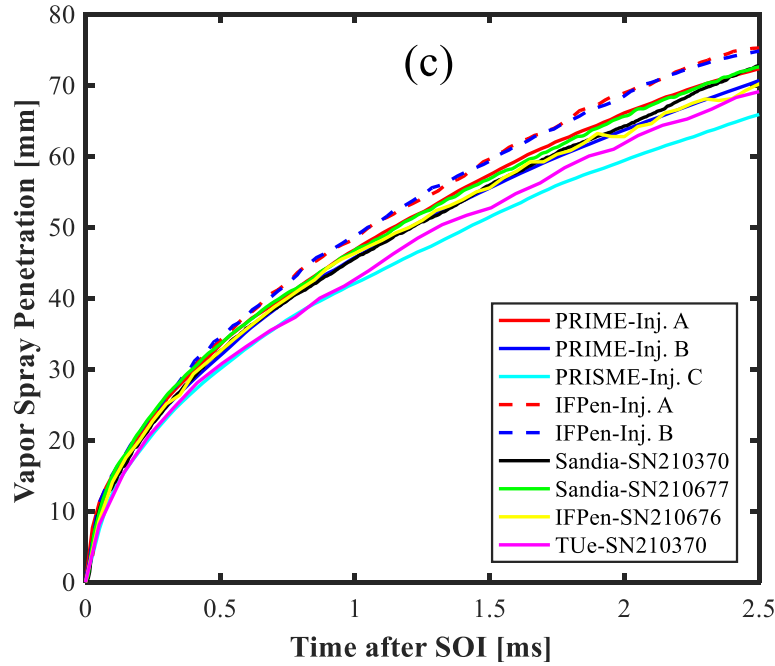


Figure 58 (a) evolution of vapor penetration of 3 ambient temperatures and its associated STD for 12 repetitive tests as a function of time for injector A, (b) evolution of average vapor penetration and comparison with IFPen data for injector A and B, (c) comparison of data from this work with data from other research institutes for all injectors at 900 K.

3.5.4 Ignition Delay

Figure 59 presents the ID values determined by using the OH* chemiluminescence signal for the three ambient temperatures. As expected, ID decreases with the increase in ambient temperature, due to the effect of the chemical reaction itself and also the effect of the fuel atomization and evaporation rate. The results obtained in the NOSE set-up at 900 K are 2.3% higher than the values provided by other research groups, with different injectors and combustion chambers. This difference is higher when data were obtained for the same injectors in the IFPen set-up, 7% and 13% for injectors A and B. At lower ambient temperature, 800 K, the difference in ID values between this work and IFPen is within the limit of the test-to-test fluctuations, represented by the error bars for injector A. However, for injector B, where the temperature field is inhomogeneous, the difference increases, confirming the strong impact of

the homogeneity of the ambient temperature on the auto-ignition ability. Interestingly, the ID of the old injector C performs similar result with other injectors for all ambient temperatures. This trend can also be observed with Bardi et al. [108], implying ID has low sensitivity on the injection parameters, i.e., spray momentum and spreading angle (at the same test fuel). However, the results globally determined in NOSE for all injectors can be considered very close to those of other research groups at 800 K. At 850 K, ID values from this work are close to CMT values but a difference around 13% compared to Sandia values. In conclusion, there is no obvious effect of the use of injector on the ID; some other parameters such as temperature field and perhaps the presence of residual species in the case of the pre-combustion chamber may also have an impact on the ID determination. The statistical significance of difference between PRISME results and ECN database, are presented by the student-t test values in **Table 18**. Only 900 K is investigated due to enough data for testing. As the results, the probability of student-t test (P-value) is higher than 0.05, which confirms that there is no significant difference of ID at 900 K between PRISME result and ECN database.

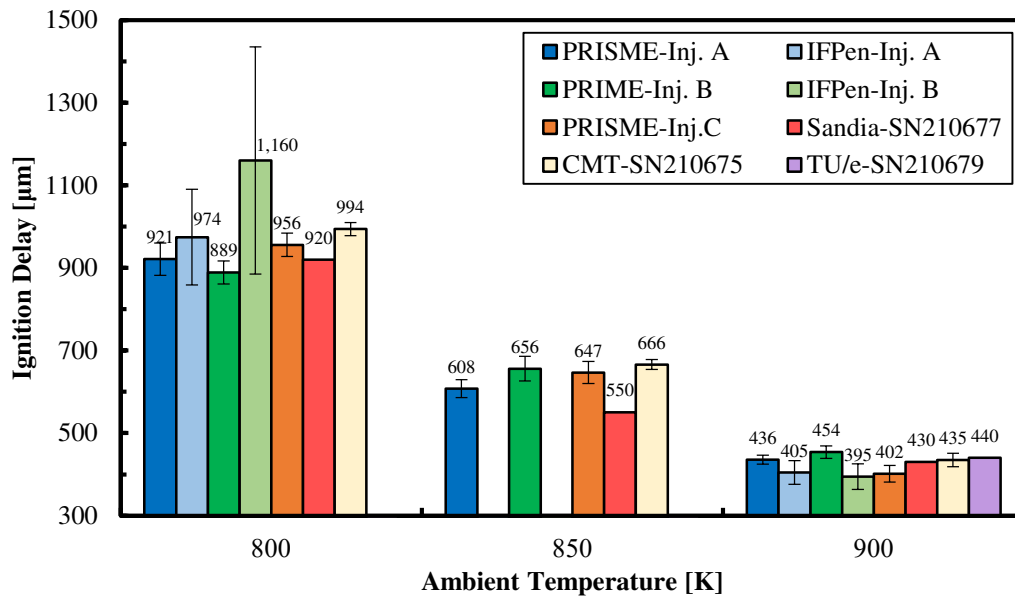


Figure 59 Measured ID values versus ambient gas temperature for different injectors compared to ECN data.

Table 18 The Student-t test result of ID for all injectors at 900 K.

Name	Test Number	Mean [mm]	STD [mm]	t-value	Probability (P-value)
ID of all Injectors	40	428	28.8	-0.839	0.41
ID of Injector A	12	436	10.7		

Null hypothesis (H0) : Mean of ID from all injectors = Mean of ID from injector A. Reject the null hypothesis, if $P < 0.05$

3.5.5 Lift-Off Length

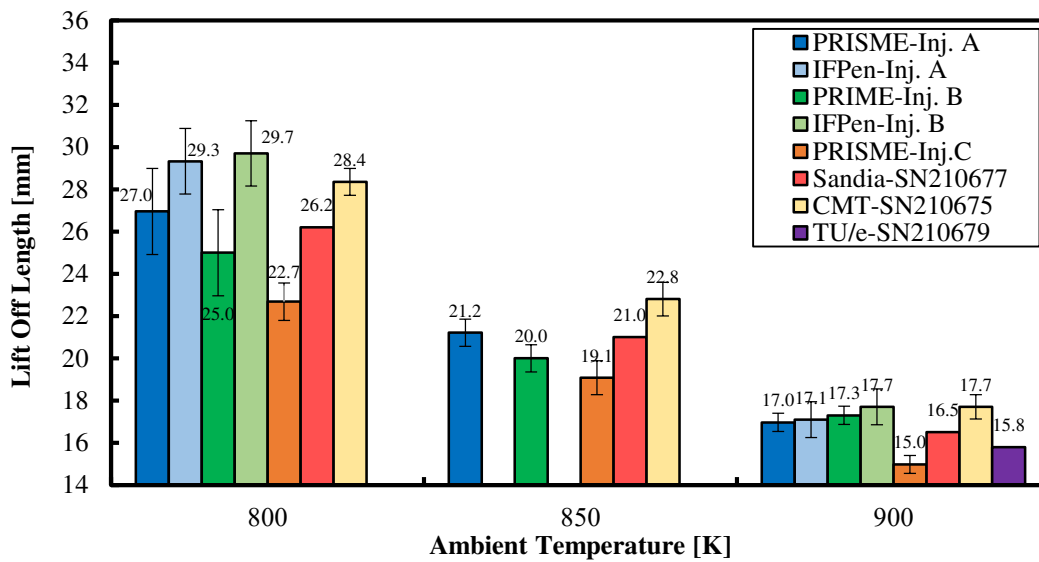


Figure 60 Comparison of measured LOL versus ambient gas temperature for different injectors with measurement available from ECN.

Figure 60 shows the experimental result of LOL as a function of ambient temperatures. As expected, by increasing ambient temperature LOL is shortened due to the combined effects of faster evaporation and mixing processes and local reaction rate, allowing the flame to stabilize closer to the injector [73]. As already mentioned, Injectors A and B were also studied by IFPen so the values can be directly compared. First, all the values determined during this work are lower, with at 900 K, differences of 0.5% and 2.3% for injectors A and B respectively and at 800 K, 8.5% and 18.8%. This difference may be due to the residual species in the pre-

combustion chamber and their effect on kinetics and/or to the flow fields inside the chambers. On the other hand, as the ambient temperature condition in NOSE was different during experiments with injectors A and B (homogeneous and non-homogeneous field respectively), it can be concluded that the temperature field has a strong impact on combustion parameters, whether ID or LOL. For the ‘pre-used’ injector C, LOL is always the lowest at all ambient temperatures due to its lower spray momentum as presented by the lower MFR result, inducing stabilization of the flame closer to the injector tip as previously observed in [108]. The data available from ECN were also added for a global comparison even if it is not the same injector (but the same nominal characteristics) and the same kind of vessel. Without considering values from Injector C, average values and standard deviations from all the data and for each temperature were calculated: at 800 K, the average value of LOL is 27.6 mm with 6.9% of standard deviation, at 850 K 21.8 mm with 3.78% STD and at 900 K, 17.2 mm with 2.7% STD (or 17 mm with 4% STD if the TU/e value is considered). It can be concluded that the results obtained in this work are in good agreement with the ECN data base: the values of LOL obtained with Injector A differ by less than 2% from the average values. However, in order to confirm this conclusion, the Student-t test distribution was used to investigate the statistical significance of difference between PRISME results and ECN database of injector A due to enough data to test, as presented in **Table 19**. As seen, the probability of student-t test (P-value) is higher than 0.05, which confirms that there is no significant difference of LOL at 900 K between PRISME result and ECN database. In **Figure 61**, the linear dependency between ID and LOL is clearly highlighted for all ambient temperatures and all the data are very close to each other, as can be seen with the linear regression obtained without Injector C data.

Table 19 The Student-t test result of LOL for all injectors at 900 K.

Name	Test Number	Mean [mm]	STD [mm]	t-value	Probability (P-value)
LOL of all Injectors	40	16.6	1.19	-1.17	0.25
LOL of Injector A	12	17	0.393		

Null hypothesis (H0) : Mean of LOL from all injectors = Mean of LOL from injector A. Reject the null hypothesis, if $P < 0.05$

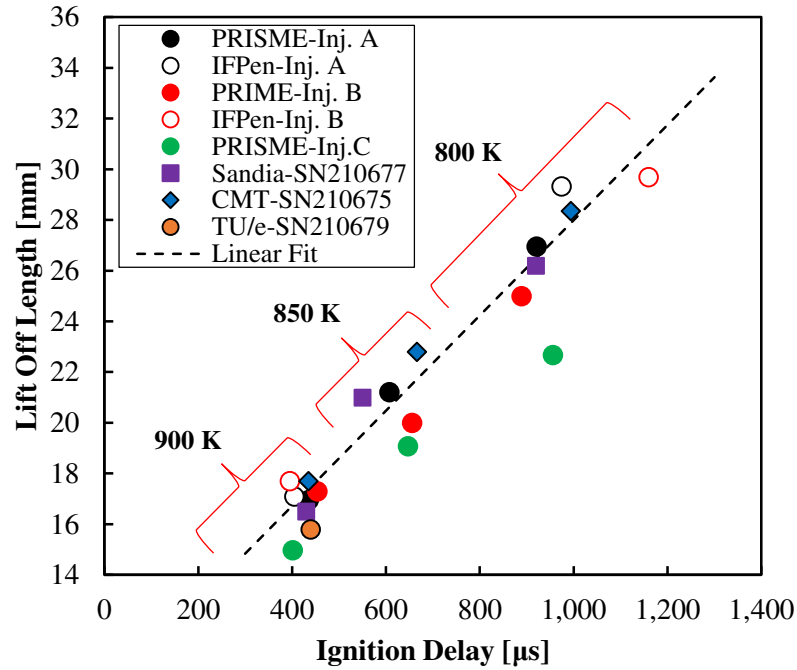


Figure 61 The relationship between ID and LOL, which compares between different data available from ECN.

3.6 Conclusion

The experimental results obtained in NOSE were compared with those obtained by IFPen and other from ECN database. In the case of injector A, characterized at different homogeneous ambient temperatures, the good agreement with results from ECN database are obtained which confirms the high accuracy of our experimental set-ups and our adaptation of the post-processing. Globally, it can be concluded that:

- 1) The values of the liquid lengths for the three injectors are globally good agreement with all values from other research institutes, with a difference lower than 1 mm.
- 2) The average vapor spray evolutions are globally in the same order of magnitude for all data, even if the results from IFPen are longer after 0.5 ms after SOI. But the use of an ‘old’ injector performs appreciably lower evolution than all results due to its lower MFR and the larger injector hole diameter.

- 3) All ignition delays estimates are globally the same range at 850 and 900 K, without any impact of the use or shape of the injector. This implies that ID has low sensitivity on the injection parameters, i.e., spray momentum and spreading angle (at the same test fuel). But a more pronounced difference for the lift-off-length was founded as a function of the injector hole shape, especially when the ambient temperature is lower than 900 K. The change in the injector hole shape for long pre-used injector can induce shorter LOL for all ambient temperatures, due to lower spray momentum of the lower MFR.
- 4) By changing the operating conditions, the effect of the temperature inhomogeneity in combustion processes was confirmed, while no effect on macroscopic spray parameters was observed.

CHAPTER 4

SPRAY AND COMBUSTION CHARACTERIZATION OF ABE20 COMPARED TO ALCOHOL BLENDS

As reviewed in **Chapter 1**, several studies present some results about the high potential of ABE and butanol diesel blends to reduce simultaneously soot and NO_x. There is not yet a complete comparative study of these fuels on spray and combustion behaviors to get better understanding on the effect of fuel properties. Therefore, the objective of **Chapter 4** and **Chapter 5** is to investigate the effect of fuel properties of ABE mixture and alcohol fuels, blended with n-Dodecane on the spray and combustion at HPHT conditions. In this chapter only ABE20 was considered and compared with other alcohol blends, the effect of the ABE ratio will be considered in next chapter.

4.1 Fuel Characteristics

The ABE mixture is composed of 30%v of acetone, 60%v of butanol and 10%v of ethanol, as the most usual mixture obtained from the intermediate fermentation of butanol production [11], [12], [13]. For that, acetone with 99.8% purity from SupraSolv® MS, butanol and ethanol with 99% and 99.8% purity from ACROS ORGANICS were used to prepare ABE mixture. Different blends in n-Do100 were selected: 20%v ABE (ABE20), 20%v Butanol (Bu20), 40%v Butanol (Bu40). Last, the fuels matrix was completed by a blend of 20%v butanol and 20%v ethanol (Bu20Eth20) to evaluate the effect of oxygen molecule content, and a 20%v of ethanol (Eth20) to consider the effect of ethanol itself in Bu20Eth20.

Table 20 summarizes the fuel properties of all tested fuels. First, it can be noted that the density is similar for all fuels with less than 3% of the variation. But up to 25% of the difference is induced by the use of difference blends for the viscosity. Moreover, the viscosity values for Bu40 and Bu20 are the highest ones and the closest to n-dodecane. The vapor pressure is mainly affected by the ethanol content, so in the case of ABE20, it is more than 100 times those of n-

Do100. But it should be noted that the latent heat of vaporization is the same for the ABE20 and Bu20, but 13% higher than dodecane. The lower heat values are identical for ABE20 and Bu20, but any alcohol blends lower than the value for n-dodecane. Moreover, their stoichiometric mixture fractions (Z_{st}) are also similar and the closest one to the dodecane due to slight difference of molecular weight and stoichiometric coefficients, as considered from **Eq. 20**. So, by analyzing these different parameters as a function of the different blend fuels, firstly it can imagine that ABE20 and Bu20 will provide similar combustion characteristics, which is not so far from the dodecane one, even if liquid phase would be not so evident.

It should be noted that, the measurements in this chapter were performed with only the pre-used injector C. Therefore, the experimental results presented in **Chapter 3** for n-dodecane of injector C are considered as reference data in order to compare with other alcohol fuels. All testing conditions for all parameters and fuels are summarized in **Table 21**.

Table 20 Fuel properties of single fuels and blended fuels in comparison with n-dodecane [15], [135], [136], [137], [138].

Properties	n-Do100	Acetone	Butanol	Ethanol	ABE20	Bu20	Eth20	Bu40	Bu20Eth20
Molecular formula	C ₁₂ H ₂₆	C ₃ H ₆ O	C ₄ H ₁₀ O	C ₂ H ₆ O	C _{8.5} H _{18.6} O _{0.4} ^a	C _{8.9} H _{19.9} O _{0.4} ^a	C _{7.1} H _{16.1} O _{0.5} ^a	C ₇ H ₁₆ O _{0.6} ^a	C _{7.8} H _{18.3} O _{0.9} ^a
Density at 15°C (kg/m ³)	752.8	789	813.3	794.1	760.7	763.3	758.8	774.9	770.6
Viscosity at 15°C (mm ² /s)	2.032	0.149	4.119	1.489	1.642	2.124	1.881	2.527	2.077
Lower heating value (MJ/kg)	44.1	29.6	33.1	26.8	41.5 ^b	41.8 ^b	40.5 ^b	39.5 ^b	38.3 ^b
Cetane number	74	-	17	8	-	-	-	-	-
Boiling point (K)	489	329	391	351	464 ^b	468 ^b	460 ^b	448 ^b	440 ^b
Vapor pressure at 298 K (kPa)	0.02	30.80	0.58	7.91	2.17 ^b	0.14 ^b	1.66 ^b	0.25 ^b	1.76 ^b
Latent heat of vaporization at 298 K (kJ/kg)	362	518	582	904	411 ^b	409 ^b	475 ^b	454 ^b	520 ^b
Oxygen concentration (% by mass)	-	27.6%	21.6%	32%	5.2%	4.6%	7.3%	9.1%	11.7%
Stoichiometric mixture fraction, Z _{st} (-)	0.0460	-	-	-	0.0489	0.0485	0.0500	0.0512	0.0528

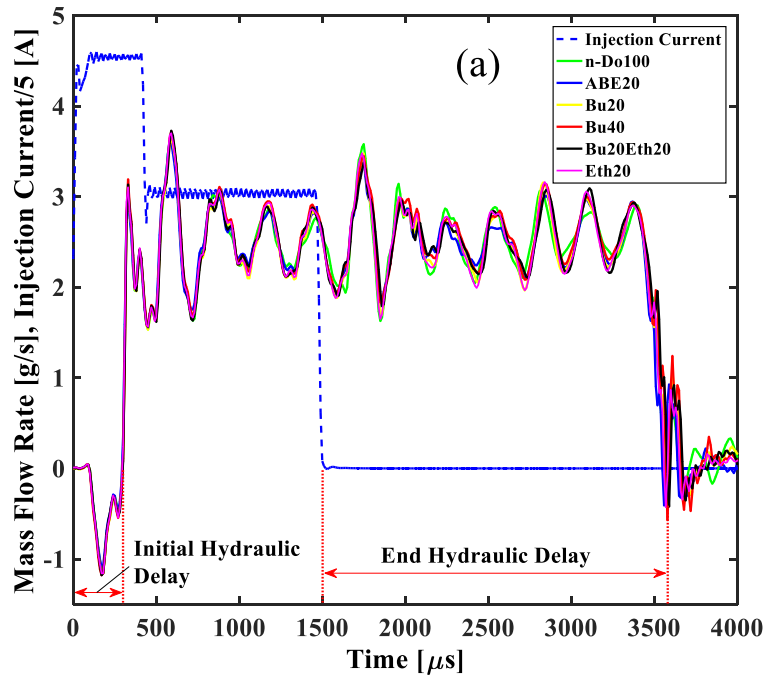
Note: ^a Equivalent formula based on mole fraction.

^b Properties estimated from mass fraction of single-component fuels in the alcohol blends.

Table 21 Testing conditions for all fuel blends

Fuels	Ambient Condition at SOI timing	Estimated parameters (Measurement technique)
• n-Do100 (reference fuel) • ABE20 • Bu20 • Bu40 • Bu20Eth20 • Eth20	• P_{amb}: 60 bar • P_{inj}: 1500 bar • T_{inj}: 293 K • Injection Duration: 1.5 ms • Injection number: 20 injections/test • Testing Number: 3 tests	• Mass flow rate (MFR) • Hydraulic delay • Cd
	• P_{amb}: 60 bar • T_{amb}: 800, 850, 900 K • ρ_{amb}: 22 kg/m³ • P_{inj}: 1500 bar • T_{inj}: 363 K • Injection Duration: 1.5 ms • Testing Number: 12 tests	Non-reactive condition (Pure N2) Liquid length penetration (DBI) Vapor spray penetration (Schlieren) • Spreading spray angle (Schlieren)
		Reactive condition (15% v O2/ 85% v N2) • Ignition delay (OH* chemiluminescence) • Lift-off length (OH* chemiluminescence)

4.2 Mass Flow Rate



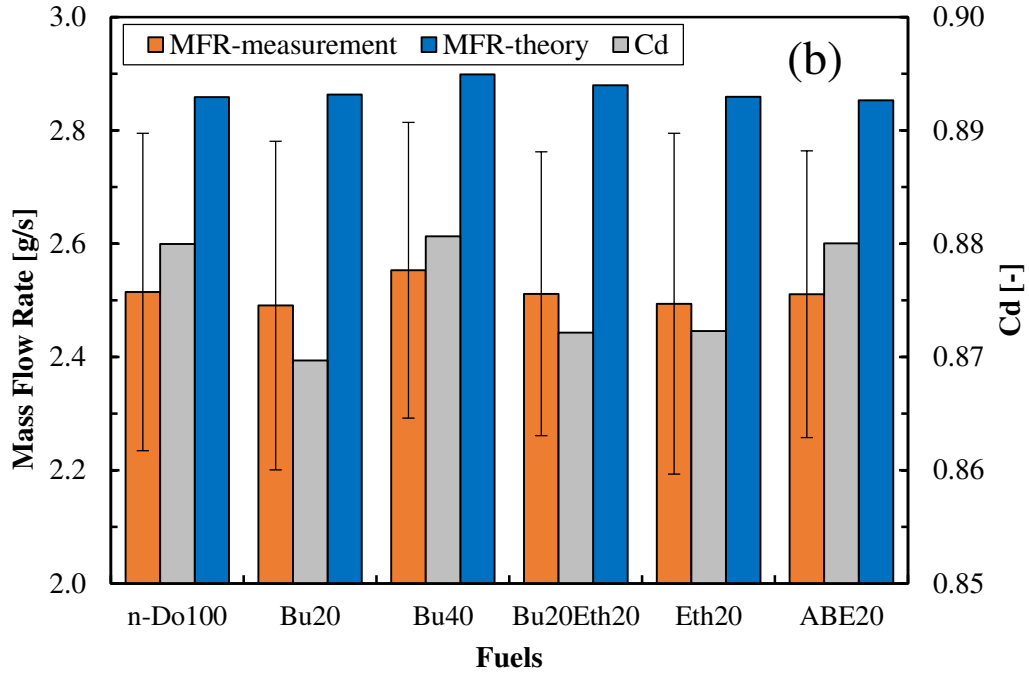


Figure 62 Measured and theoretical mass flow rate at Spray-A conditions: (a) temporal averaged MFR and injection current after SOI for all fuels, (b) averaged MFR calculated between 2 and 3 ms after SOI, theoretical MFR and Cd. Error bars indicate standard deviation during the averaging time.

Figure 62 (a) shows the evolution of measured MFR for all tested fuels as a function of time after SOI. The MFR profiles are globally similar for all fuels, and present the identical initial and end hydraulic delay values, respectively of 310 μ s and 2080 μ s with 0.5% of variation only. Because they have the small difference of fuel density, as the fuel density is the unique fuel property driving the mass flow rate at high injection pressures (from Dernet et al. [58]). The average MFR values deduced from the temporal evolution, **Figure 62** (b)-in orange, are all around 2.51 g/s with the highest value for the ‘highest’ relative dense fuel, Bu40, i.e., 3% higher to the value of n-Do100. Although this difference could be considered within the uncertainties limit due to the measurement technique itself, the theoretical MFR (in blue) calculated by **Eq. 30** remains higher. The difference between measured and theoretical MFR can also be represented by the discharge coefficient (Cd). The variation of Cd presents less than 1% for all fuels around the average value of 0.88, with a maximum of Bu40.

$$\dot{m}_{th} = A_f \cdot \sqrt{(P_f - P_a) \cdot \rho_f} \quad \text{Eq. 30}$$

4.3 Macroscopic Spray Characterization

4.3.1 Liquid Length Penetration

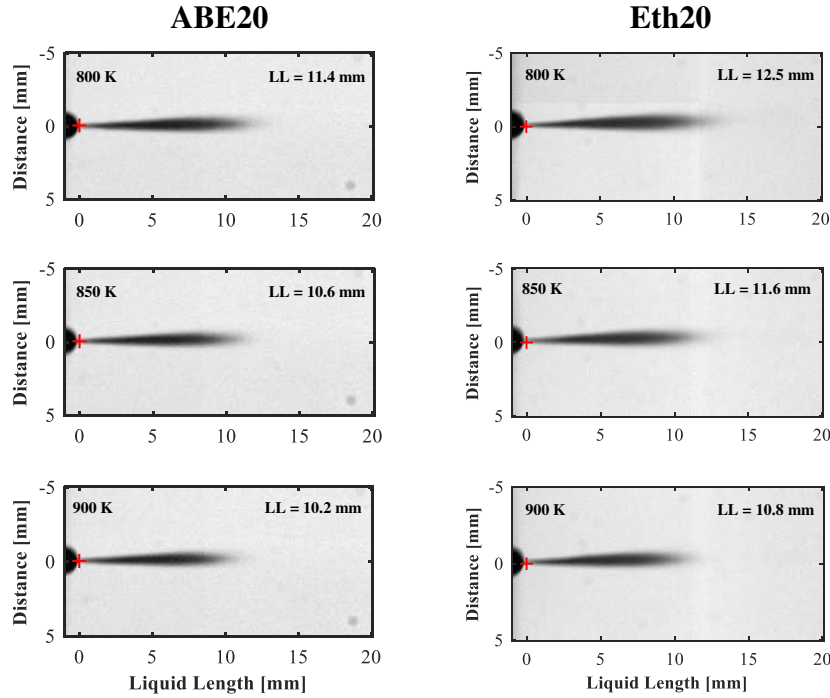
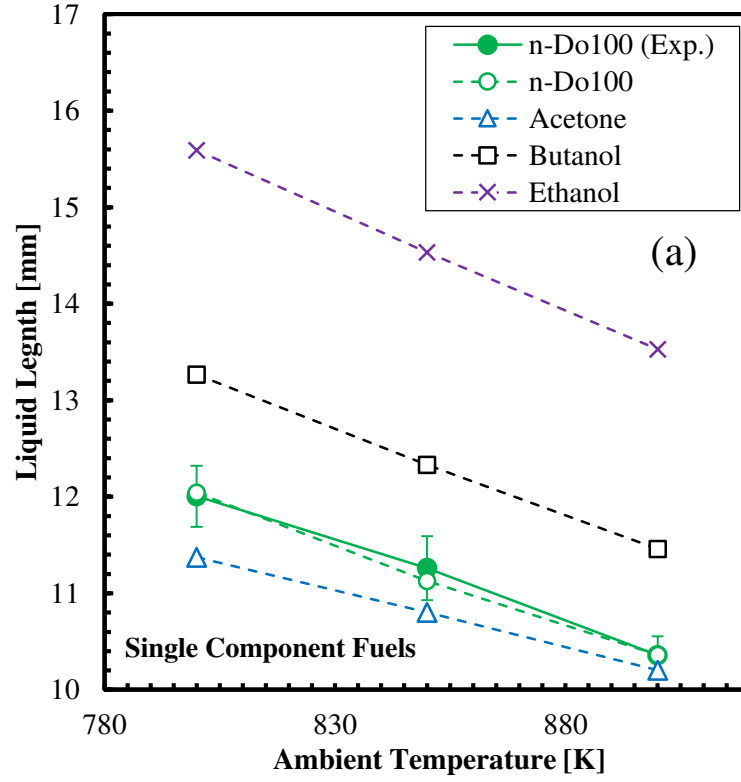


Figure 63 Example of average DBI images for ABE20 and Eth20 for 3 ambient temperatures.

Figure 63 illustrates some averaged images of liquid phase obtained by DBI during the steady state of injection for ABE20 and Eth20 which are presented for the shortest and longest LL, respectively. The feature spray of both fuels is similar with only a small difference of LL around 1 mm, i.e., less than 10% variation. To help the analysis, the LL of single component fuel was estimated from the fuel properties (shown in **Table 20**) by using the well-known scaling law correlation suggested by Naber and Siebers as [34], [44] (**Eq. 6**). The arbitrary constant A was determined by fit the experimental data and set to 1.7 for all fuels, due to the best fit with

the experimental result of n-Do100. To determine the transfer number, B , the steady-state value of surface temperature, T_s is solved by using “Graphic Method”, as described in [139] and described more details in **Appendix C**.



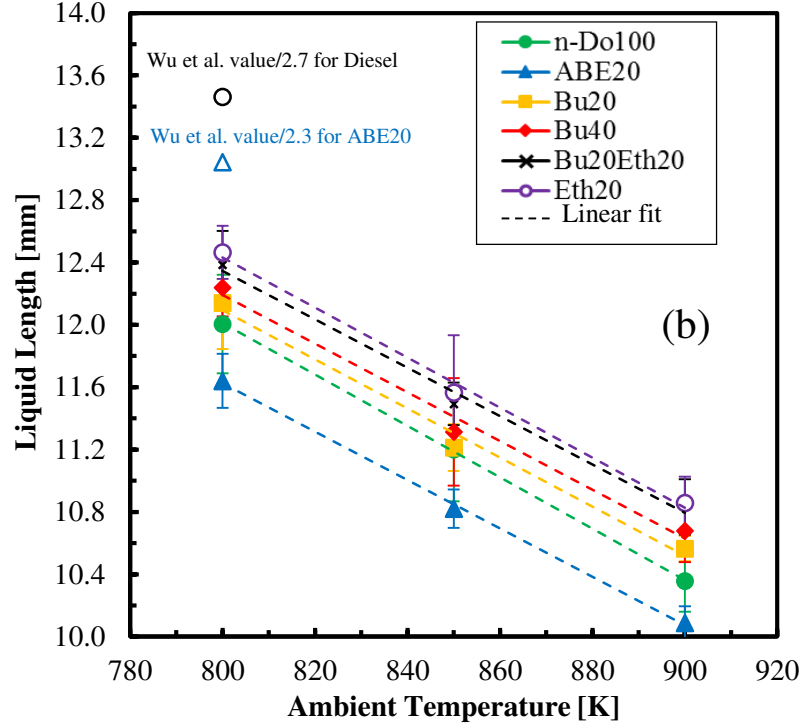


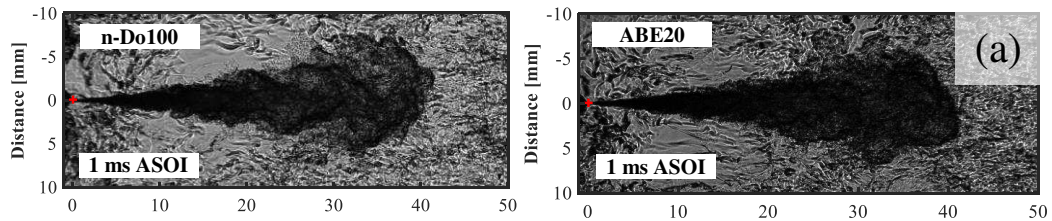
Figure 64 Liquid length results: (a) estimated values for single-component fuels from **Eq. 6** and (b) experimental values for non-reactive conditions for all fuel blends at 3 ambient temperatures. Error bars represent the variation around the average of 12 experimental tests.

The simulated results of single-component fuels in **Figure 64** (a) illustrate the shortest LL are obtained for the highest ambient temperature for all fuels. Indeed, as well known, the increasing of the energy entrainment as a function of the ambient temperature increases the vaporization rate, related to the increase of mass and thermal transfer between ambient and drops of spray. So, the shorter LL is expected at higher temperatures. From the model, LL is dominated by two main properties of fuel, considered in transfer number (B): the volatility (boiling point and vapor pressure) which is considered as the mass transfer from drops of spray to ambient gases, and the latent heat of vaporization (L_v) which is considered as the heat transfer from ambient gases to drops of spray. For the highest volatile fuel, acetone, the mass transfer from drops of spray to ambient gases is easier for lower volatile fuel, leading to shorter LL. While the highest value of L_v for ethanol induces a high local cooling effect, decreasing the local ambient gas temperature and surface temperature leading to decreasing the heat transfer from

ambient gases to fuel drops. Therefore, the reduction of the vaporization rate and a longer LL are expected. As butanol presents properties between both extrema fuels, the LL is between acetone and ethanol. While the lower volatility, n-Do100, has LL between acetone and butanol.

The experimental results for all blends in **Figure 64** (b) show that for ABE20 LL of spray is the shortest for all ambient temperatures and the highest for Eth20 and Bu20Eth20. The shortest of ABE20 is mainly due to the highest volatility of acetone in ABE20 as shown in **Table 20**, as previously observed in [13], [15], [35]. In the case of alcohol blends, the rank of LL is relative to the rank of L_v (**Table 20**): higher L_v provides longer LL as decreasing B coefficient in **Eq. 30**. It is due to the cooling effect, leading to lower heat transfer as explained in the case of single-component fuels. Therefore, due to the lower L_v of Bu40, compared to Eth20 and Bu20Eth20, a shorter LL is obtained. However, for a similar value of L_v , the transfer number B is more dominated by the volatility characteristic as the boiling point and vapor pressure. Even though L_v of Bu20Eth20 is higher than of Eth20, its boiling point is lower and its vapor pressure is in a similar level, leading to higher B and shorter LL. For ABE20 and Bu20, even if the boiling point and L_v are in the same order of magnitude, as ABE is more volatile due to higher vapor pressure, it leads to a shorter LL. The LL results of Wu et al. [13] for diesel and ABE20, estimated of 2.5 after SOI, at the ambient temperature 800 K and oxygen content 16% are added in **Figure 64** (b). Globally as in this study, ABE20 provides shorter LL than diesel. Nevertheless, it is not possible to compare the quantitative values (strongly higher from Wu et al. than from this study) as their ambient density was lower (14.8 kg/m^3) and the injector hole was bigger ($145 \text{ }\mu\text{m}$).

4.3.2 Spray Angle



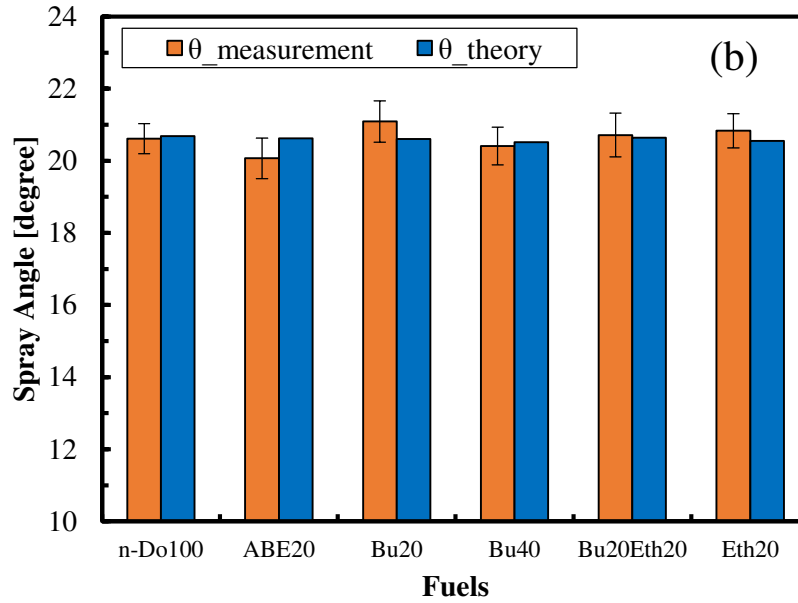
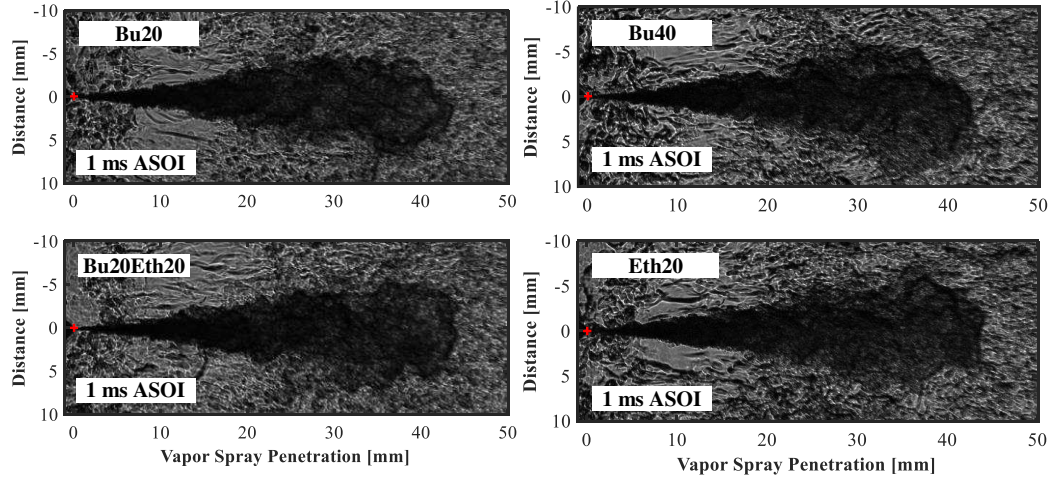
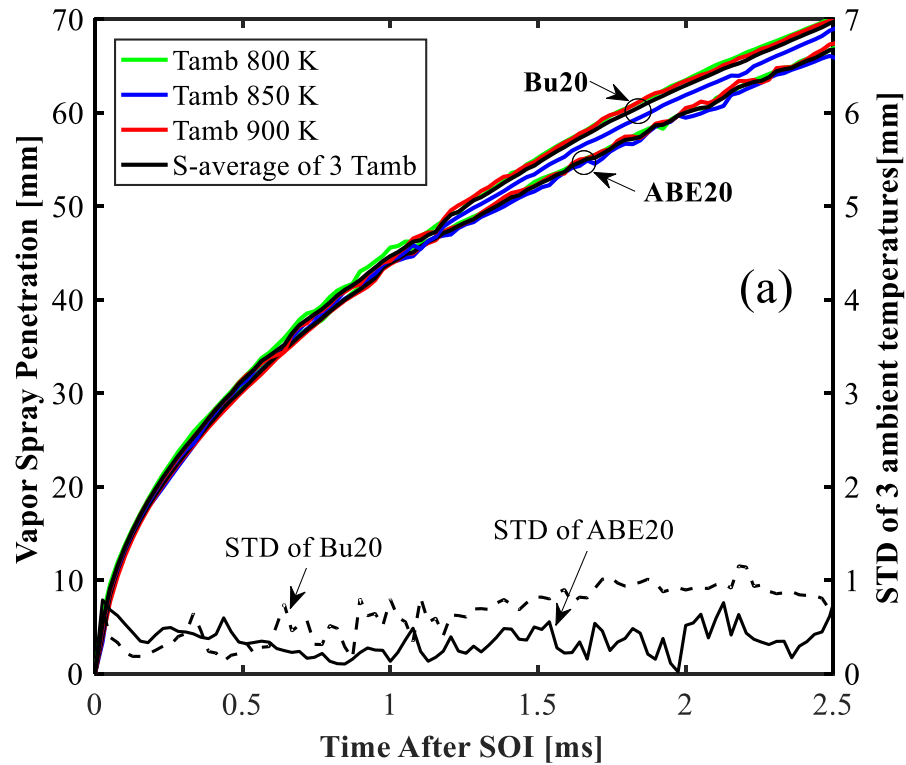


Figure 65 Schlieren images and spray angle result for all fuels at $T_a = 900$ K: (a) Schlieren images at 1 ms after SOI, (b) Comparison result of the experimental spray angles during stabilized period 1.0 to 2.0 ms and the theoretical value estimated by **Eq. 16**. Errors bars represent standard deviations from 12 experimental tests.

Figure 65 (a) presents examples of Schlieren images for all fuels, at 1 ms after SOI, $T_a = 900$ K. The red-cross symbolizing presents the position of injector tip. The contrast between the ambient gases background (gray) and the spray region (black) is due to the difference of the

refractive index due to the different density. The global shape of spray is similar for all fuels, especially of the spreading spray angle. The experimental averaged value of the spray angle (plotted in **Figure 65** (b)-in orange) is around 20.6 degrees with 1.7% of variations due to the low fuel density variation itself around 3%. The theoretical values (in blue) were calculated from the empirical correlation suggested by Siebers [34] as in **Eq. 16**. The c is an empirical constant recommended to be set to 0.26 for three fuels (heptamethylnonan, n-hexadecane and a standard diesel fuel) [34]. In the case of n-Do100 and alcohol blends studied in this study, c was set to 0.37 to minimize the difference between theoretical and measurement values. As the ambient density was maintained constant at 22.8 kg/m^3 for all conditions, the variation of the spray angle is only relative to fuel density variation. From the **Eq. 16**, the difference in fuel density involves a very low difference of 0.3% of the spray angle value.

4.3.3 Vapor Spray Penetration



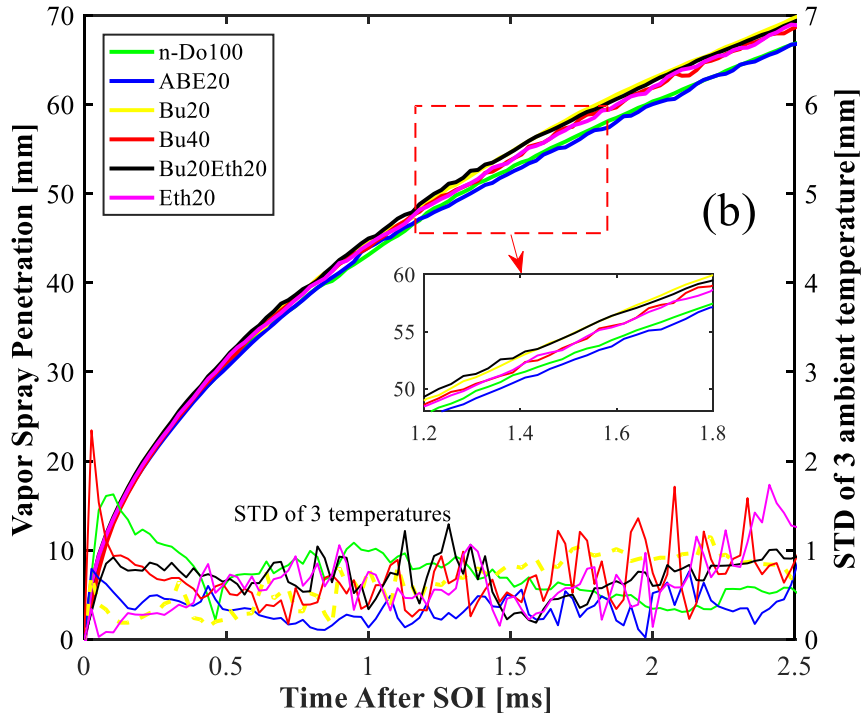


Figure 66 Vapor spray penetration in non-reactive conditions (a) for ABE20 and Bu20 for 3 ambient temperatures (b) for all blends, average and standard deviations on the 3 temperatures.

Figure 66 (a) shows the temporal evolution of vapor spray penetration, S , after SOI for ABE20 and Bu20 for 3 ambient temperatures in non-reactive condition. The difference for the ambient temperatures is very small as indicates the standard deviation from the average of the three evolutions (less than 1.5 mm or 3% in average). Indeed, the vapor spray penetration depends mainly on the spray momentum, mainly controlled by the injection pressure and the ambient gas pressure. For ambient temperatures of 800, 850 and 900 K, the ambient pressure changes respectively as 54.2, 59.0 and 60.9 bar to maintain an ambient density at 22.8 kg/m^3 , as seen in **Table 9**. Therefore, the small difference in the pressure drop at the injector tip for the 3 ambient temperatures leads to a very similar S evolution. The average of S obtained from the 3 ambient temperatures is plotted for all test fuels to compare the effect of fuel properties in **Figure 66** (b). Due to the small difference in fuel density, S can be considered similar for all blends especially until 1 ms after SOI. However, around 0.5 ms later the blends with higher fuel

density, i.e., Bu20, Bu40 and Bu20Eth20 have a slightly further S due to higher momentum. However, the rank of S from the first group of blends does not agree with the density rank. The simulation code, available on ECN website, based on the model of the Musculus and Kattke [61], was used to simulate the effect of fuel on S. As example, comparative results between experimental and simulated data are presented in **Figure 67** for n-Do100 and Bu40 to illustrate fuel density effect. The difference between simulation and experimental data is small (less than 1.5% in average for n-Do100 and 1.0% for Bu40) and between both fuels, maximum of 4% which is in good agreement with the 3% of the difference in fuel density.

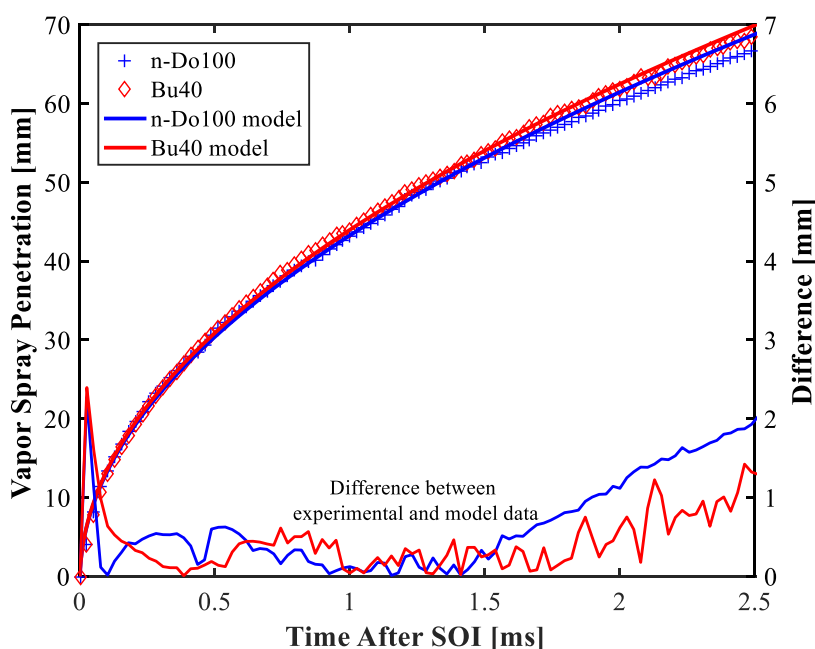
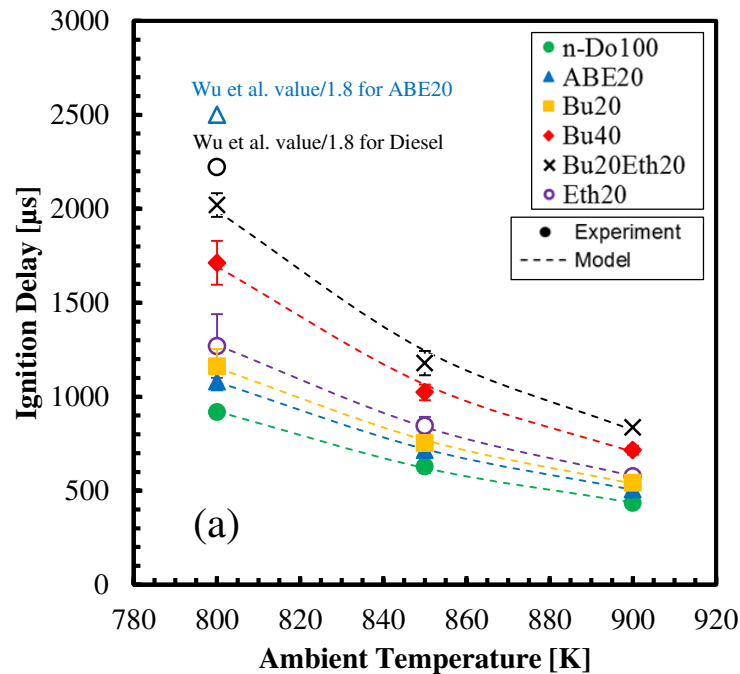


Figure 67 Comparison between experimental and simulated results of the vapor spray penetration for n-Do100 and Bu40.

4.3.4 Ignition Delay

The experimental results of the ID for all fuels as a function of ambient temperature are plotted in **Figure 68** (a). According to power-law empirical correlations of Pickett and coworker presented in **Eq. 31** [69], [73] (see more details in **Chapter 1**), the accuracy of the experimental results are validated by the trend of the simulated ones (dot line), which matched very well with

experimental results. The ID values are the main flame ignition delay, corrected by the hydraulic delay obtained from Schlieren images in each test. As expected, ID for all fuels decreases as the ambient gas temperature increases due to the higher reaction rate [69], [71]. The rank of the fuels from the longest to shortest ID is as follow: Bu20Eth20/Bu40/Eth20/Bu20/ABE20/n-Do100. As the ignition delay is composed of physical and chemical ignition delays, the physical delay is dominated by spray atomization and vaporization process, while the chemical delay is influenced by the chemical reaction rate. Indeed, the ability of auto-ignition is mainly linked to the Cetane Number (CN). In the case of simple alcohol component blends, a higher proportion of butanol, Bu40 as its CN is equal to 17 provides higher ID than Bu20 and Eth20, while the highest CN of 74, n-Do100 has the lowest ID. In the case of Bu20Eth20, even if it is difficult to estimate the CN, the rank of ID indicates that the CN is certainly the lowest one. In the case of ABE20, it is first confirmed that the ID is lower than other kinds of alcohol blends for all ambient temperatures. Even though the CN of ABE20 is not known, it should be lower than n-Do100 due to the different components with lower CN, inducing longer ID.



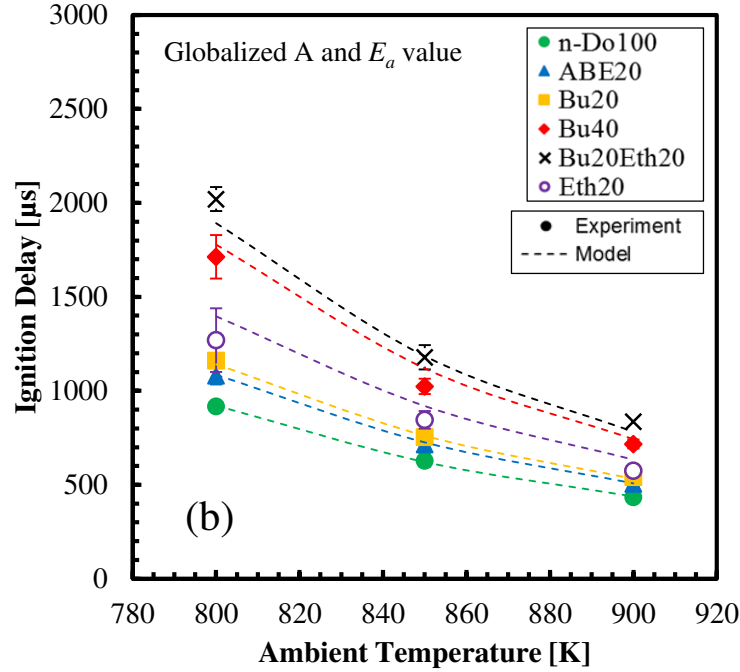


Figure 68 Experimental and simulated data of ignition delay: (a) for all fuel blends as a function of the 3 different ambient temperatures, with error bars from 12 experimental tests and (b) the simulated data calculated by using the globalized A and E_a values.

According to the empirical correlation given by Pickett and coworkers presented in **Eq. 18**, the original version takes into account the stoichiometric mixture fraction, Z_{st} to estimate the effect of oxygen concentration in the ambient gases [69], [73]. However, even if the oxygen concentration in ambient gas in this work was set constant at 15%v for all ambient conditions, the Z_{st} of each fuel is not constant as presented in **Table 20**, because its determination (**Eq. 20**) does not only take into account on oxygen content in the ambient gases but also oxygen content in fuel especially alcohol blends. As a result, the Z_{st} is increased by increasing of oxygen content in fuel. Moreover, the relationship between the oxygen content in fuel and ID presented the opposite trend with the oxygen content in the ambient gases and ID: increasing of the oxygen content in fuel performed the longer ID, while ID shortened by increasing oxygen in ambient gases. Therefore, to avoid this ambiguity the Z_{st} is not presented in the empirical correlation of ID and LOL in this study, as presented by:

$$\tau_{ID} = A \cdot \exp\left(\frac{E_a}{RT_a}\right) \cdot \rho_a^{-1.3} \quad \text{Eq. 31}$$

To clearly explain about ID results, the pre-exponential constant (A) and the apparent activation energy (E_a) of the empirical correlation **Eq. 31** for all fuels are presented in **Table 22**. The value of E_a provides an indication about the energy needed to start the auto-ignition process [10], [140]. The ID results are significantly related to E_a values: the ID for n-Do100 is the shortest with lowest the E_a (44.7 kJ.mol⁻¹), while it is the longest one for Bu20Eth20 with highest E_a (52.9 kJ.mol⁻¹). For 20%v blends, E_a values are in the same range around 46.2 kJ.mol⁻¹. Meanwhile, E_a of the 40%v blends is around 52.6 kJ.mol⁻¹. The pre-exponential factor, A takes into account the effect of fuel properties on the complex phenomena of ID process. From **Table 20**, to find a link between A and fuels properties is not evident. The rank of ID follows the order of E_a , representative of the chemical reaction process. Moreover, as the ambient temperature for this study is strongly higher than the boiling temperature of all fuels, the atomization and vaporization processes induce a short physical ignition delay.

The results of Wu et al. [13] indicated in **Figure 68** (a) confirm the longer ID for ABE20 than diesel fuel. Sure the blend was not done in n-dodecane, therefore it was not expected a perfect quantitative agreement, but the difference between diesel and n-dodecane is too high. In fact, the values of ID are not the same range, not only due to the operating conditions (i.e. the fuel) but also to the different measurement technique for ID, i.e., it was determined from the heat release rate and the fact that these values were not corrected by the hydraulic delay of injection.

The values of A and E_a are averaged for three groups: single fuel (n-Do100), 20%v blend and 40%v blend as presented in **Table 22**. The ID estimates by considering these average values of A and E_a are plotted in **Figure 68** (b). A good agreement with the experimental data is obtained for all fuels with the value of R^2 (the coefficient of the correlation), higher than 0.97, as shown in **Table 22**, except for Eth20. Indeed, the estimated data are slightly higher, especially at lower ambient temperature. To improve more the correlation, more data are necessary by completing the fuel matrix and wide the operating conditions range.

Table 22 Estimate of Arrhenius coefficients of ignition delay for all fuels.

Fuel	A [μ s]	E_a [kJ/mol]	R^2 [-]
n-D100	65.1	44.7	0.99
ABE20	67.3	45.5	0.99
Bu20	69.2	45.8	0.99
Eth20	60.6	47.3	0.99
Bu40	37.9	52.3	0.99
Bu20Eth20	40.6	52.9	0.99
Globalized A and E_a value			
ABE20	65.7	46.2	0.99
Bu20			0.99
Eth20			0.92
Bu40	39.2	52.6	0.97
Bu20Eth20			0.97

4.3.5 Lift-Off Length

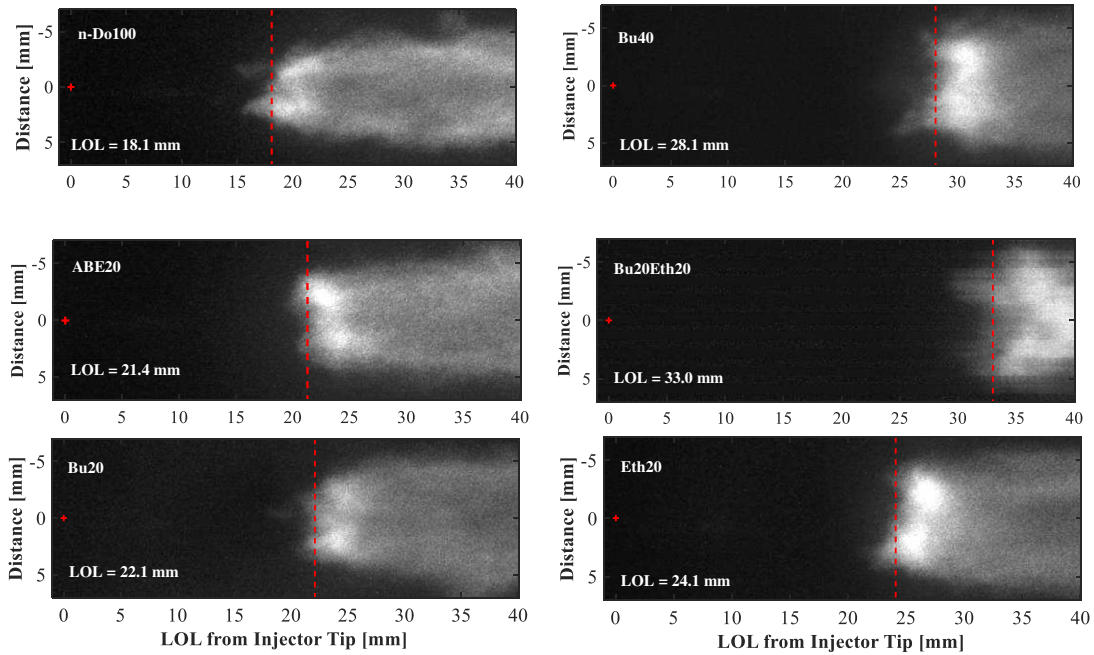


Figure 69 Examples of OH* images for all fuel blends at ambient temperature 850 K. The red line indicates the average LOL.

Figure 69 illustrated some OH* chemiluminescence images during quasi-steady period of mixing-controlled combustion for all fuels at 850 K. The stabilized flame position of ABE20 and Bu20 are the closest to the position of n-Do100 but this position moves further to downstream for the other alcohol blends.

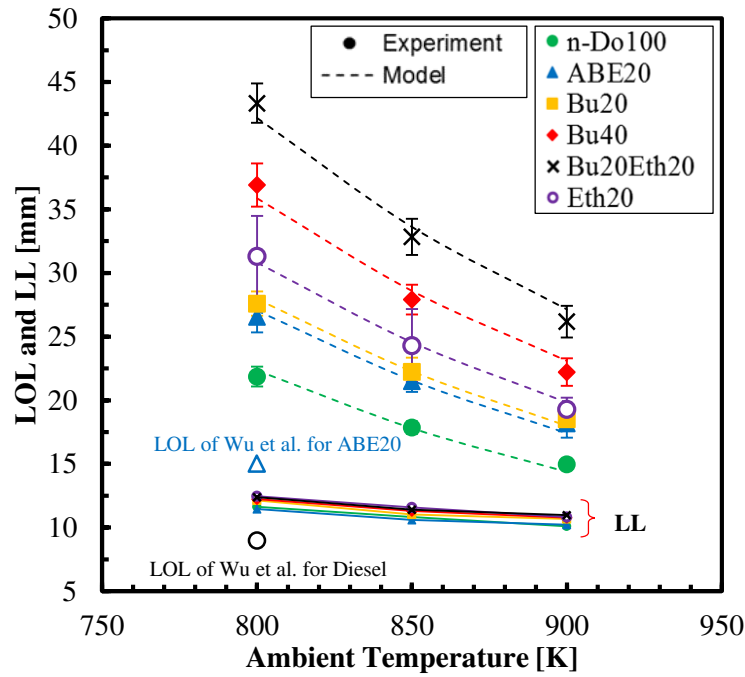


Figure 70 LOL and LL results for 3 ambient temperatures and all fuel blends. Error bars indicate statistical standard deviation from 12 tests.

Figure 70 presents LL and LOL values obtained for all conditions and fuels. As all LOL are longer than LL for all fuels, most of the fuels are completely vaporized before reaching the reaction zone, especially at the highest ambient temperature. This implies that the fuel properties involved the fuel atomization and vaporization, i.e. the volatility and the latent heat of vaporization, would be less effect on the stabilized flame location. As seen in several works [15], [69], [71], [76], an increase of ambient temperature results in a faster local reaction rate, allowing the flame to stabilize closer to the injector but this effect does not seem linear. This is also combined with faster evaporation and mixing processes, due to shorter LL with the increase

of ambient temperature. The LOL empirical correlation of Pickett and coworkers [69], [73] in **Eq. 19** was considered to evaluate LOL. As described before in **Eq. 31**, the Z_{st} does not take into account for this study. Therefore, it can be rewritten by **Eq. 32** and the simulated LOL results are plotted in dot-line which matched very well with experimental results.

$$LOL = C \cdot T_a^{-3,74} \cdot \rho_a^{-0,85} \cdot d^{0,34} \cdot U^1 \quad \text{Eq. 32}$$

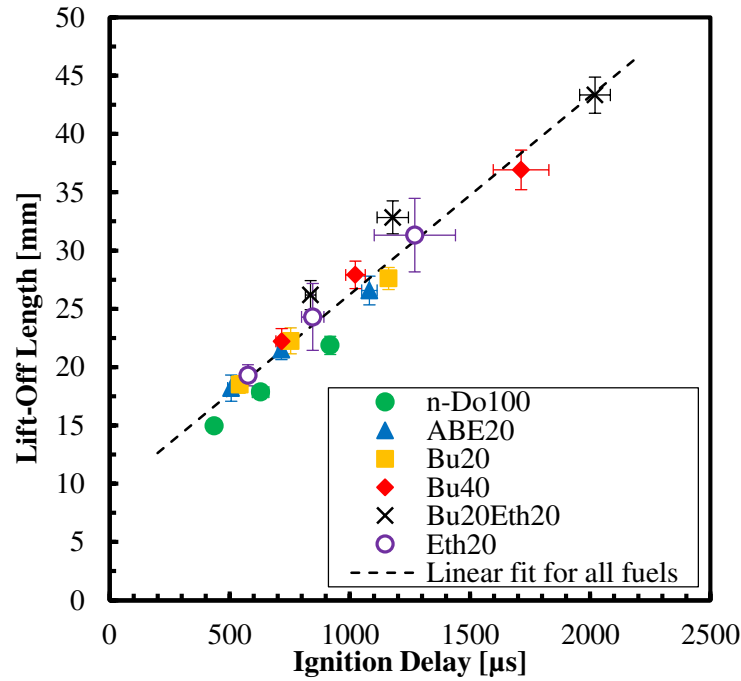


Figure 71 Evolution of LOL as a function of ID for all test fuels.

The rank of LOL from the longest to shortest is Bu20Eth20/Bu40/Eth20/Bu20/ABE20/n-Do100, similar to the ID one. This is highlighted by **Figure 71**, where the linear dependency between ID and LOL is evident for all fuels as found in [69], [68]. By following the assumption of Donkerbroek et al. [68], the upper limit of LOL can be obtained by balancing fuel injection velocity and flame speed. When the ambient temperature and density are sufficiently high to promote auto-ignition before the fuel reaches

the lift-off location, the LOL is likely governed by ignition chemistry. Therefore, the LOL is pulled close to the injector tip. This implies which fuel has a higher ability of auto-ignition, i.e., higher CN (or shorter ID) will have a shorter LOL. The LOL results from Wu et al. are also indicated in **Figure 70**. As in their work [10], LOL was not constant and decreased as a function of time. Therefore, to compare with the present study, the values given here from Wu et al. data are estimated at 4.5 ms after SOI, to avoid the transient phase during the start and the stop of injection. The LOL for ABE20 is also longer than diesel but strongly shorter than the present work, mainly due to the difference of measurement technique (natural flame luminosity for all spectrum 400-1000 nm).

To compare the effect of fuel on LOL, a “ LOL_{scaled} ” can be calculated from the LOL results, $LOL_{measured}$, normalized by a reference condition. As only the ambient temperature varies in this study, the reference condition T_{ref} is taken at 900 K. Then, the empirical correlation given by Pickett and coworkers [69], [73] in **Eq. 32** can be rewritten in **Eq. 33**:

$$LOL_{scaled} = LOL_{measured} \left(\frac{T_{ref}}{T_{amb}} \right)^{-3.74} \quad \text{Eq. 33}$$

with T_{amb} the ambient temperature. In **Figure 72**, the average value of LOL_{scaled} is plotted as a function of the oxygen mass content in fuel for the 3 ambient temperatures. As expected from previous works [69], [71], the increase of oxygen content in fuel leads to a longer LOL for all ambient temperatures. According to the assumption of Manin et al. [71], they computed the flow velocity of spray and the distribution of the stoichiometric mixture fraction (Z_{st}) from the Musculus and Kattke model. They found that at one given residence time, higher Z_{st} provides higher flow velocity value and a mixture fraction distribution, closer to the spray axis. So, as Z_{st} increases with the increase of oxygen content in fuel, the further LOL of the highest oxygen content fuel would be expected to stabilize downstream, as the air-fuel mixture travels further away along the stoichiometric mixture fraction contour because of higher flow velocity on this contour. This assumption is clearly found in the case of similar Cetane Number and different oxygen content in fuel. But in the case of different CN of fuel, the trend of LOL is related to CN. This implies that the CN would be the main dominating fuel properties on LOL, while the oxygen content in the fuel can be considered as a minor property. Therefore, the longer LOL of

alcohol fuels would be induced by the combined effect of the lower CN and higher oxygen content.

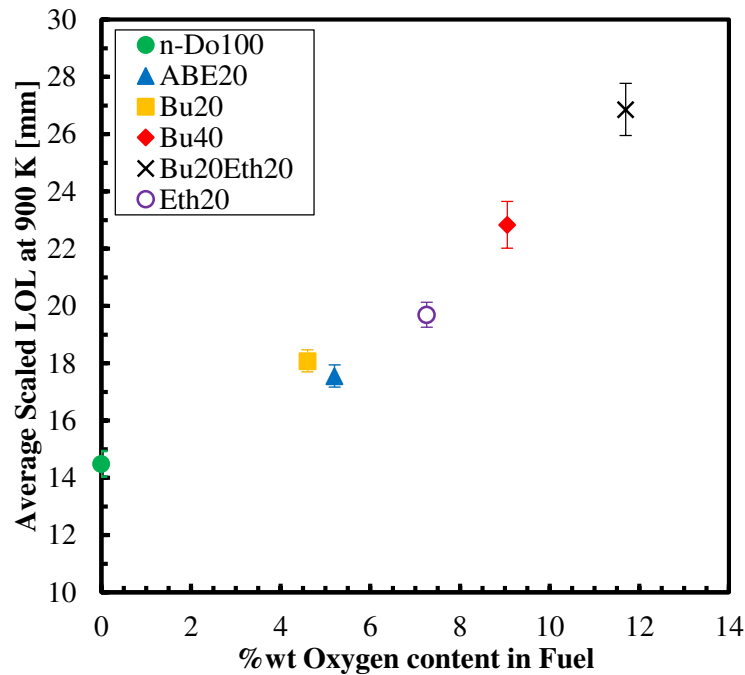


Figure 72 Effect of fuel properties on scaled LOL as a function of %wt oxygen content in fuel, at the reference condition 900 K.

4.4 Conclusion

The characterization of spray and combustion parameters of different alcohol blends (ABE20, Bu20, Bu40, Bu20Eth20 and Eth20) were investigated and compared to n-Do100. The main conclusions are summarized:

- 1) Due to the slight difference in fuel density, the mass flow rate, the vapor spray penetration and the spray angle can be considered similar for all fuels blends.
- 2) ABE20 presents a shorter liquid length compared to other fuels due to its highest volatility, which favors the vaporization process. Moreover, as its ability of auto-ignition (cetane number) is expected higher than the other alcohol blends, its lift-off length and ignition delay are also closer to pure n-Do100 for all ambient temperatures, which concludes the high possibility of using ABE20 as Diesel substitute fuel.

- 3) The linear relationship between the lift-off length and ignition delay for all conditions is verified for all fuels, even if their oxygen content is different. The lift-off length is strongly linked to the auto-ignition ability of the fuel but also to the oxygen content in fuel. However, it seems that the latent heat of vaporization and the volatility of fuels have also to be considered due to the effect on the evaporation process in upstream of lift-off length, to predict the effect of blends.
- 4) The increase of butanol and the addition of ethanol in blends increase the LL due to the cooling effect from the latent heat of vaporization, and LOL and ID because of the lower ability of auto-ignition and higher oxygen content for all blends. Due to the presence of Acetone in ABE, the competition between all properties of fuel components in the blending fuel provides different behaviors of ABE spray.

CHAPTER 5

EFFECT OF ABE-DODECANE BLEND IN DIFFERENT VOLUME RATIO ON DIESEL SPRAY AND COMBUSTION CHARACTERISTICS

5.1 Introduction

In the previous chapter, the specificities of ABE20 spray and combustion were studied in comparison to different alcohol blends. As Bu20 and ABE20 can be considered as a fuel for CI engine due to the spray and combustion characteristics close to n-dodecane. However, according to the suggestion of Wu et al. about the critical ratio of ABE in the blend [13], this chapter will present a study of the non-linear behavior of the blending ratio of ABE, especially focused between 20%v and 50%v, in order to reveal the suitable ratio of ABE for CI engine. Various volume fractions of ABE (20%v, 30%v, 40%v and 50%v) were selected to blend with n-dodecane (n-Do100), labeled as ABE20, ABE30, ABE40, ABE50, respectively. The ratio of Acetone-Butanol-Ethanol mixture was 3:6:1 with the same single fuel components used in **Chapter 4**. The physical properties of all pure fuels and blends are summarized in **Table 23**. Values of density and viscosity were measured by Anton Paar model SVM™ 3000. It can be noted, the density of the blend fuel increases as ABE quantity increases but only 3.1% of the difference between n-Do100 and ABE50 can be observed. As expected, the increase of ABE quantity decreases the viscosity and the boiling point, due to the increase of alcohol fuels in the blend. Both of the vapor pressure and the latent heat of vaporization (L_v) dramatically increase with the ABE ratio: up to 250% of different between n-Do100 and ABE50 for vapor pressure, and up to 33% for L_v . Last, the oxygen content and Z_{st} increase as a function of ABE content. It can be noted that the values are in the same range of other alcohol blends studied in **Chapter 4**, allowing stronger analysis about the effect of these parameters on combustion characteristics.

All fuels were investigated in the NOSE at the high-pressure and high-temperature conditions of the Spray-A, defined by ECN. For all experimental conditions, set-ups and post-processing were carried out the same as characterization alcohol blends in **Chapter 4**, summarized in **Table 24**.

Table 23 Fuel properties [15], [135], [136], [137], [138].

Properties	n-Do100	Acetone	Butanol	Ethanol	ABE20	ABE30	ABE40	ABE50
Molecular formula	C ₁₂ H ₂₆	C ₃ H ₆ O	C ₄ H ₁₀ O	C ₂ H ₆ O	C _{8.5} H _{18.6} O _{0.4} ^a	C _{7.3} H _{16.3} O _{0.5} ^a	C _{6.4} H _{14.4} O _{0.7} ^a	C _{5.7} H _{12.8} O _{0.7} ^a
Density at 15°C [kg/m ³]	752.8	789	813.3	794.1	760.7	766	771	776
Viscosity at 15°C [mm ² /s]	2.032	0.149	4.119	1.489	1.642	1.558	1.471	1.388
Lower heating value [MJ/kg]	44.1	29.6	33.1	26.8	41.5 ^b	40.2 ^b	38.9 ^b	37.7 ^b
Cetane number [-]	74	-	17	8	-	-	-	-
Boiling point [K]	489	329	391	351	464 ^b	451 ^b	439 ^b	427 ^b
Vapor pressure at 298 K [kPa]	0.02	30.80	0.58	7.91	2.17 ^b	3.22 ^b	4.25 ^b	5.28 ^b
Latent heat of vaporization at 298 K [kJ/kg]	362	518	582	904	411 ^b	435 ^b	459 ^b	482 ^b
Oxygen concentration [% by mass]	-	27.6%	21.6%	32%	5.2%	7.7%	10.3%	12.7%
Stoichiometric mixture fraction, Zst [-]	0.0460	-	-	-	0.0489	0.0506	0.0522	0.0540

Note: ^a Equivalent formula based on mole fraction.

^b Properties estimated from a mass fraction of single-component fuels in the alcohol blends.

Table 24 Testing condition summarization for the ABE-dodecane blends.

Fuels	Ambient Condition at SOI timing	Studying Parameters and Measurement technique
• n-Do100 (reference fuel) • ABE20 • ABE40	• P_{amb}: 60 bar • P_{inj}: 1500 bar • T_{inj}: 293 K • Injection Duration: 1.5 ms • Injection number: 20 injections/test • Testing Number: 3 tests	• Mass flow rate • Hydraulic delay • Cd
• n-Do100 (reference fuel) • ABE20 • ABE30 • ABE40 • ABE50	• P_{amb}: 60 bar • T_{amb}: 800, 850, 900 K • ρ_{amb}: 22 kg/m³ • P_{inj}: 1500 bar • T_{inj}: 363 K • Injection Duration: 1.5 ms • Testing Number: 12 tests	Non-reactive condition (Pure N2) • Liquid length penetration (DBI) • Vapor spray penetration (Schlieren) • Spreading spray angle (Schlieren)
		Reactive condition (15% v O₂/ 85 % v N₂) • Ignition delay (OH* chemiluminescence) • Lift-off length (OH* chemiluminescence)

5.2 Mass Flow Rate

As presented in the previous chapter, MFR mainly depends on the fuel density, therefore only ABE40 was selected to measure the MFR in order to compare with the n-Do100 and ABE20 which is presented in the previous chapter. **Figure 73** (b) presents the temporal evolution of measured MFR as a function of time for these 3 fuels. According to the criterion to determine the initial hydraulic delay, the same start and end of injection was found around 304 μ s and 3500 μ s or less than 1% of the variation. The MFR profile indicates a similar global trend, with a slight difference in fuel density. This is confirmed in **Figure 73** (b) as the average MFR of ABE blends is higher than n-Do100 (between 2.2% and 4.3% related to 1% to 2.4% of density increase), as predicted the theoretical MFR calculated from **Eq. 3 (Chapter 1)**. The difference between measured and theoretical MFR can be considered as the discharge coefficient (Cd), which slightly increases with the increasing of ABE ratio in the blend. This confirms that the fuel density is the unique fuel property driving the MFR at high injection pressure as presented in the previous study [58], [141].

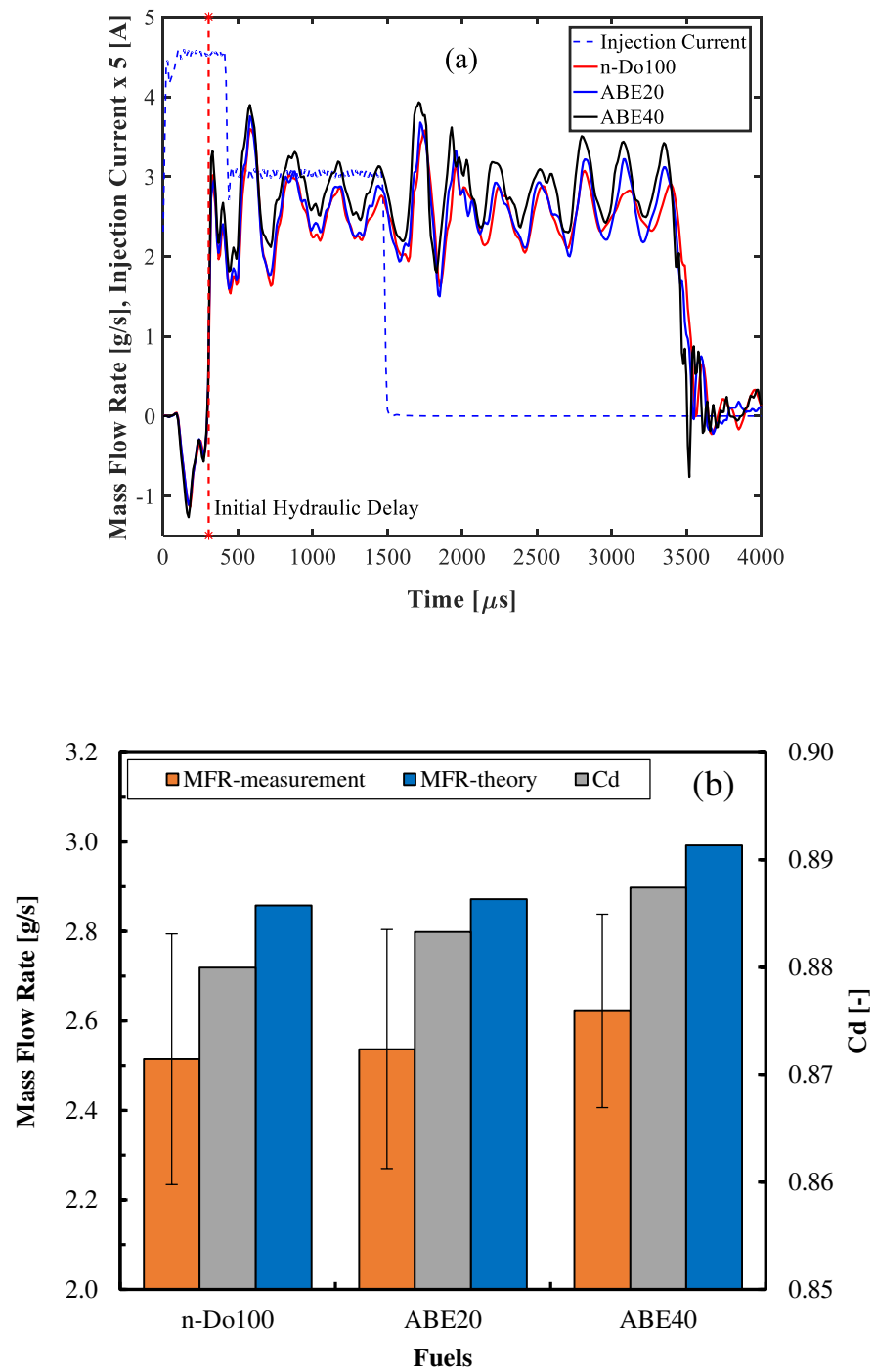


Figure 73 Mass flow rate results: (a) MFR profile and (b) averaged MFR, theoretical MFR and Cd.

5.3 Macroscopic Spray Characterization

5.3.1 Liquid Length Penetration

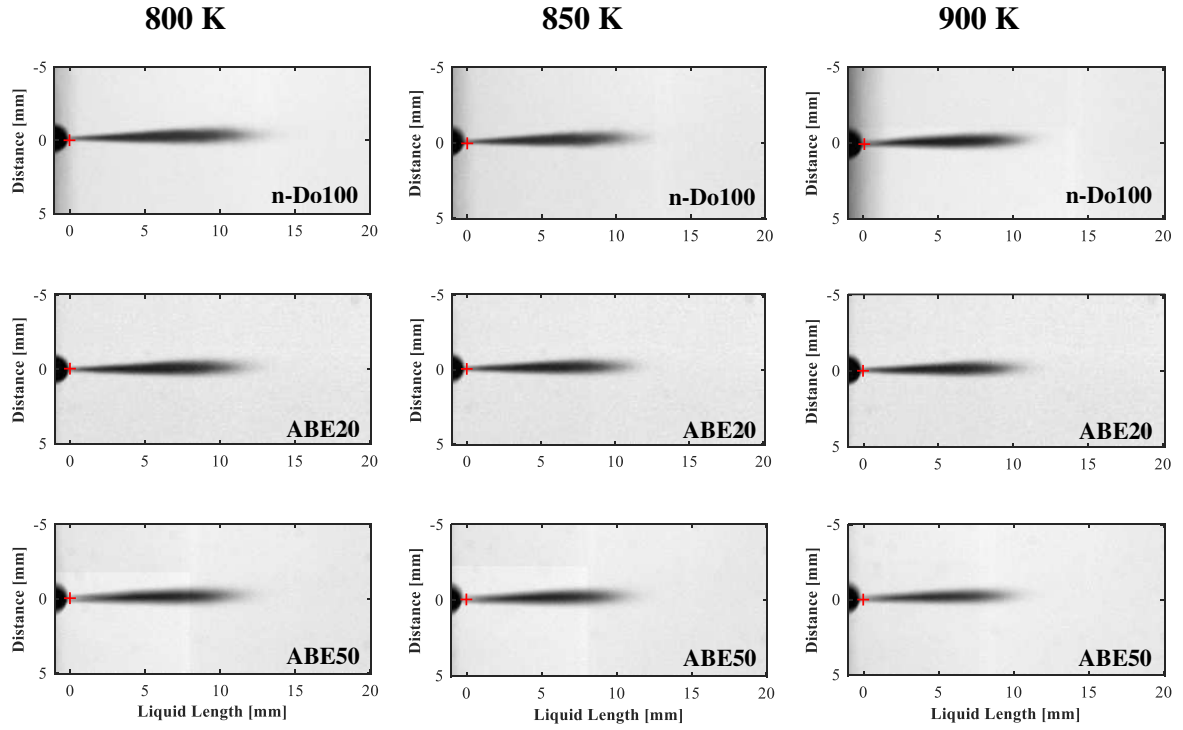


Figure 74 Average DBI images at the three ambient temperatures for n-Do100, ABE20 and ABE50.

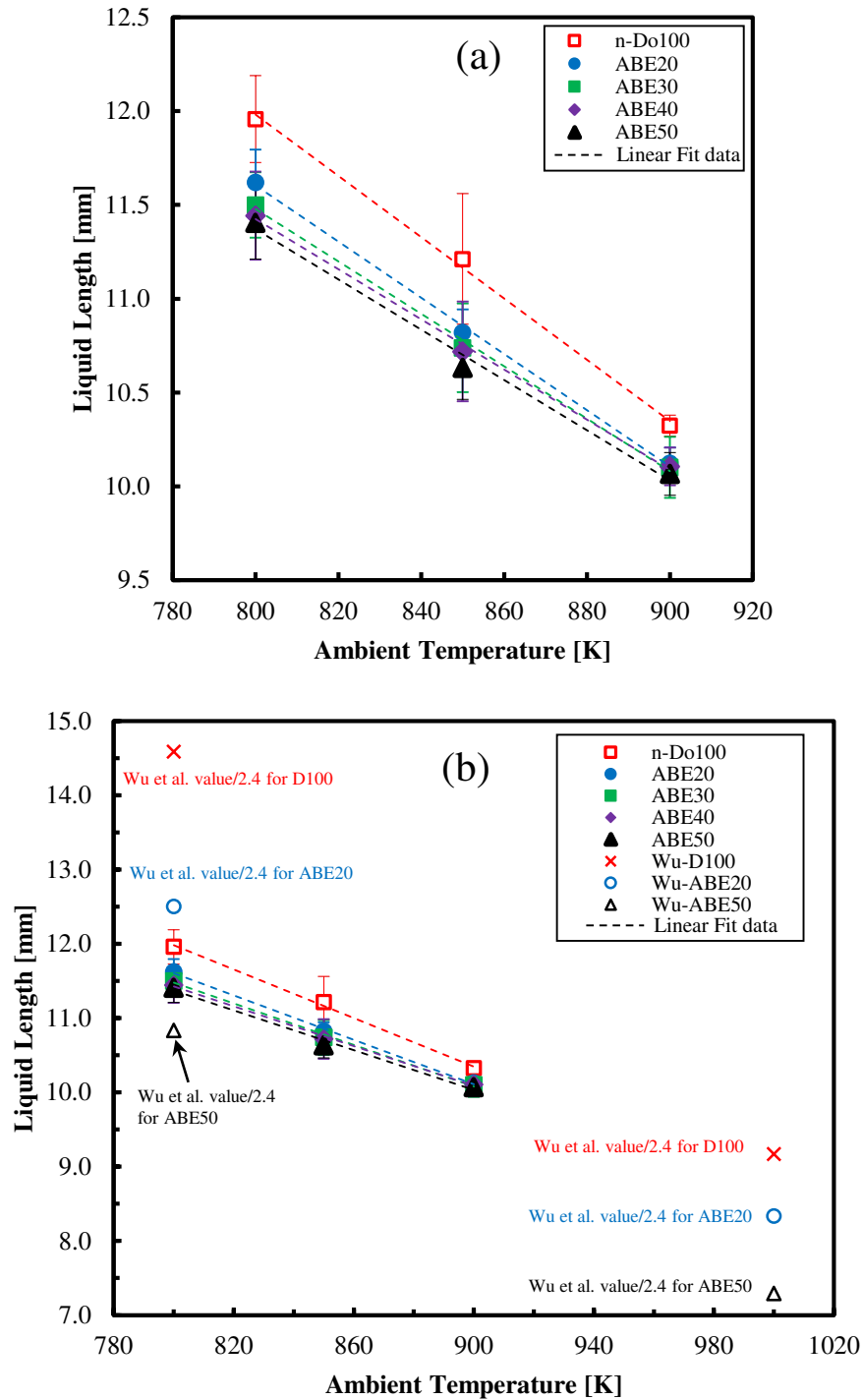
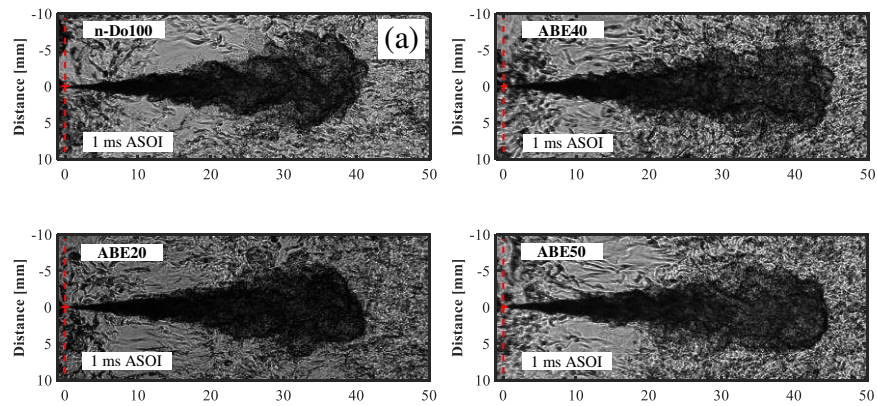


Figure 75 Experimental results of liquid lengths: (a) all ABE blends, the dot-lines represent the linear-fit as a function of the ambient temperatures, and (b) comparison with Wu et al.'s experimental results at 800 and 1000 K [13].

Figure 74 illustrates an example of averaged images of liquid phase of 3 fuels obtained by DBI during the steady state of injection for the 3 ambient temperatures. The experimental LL for all fuels are plotted in **Figure 75** (a): as expected ([13], [33], [35]), the increase of the ambient temperature induces a shortening of LL due to the increase of the energy entrainment with the increasing of ambient temperature. Therefore, the vaporization rate relates to the increasing of mass and thermal transfer between liquid fuel and ambient gases which is illustrated in the simulated LL of single component fuel estimated by using the Naber-Siebers scaling law correlation [34], [44] in **Figure 64** (a).

As expected, the LL results for ABE blends are shorter than n-Do100 due to the higher volatility of ABE fuel and higher acetone in the blends, requiring less energy to vaporize the liquid fuel. The data from Wu et al. [13], for diesel, ABE20 and ABE50 are plotted to compare with this study in **Figure 75** (b), but at different ambient conditions: 16%v of oxygen and at 800 and 1000 K. According to they plotted in their paper only temporal evolution of LL, to compare their result with this study, the data at 2.5 ms after SOI were extracted. It can be expected, their trend as a function of the ambient temperature and of the ABE content are accorded with this work, but the quantitative values are absolutely not in the same order of magnitude. Due to the efforts dedicated during ECN France to reach ECN standards, the values from this study have to be more realistic.

5.3.2 Spray Angle



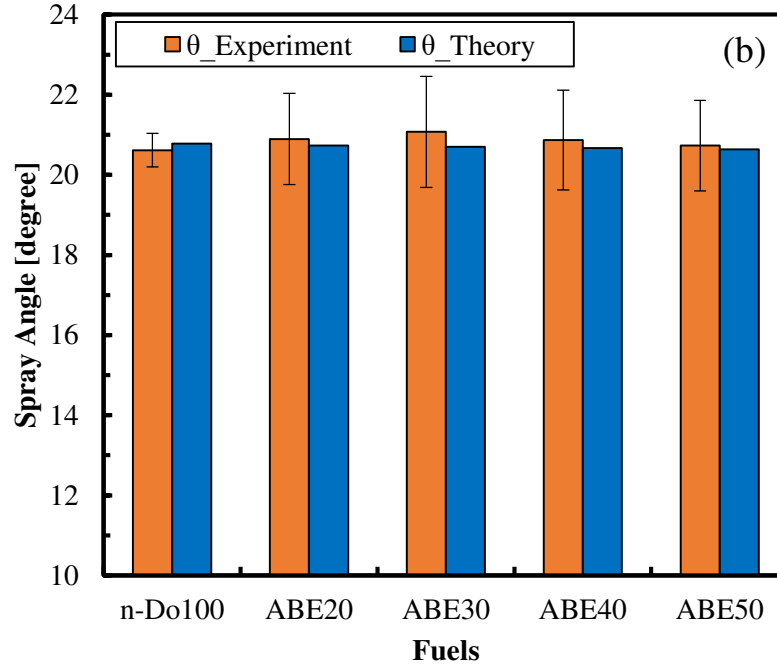
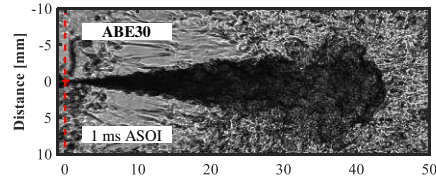
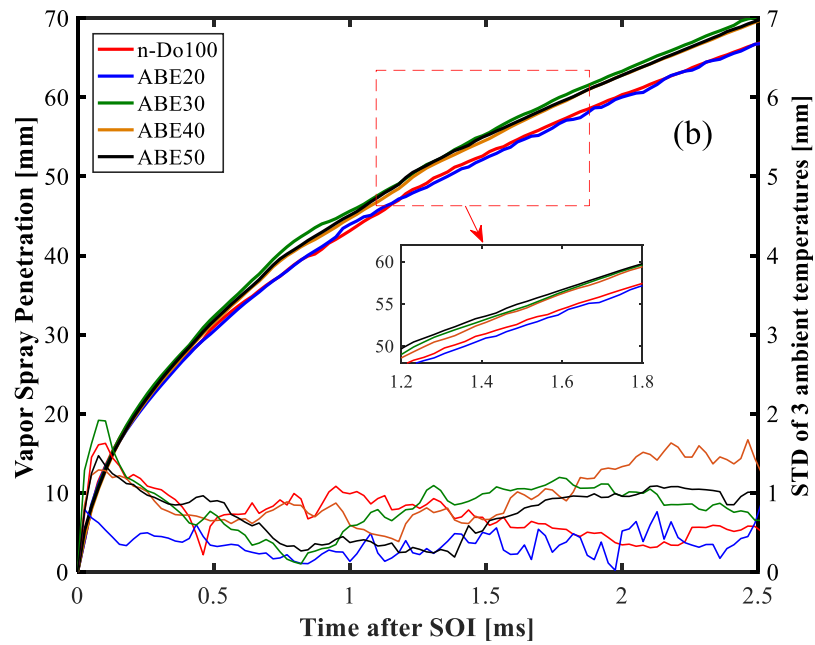
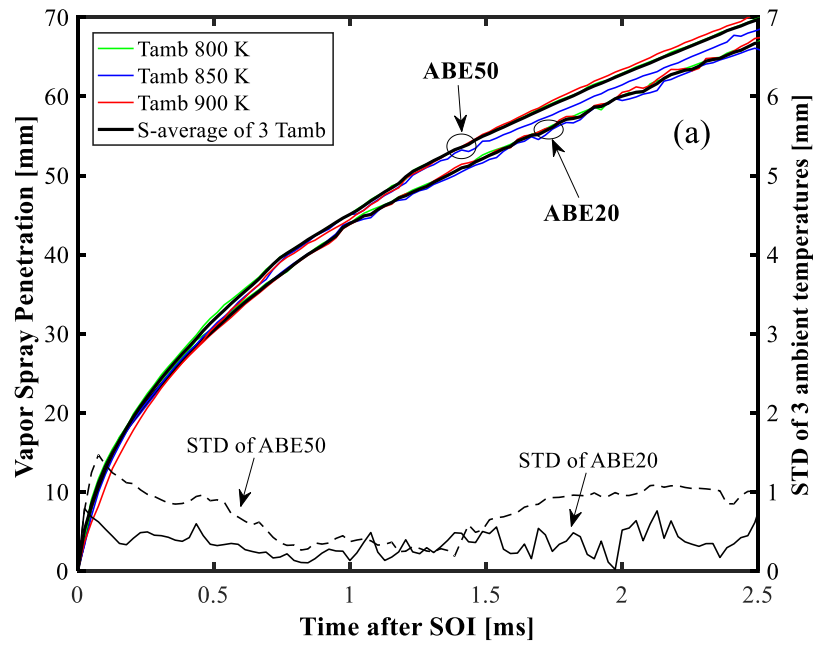


Figure 76 (a) Example of Schlieren images for different blends, 1.0 ms after SOI at $T_a = 900$ K, (b) the mean spray angle averaged from the 3 ambient temperatures and during 1.0 to 2.0 ms after SOI. The error bars represent the standard deviation from results obtained at 3 ambient temperatures.

From **Figure 76** (a), the contrast between the ambient gases background (gray) and the spray region (black), provided by the Schlieren set-up, is sufficient to study on the vapor phase of spray. The spray shape is similar for all fuels, especially the spreading spray angle. As shown in **Figure 76** (b), the average spray angle is around 20.7 degrees for all fuels with a variation of 5% which is similar to the variation of fuel density (around 3%). A good accuracy is also obtained between the experimental data and simulated results, estimated from Siebers' empirical correlation [34] (less than 3% of difference).

5.3.3 Vapor Spray Penetration



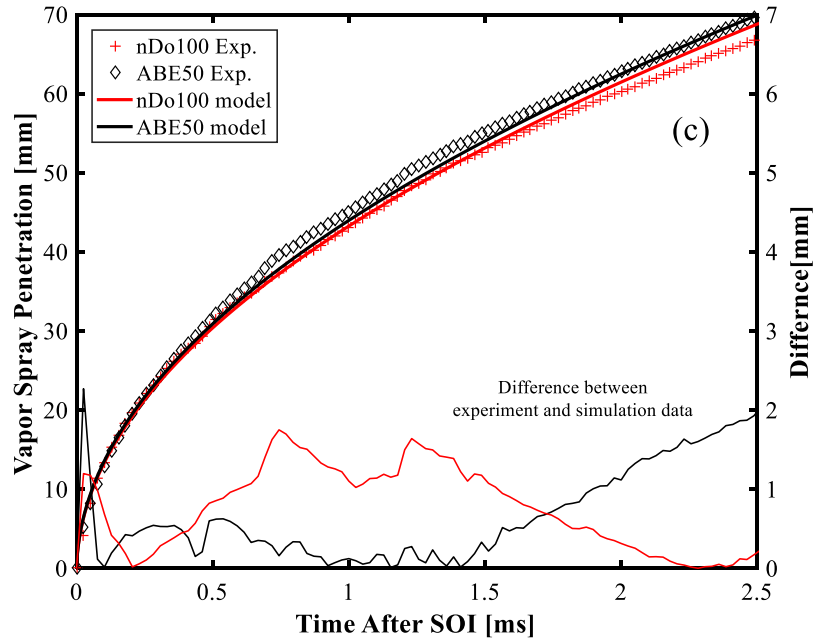


Figure 77 Vapor spray penetration results in non-reactive condition: (a) ABE20 and ABE50 for three ambient temperatures, (b) averaged results for all blends and (c) comparison between experimental and simulated results for n-Do100 and ABE50.

To investigate the effect of ambient temperature, the temporal evolution of vapor spray penetration, S for three ambient temperatures of ABE20 and ABE50 is plotted in **Figure 77** (a). A slight difference can be observed as a function of the ambient temperature, with a standard deviation lower than 1.4 mm in average, for all fuels. In fact, the vapor spray penetration depends mainly on the spray momentum, controlled by the injection pressure and the ambient gas pressure. But, as for different ambient temperatures, in order to maintain the ambient density at 22.8 kg/m^3 , the ambient pressure was changed respectively to 54.2, 59.0 and 60.9 bar. Therefore, the small difference in the pressure drop at the injector tip for the three ambient temperatures leads to a very similar S evolution. In **Figure 77** (b), it can be seen that the evolution of S is similar from SOI to 0.5 ms. But, after 0.5 ms, the higher density of ABE blends (as ABE30, ABE40, and ABE50) starts to separate and slightly further S due to higher momentum as presented a little bit higher MFR and spray angle, while the lower fuel density such as n-Do100 and ABE20 induces slightly shorter S .

To investigate the effect of fuel properties on the evolution of S, the simulation code of Musculus and Kattke [61] model was used to evaluate the temporal evolution of S. **Figure 77** (c) presents the comparison between the experimental and simulated results for two fuels, i.e. n-Do100 and ABE50 because of maximum and minimum S. It can be seen that there is a good agreement between the experimental and simulated results as the difference lower than 2 mm for both fuels. In a comparison of the simulated results between two fuels, the difference only 1.6% can be observed in average due to the slight difference in fuel density, spray angle and Cd.

5.4 Combustion Characterization

5.4.1 Ignition Delay

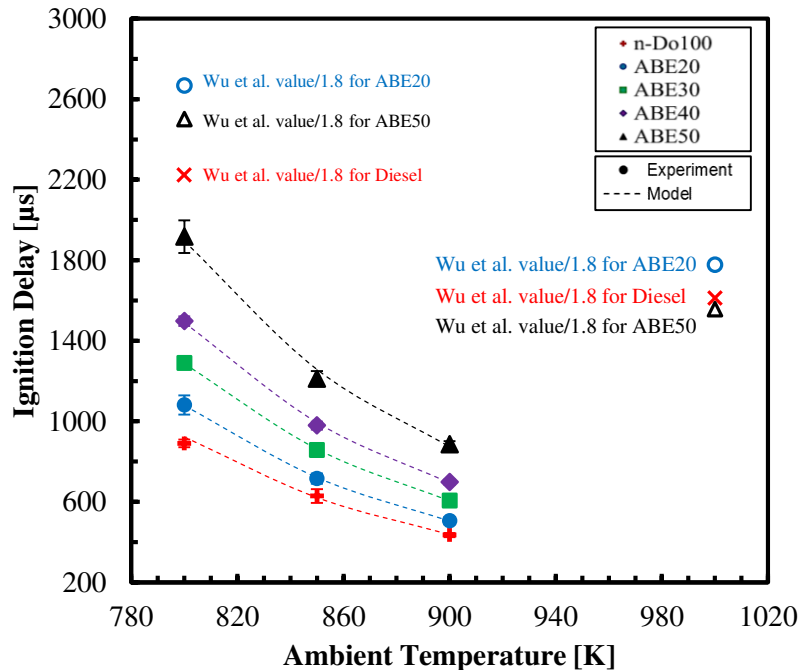


Figure 78 Comparative result between experimental (symbols) and simulated (dot-line) results of the ignition delay for all fuel blends. Wu et al.'s experimental results of 800 and 1000 K were also plotted (values are divided by 1.8).

Figure 78 represents the experimental results of the hot flame ignition delay for all fuels as a function of ambient temperature. The ID values in this graph are the absolute ID, corrected

by the hydraulic delay of the injection. The estimated results from the empirical model proposed by Pickett and coworkers [69] are also plotted as a dot-line to validate the accuracy of the experimental results. The ID is mainly dominated by the ambient conditions, i.e., T_a and ρ_a . A very good agreement is observed between simulated and experimental results for all fuels, with a difference lower than 2%. As expected, ID for all fuels increases with the ambient gas temperature decrease, especially at 800 K. This would be related to the fact that the lower ambient temperature induces a slower chemical reaction rate, the energy entrainment on the spray and atomization process to promote the auto-ignition process [69], [108]. **Figure 78** also shows the ignition delay increases with the increase of the quantity of ABE in the blends. Generally, ID is composed of physical and chemical ignition delays: the physical delay is dominated by spray atomization and vaporization process, while chemical delay due to the chemical reaction rate is linked to the cetane number (CN). Although the CN of ABE blends does not known, it should be lower than n-Do100 and decreases as a function of the quantity of ABE in the blend.

Moreover, the rank of IDs can be more explained by considering **Eq. 31**, as presented in

Table 25. As seen, the value of E_a and A increase as a function of blending ratio of ABE, indicating the high inhibition of the auto-ignition process for the higher ABE blends. The E_a indicates the energy needed to start the auto-ignition process [70], [140], ID is strongly related to E_a in the same rank: n-Do100 presents the shortest ID and the lowest E_a , while E_a increases by increasing quantity of ABE in the blends. This means that the increase of ABE quantity requires more energy to start the auto-ignition process, inducing a longer ID. However, the constant (A) represents the effect of fuel properties on the physical ID process, which is more impact to the ABE ratio. Although the highest ABE ratio has the highest volatility to promote the atomization and vaporization processes (i.e., shorter LL than n-Do100), the significant difference of the latent heat of vaporization induces a higher cooling effect on the local ambient temperature, which inhibits the auto-ignition process. Therefore, the combine effect of E_a and A induces the longer ID for the high ABE ratio.

The ID data of diesel, ABE20 and ABE50 determined by Wu et al. [13] at conditions 16%v of oxygen for 800 K and 1000 K are also plotted in **Figure 78**. Sure, as expected due to the different experimental techniques without the requirement of ECN standard, the values are

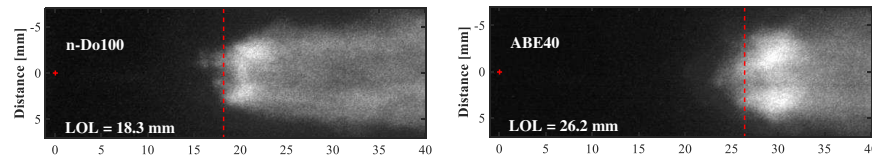
not in the same order. But the trend of ID as a function of the ABE volume in the blend is the inverse to those highlighted by this study. It can be seen that the trend of ID in this work is not agreement with the results of Wu et al. The trend of ID is not related with the increase of ABE ratio, i.e., ABE50 is the shortest value at 1000 K, while ID of ABE50 is shorter than ABE20 at 800 K. Even though ABE50 has the highest fuel volatility to improve the atomization and spray process, its CN is the lowest one as well as the highest latent heat of vaporization, leading to a longer ID.

Table 25 Arrhenius coefficients of ignition delay for ABE blends.

Fuel	A [μ s]	E_a [kJ/mol]	R^2 [-]
n-Do100	65.1	44.7	0.99
ABE20	67.3	45.5	0.99
ABE30	79.6	45.6	0.99
ABE40	89.2	45.8	0.99
ABE50	104.0	46.3	0.99

5.4.2 Lift-Off Length

Figure 79 illustrates the OH* chemiluminescence images during quasi-steady period of mixing-controlled combustion for all fuels at 850 K. As expected, the stabilized flame location of ABE blends (red-dot line represents) moved further to downstream by increasing the ratio of ABE in the blend.



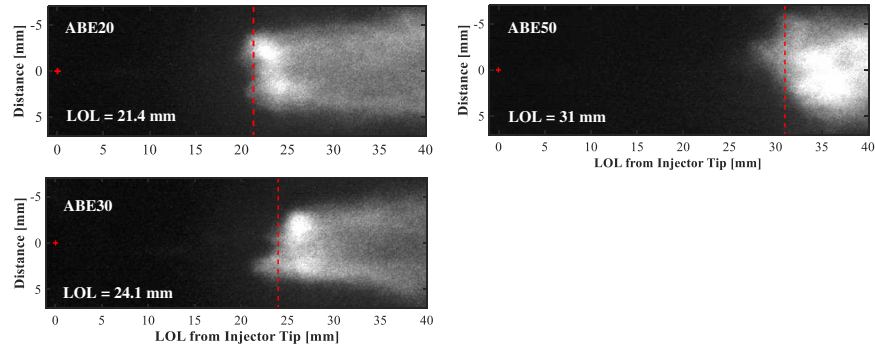


Figure 79 OH* chemiluminescence images during quasi-steady period for all fuels at 850 K

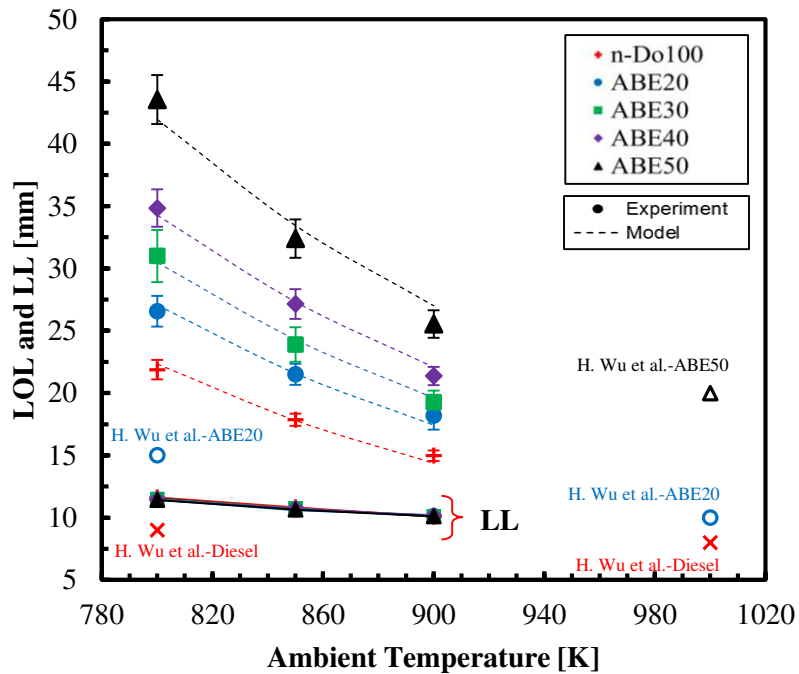
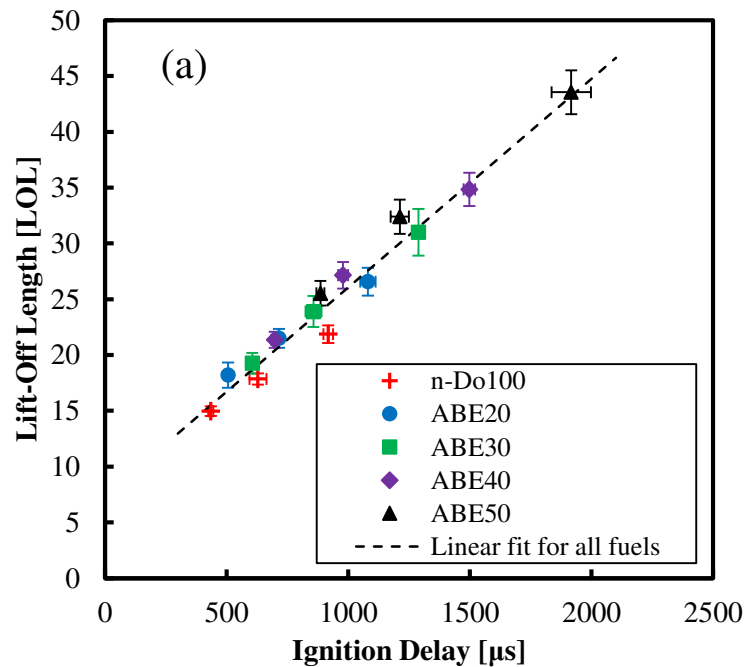


Figure 80 LOL and LL result for three ambient temperatures and all fuel blends. Error bars indicate statistical standard deviation for 12 tests.

The experimental results of the LL and LOL for all fuels as a function of ambient temperature in **Figure 80**. As expected, LL is shorter than LOL for all fuels, which implies that the most of the fuel is completely vaporized before reaching reaction zone of combustion. Therefore, the fuel properties involved on the atomization and vaporization processes, i.e., volatility (boiling point and vapor pressure) and latent heat of vaporization would be less effect on the flame stabilizing process. To validate the accuracy of the experimental results, the

simulated LOL from the power-law relationship suggested by Siebers and coworkers [69], [73], [76] are plotted in dot lines. For that, the constant c was determined from the best fit with experimental data and a very good agreement between experimental and predicted data is obtained. As well known, the LOL for all fuels decrease as a function of the increase of ambient temperature, due to a faster local flame reaction rate at high temperature, allowing the flame to stabilize closer to the injector. Similar to the ID results, LOL increases with the increase of ABE ratio in the blends with the shortest value for n-Do100.

The experimental results of Wu et al. [10], [13] are also plotted, by considering their data 4.5 ms after SOI in **Figure 80**. Contrary to the results of ID, the effect of ABE ratio on LOL is in a good agreement with this present study, adding more doubts about the ID results from Wu et al. As seen in several works [13], [69], [71], the strong linear relationship between LOL and ID can be observed in this study (see **Figure 81** (a)). Generally, the upper limit of LOL can be obtained by balancing injection velocity and flame speed. When the ambient temperature and density are sufficiently high to promote auto-ignition before the fuel reaches the lift-off location, the LOL is likely governed by ignition chemistry [68]. Therefore, the LOL is pulled closer to the injector tip. It implies that a fuel with a higher ability of auto-ignition, i.e. higher CN or shorter ID will have a shorter LOL.



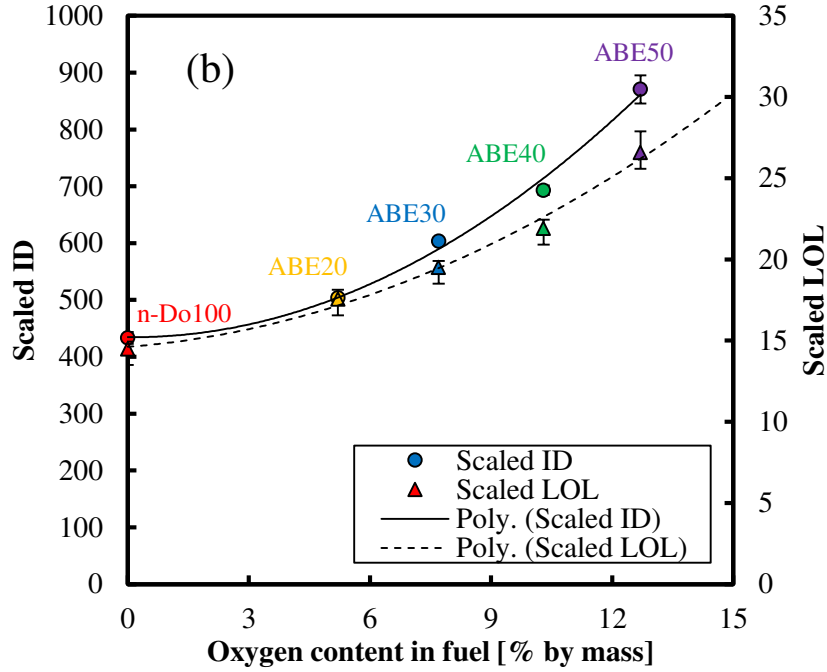


Figure 81 Relationship of ID and LOL: (a) evolution of LOL versus ID for all ABE blends, (b) the scaled ID and LOL evolution as a function of oxygen content in fuel. The details of calculating scaled ID and LOL was presented in **Eq. 33**. The fit curves are fitted by the second order of polynomial function.

The oxygen content in fuel clearly affects the combustion parameters as ID and LOL. As the oxygen content increases, the ID and LOL for Diesel conditions strongly increase, as presented in **Figure 81** (b), as also previously seen in **Chapter 4**. According to results of Manin et al. [71], the oxygen content in fuel affected ID only for the same rank of CN at the low ambient temperature (750-800 K), but in other cases, i.e. $T_a > 800$ K, ID generally follows the rank of CN even though some fuels have a high oxygen concentration. As the T_a was carried out between 800 and 900 and the predicted CN for all fuels was not similar range, thus the oxygen content would be less effect on ID for this work. On the other hand, Manin et al.'s results [71] indicated the effect of the oxygen content is more significant on LOL than on ID for fuels with similar CN level. By computing the flow velocity of spray and the distribution of the stoichiometric mixture fraction, Z_{st} from the Musculus and Kattke model, they found that for

one given residence time, higher Z_{st} provides higher flow velocity value and a mixture fraction distribution, closer to the spray axis. So, as Z_{st} increases with the increase of oxygen content in fuel, the further LOL of the higher oxygenate content fuel would be expected to stabilize at a downstream location, as the air-fuel mixture traveled further away along the stoichiometric mixture fraction contour because of higher flow velocity on this contour. Therefore, the combined effect of lower CN and higher oxygen content induces the increasing LOL of the higher ABE ratio.

From the experimental results, it can be observed that the changing behavior of combustion characteristics as a function of the ABE ratio does not discover in this study as mentioned by Wu et al. [13], especially in ID. There is only the lowest ratio, ABE20, performed a similar spray and combustion characteristics to n-Do100, indicating the high possibility of using ABE as Diesel substitute fuel with minor modification.

5.5 Comparison between Alcohol and ABE Blends

In this part, the spray and combustion parameters of different blends presented in **Chapter 4** and **Chapter 5** are compared in order to investigate the effect of fuel properties and to discuss the feasibility of blends for CI engine. For that, butanol and ABE are compared in 20%v and 40% in blend, while Bu20Eth20 is also added for comparison. The fuel properties are given again in **Table 26**. Before discussion, it could be summarized that ABE blends have lower viscosity than other alcohol blends but higher vapor pressure. In the other hand, the boiling point, the latent heat of vaporization and the lower heating values are the same for ABE and butanol blends as a function of the volume ratio. The comparison of the properties of Bu20Eth20 is more complex, the main important characteristics are the lowest boiling point, lower heating value due to ethanol content, highest oxygen concentration and stoichiometric mixture fraction.

Table 26 Fuel properties of ABE and alcohol blends in comparison with n-dodecane [15], [135], [136], [137], [138].

Properties	n-Do10	ABE20	ABE40	Bu20	Bu40	Bu20Eth20
Molecular formula	C ₁₂ H ₂₆	C _{8.5} H _{18.6} O _{0.4} ^a	C _{6.4} H _{14.4} O _{0.7} ^a	C _{8.9} H _{19.9} O _{0.4} ^a	C ₇ H ₁₆ O _{0.6} ^a	C _{7.8} H _{18.3} O _{0.9} ^a
Density at 15°C (kg/m ³)	752.8	760.7	771	763.3	774.9	770.6
Viscosity at 15°C (mm ² /s)	2.032	1.642	1.471	2.124	2.527	2.077
Lower heating value (MJ/kg)	44.1	41.5 ^b	38.9 ^b	41.8 ^b	39.5 ^b	38.3 ^b
Boiling point (K)	489	464 ^b	439 ^b	468 ^b	448 ^b	440 ^b
Vapor pressure at 298 K (kPa)	0.02	2.17 ^b	4.25 ^b	0.14 ^b	0.25 ^b	1.76 ^b
Latent heat of vaporization at 298 K (kJ/kg)	362	411 ^b	459 ^b	409 ^b	454 ^b	520 ^b
Oxygen concentration (% by mass)	-	5.2%	10.3%	4.6%	9.1%	11.7%
Stoichiometric mixture fraction, Z _{st} (-)	0.0460	0.0489	0.0522	0.0485	0.0512	0.0528
Alcohols content in the blend (Butanol/Ethanol) [%v]	-	14% (12/2)	28% (24/4)	20% (20/0)	40% (40/0)	40% (20/20)

Note: ^a Equivalent formula based on mole fraction.

^b Properties estimated from mass fraction of single-component fuels in the alcohol blends.

5.5.1 Macroscopic Spray Parameters

Figure 82 (a) confirms the highest volatility of ABE blends enhances the atomization process and vaporization process, inducing shorter LL than n-Do100 and other alcohol fuels. The rank of LL for the alcohol blends is relative to the rank of L_v , which higher L_v provides longer LL as decreasing the transfer number, B due to the cooling effect. Therefore, Bu20Eth20 is the longest LL because of its highest L_v , while LL of n-Do100 is ranked between ABE and alcohol blends due to the balance between the lowest L_v and the lowest volatility (the highest boiling point and lowest vapor pressure).

Due to the similar fuel density (less than 3% for all fuels), mass flow rates and spreading spray angle are similar, leading to the development of the vapor phase not affected by the kind of blends, as illustrates the evolution of vapor spray penetration in **Figure 82** (b). After 1 ms of SOI, a slight increase of S , for Bu20, Bu40, Bu20Eth20 and ABE40 can be distinguished due to higher momentum while ABE20 vapor spray evolves like n-dodecane due to lower fuel density and spray angle compared to other alcohol fuels.

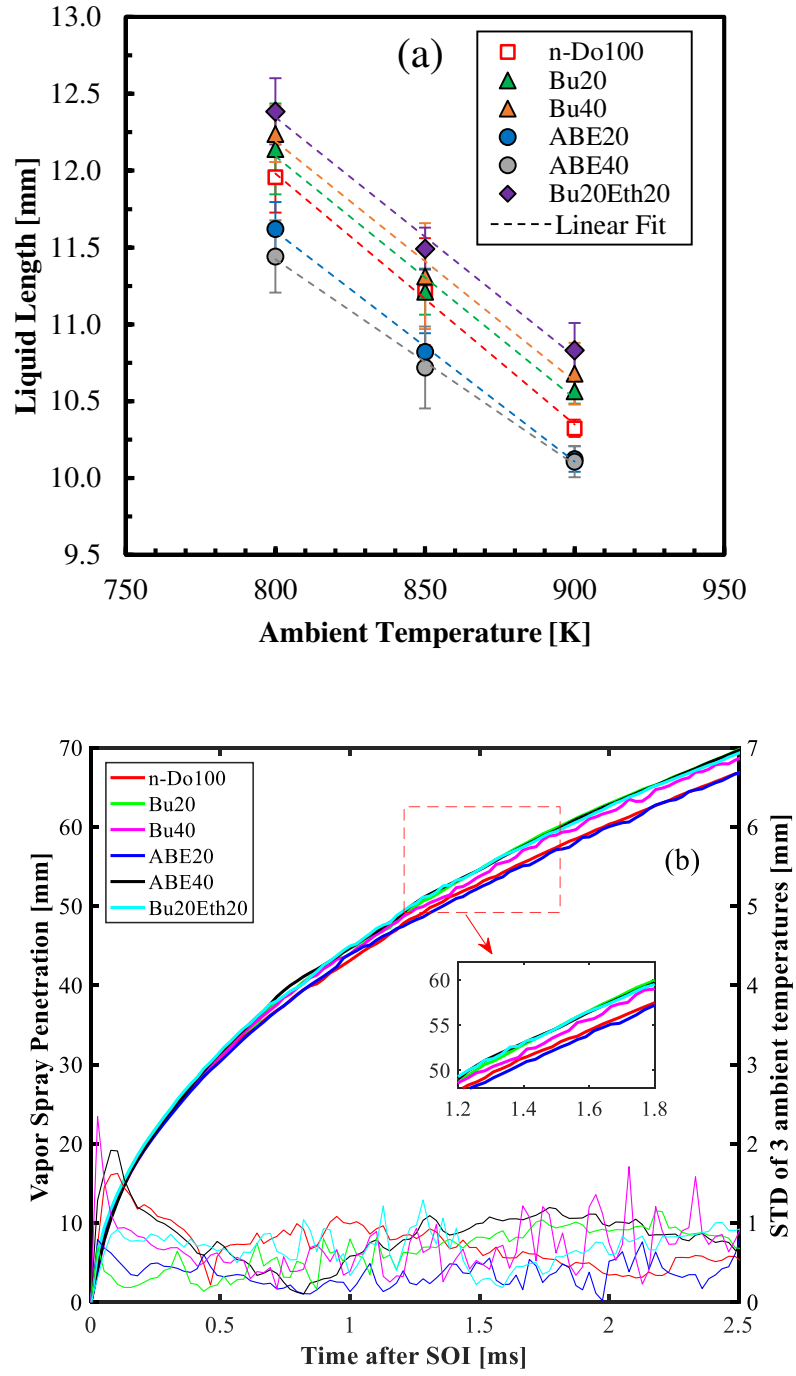


Figure 82 Macroscopic spray parameters for the alcohol and ABE blends: (a) liquid length and (b) vapor spray penetration.

5.5.2 Combustion Parameters

As the ignition delay is strongly linked to the CN, even if the CN for the blends was not measured during this study, it can be estimated that CN decreases by increasing the volume of alcohol in the blend. Therefore, as it can be seen in **Figure 83** (a), there is no surprise that n-Do100 and Bu20Eth20 provide the shortest and the longest ID respectively. However, for the same volume of blend such as ABE20 versus Bu20 and ABE40 versus Bu40, it is difficult to predict CN. For that, the ID is plotted as a function of the alcohol content (butanol and ethanol) in the blend, as seen in **Figure 83** (b). It can be observed that the ABE blends present a lower alcohol content at the same volume ratio, thus the lower CN of ABE blends could be obtained. Moreover, ABE blends obviously present shorter ID than butanol blends, especially at the low ambient temperature due to the higher enhancement of the atomization and vaporization process of ABE blends, indicating by the shorter LL. As a result, the shorter physical ID could be obtained, inducing the shorter global ID.

From the parameters estimated from ID models and presented in **Table 27**, Bu20 has slightly higher A and E_a than ABE20 leading to slightly longer ID. ABE20, Bu20 and ABE40 present the same level of E_a , but ABE40 the highest A value. As presented above, the auto-ignition timing of ABE40 would be prolonged by the fuel properties involved in the atomization and vaporization process in term of physical ID. On the other hand, Bu40 has higher E_a than ABE40 leading to higher required energy to start the auto-ignition process.

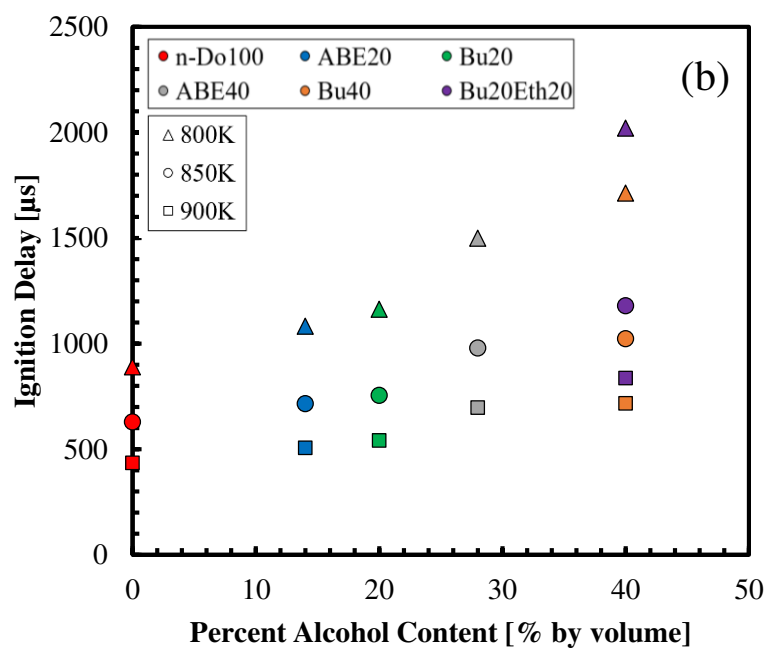
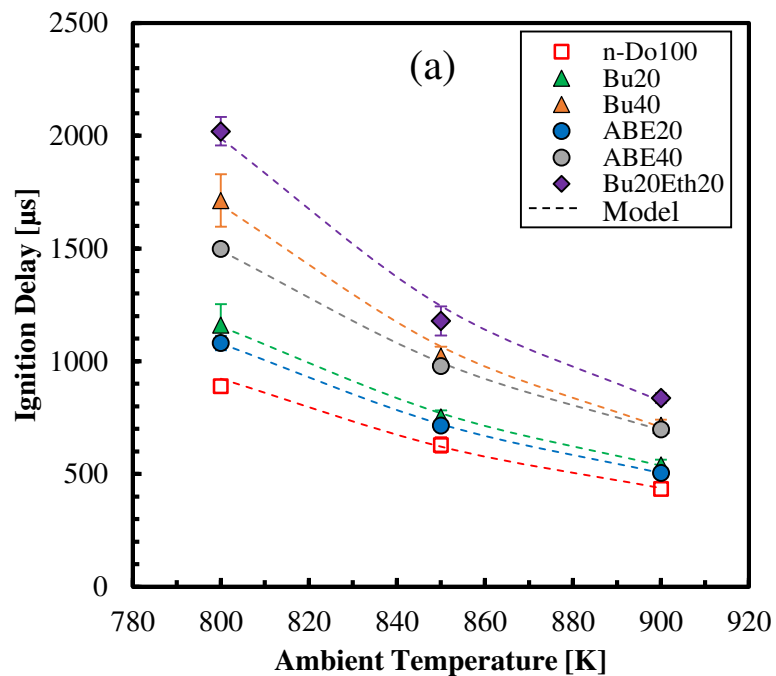
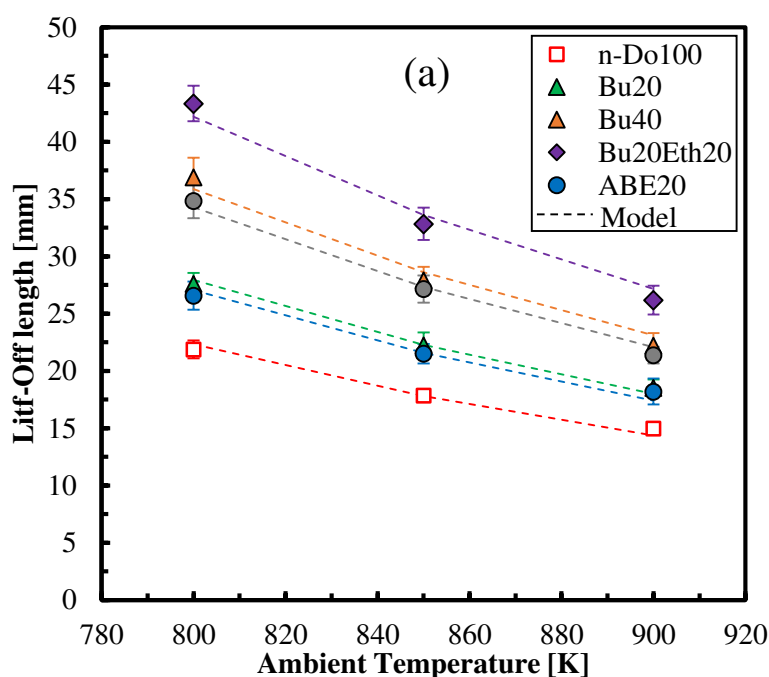


Figure 83 Combustion parameters for the alcohol and ABE blends: (a) ignition delay and (b) ignition delay as a function of alcohol content (butanol and ethanol) in the blend.

Table 27 Arrhenius coefficients of ignition delay for alcohol and ABE blends.

Fuel	A [μ s]	E_a [kJ/mol]	R^2 [-]
n-Do100	65.1	44.7	0.99
ABE20	67.3	45.5	0.99
Bu20	69.2	45.8	0.99
ABE40	89.2	45.8	0.99
Bu40	37.9	52.3	0.99
Bu20Eth20	40.6	52.9	0.99

As discussed in previous chapters, the Lift-Off-Length is mainly governed by the auto-ignition ability of the fuel, combined with the oxygen content in fuel as minor factor. From **Figure 84** (a), it can be noted that the longest LOL is obtained for Bu20Eth20 due to the lowest auto-ignition ability and highest oxygen content in the fuel, while the LOL of dodecane fuel is the lowest one. In comparison between ABE and butanol blends, the values are close as a function of the blend ratio, but a small difference can be highlighted as butanol blends generate always slightly higher LOL than ABE blends. LOL would be mainly dominated by the ability of auto-ignition as the trend of LOL is similar to the order of ID result, even if ABE blends have slightly higher oxygen content than butanol blends for the same volume ratio, as seen in **Figure 84** (b).



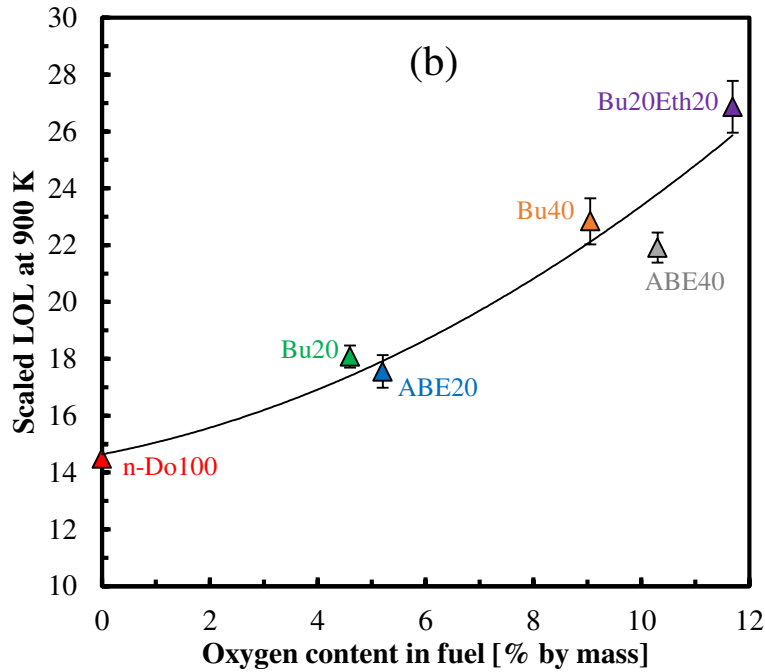


Figure 84 Combustion parameters for the alcohol and ABE blends: (a) lift-off length and (b) the scaled LOL evolution as a function of oxygen content in fuel. The details of calculating scaled LOL was presented in **Eq. 33**. The fit curves are fitted by the second order of polynomial function.

According to the experimental results, this analysis highlights the fact that 20%v of butanol and ABE can be added in diesel fuel with a little modification of the liquid and vapor spray development. Moreover, combustion characterizations, ignition delay and lift-off length, performs close to the reference fuel, n-dodecane. Last, it can be confirmed that ABE can be used instead of butanol due to its higher volatility and higher ability of auto-ignition which induces the similar spray and combustion characteristics to n-dodecane.

5.6 Conclusion

In this work, the spray and combustion characteristics of different ABE-dodecane blends from 20%v to 50%v were investigated to compare with the reference fuel n-dodecane, in High-

Pressure and High-temperature conditions of the ECN Spray-A for three ambient gas temperatures (800, 850 and 900 K). The main conclusions could be summarized as:

- 1) Mass flow rate of ABE blends is higher than n-Do100 and increases in the ABE ratio increase due to the higher fuel density.
- 2) Liquid length of ABE blends is shorter than n-Do100 and slightly decreases by increasing ABE ratio in the blend as its higher volatility enhancing the vaporization process. Due to the slight different density of each fuel, an only slight difference in vapor spray penetration and spray angle was observed.
- 3) The linear relationship between the lift-off length and ignition delay for all conditions was highlighted for ABE blends. The ignition delay and lift-off length of all ABE blends are longer than n-Do100, and increase as a function of ABE quantity in the blends, expected by the lower cetane number. The auto-ignition ability influenced the stabilized flame position as lift-off length presented the same order with ID.
- 4) ABE20 performed similar spray and combustion characteristics to n-dodedance, indicating the high possibility of using ABE as Diesel substitute fuel with minor modification.
- 5) ABE blends significantly promote the auto-ignition process when compared to butanol blends at the same volume ratio due to the enhancement in the atomization and vaporization process, which induces the shorter LOL.

CHAPTER 6

GENERAL CONCLUSION AND PERSPECTIVE

6.1 General Conclusion

To investigate the effect of fuel properties on the spray and combustion process of ABE-dodecane blends and alcohol-dodecane blends, the high-pressure and high-temperature (HPHT) chamber called “New One Shot Engine (NOSE)” was designed and developed to provide the standard condition “Spray-A” defined by ECN. To validate NOSE achieved this condition, the ambient pressure, temperature, gas field velocity were measured and characterized. The measurements of ambient thermodynamic conditions (pressure and temperature) demonstrated that NOSE can reach the standard Spray-A condition of ECN (near 60 bar, 900 K and 22.8 kg/m³) with a homogeneous ambient temperature field as indicated by the spatial distribution of temperature measurements. By adapting the compression ratio of the NOSE, the homogeneity of the ambient temperature can be obtained for other ambient temperatures (800 and 850 K). Meanwhile, the reduction of the piston head angle and the increase in the gap distance can eliminate squish effect and therefore reduce the gas velocity inside the chamber. The simulated results and PIV measurements confirm that the ambient gas velocity is below 1 m/s as required by ECN Spray-A specifications.

By using the standard operating condition of ECN Spray-A, the spray and combustion characteristics of the three injectors (A, B and C) were investigated in the NOSE. The optical techniques, post-processing and criteria to determine spray and combustion parameters recommended by ECN network were set-up to compare the experimental results with the same injector of IFPen and other data from ECN database. The experimental results showed that LL results for the three injectors are globally in good agreement with IFPen values and those of

other institutes, with a difference lower than 1 mm. For the vapor phase of spray, the average vapor spray evolutions for injectors A and B are globally in the same order of magnitude for all data, even if the results from IFPen are longer after 0.5 ms after SOI. The different result obtained for the injector C is due to its lower MFR and the larger hole of injector diameter. In the case of combustion parameters, all estimations of the ID for all injectors are globally in the same range at 850 and 900 K. The difference is more pronounced, especially, for the LOL from injectors A and B at 800 K. The ‘old’ injector C provides the shortest LOL for all ambient temperatures. Meanwhile, the changing of the operating conditions to reach 800 and 850 K targets, the effect of the inhomogeneity of the temperature field in combustion processes was confirmed, while no effect on macroscopic spray parameters was observed. For the last conclusion in this part, all parameters determined from the experimental results of injector A characterized in the homogeneous ambient temperature are similar to those of the ECN database. According to these experimental results, it can be confirmed that the high accuracy of the experimental set-ups and post-processing obtained in this study.

As reviewed, even if several studies present some results about the high potential of ABE and butanol diesel blends to reduce simultaneously soot and NO_x, there is not yet a complete comparative study of these fuels on the diesel spray and combustion behaviors to understand better the effect of fuel properties. Therefore, the characterization of spray and combustion parameters of different alcohol blend fuels were investigated and compared to n-Do100 in the high-pressure and high-temperature conditions. From the experimental result, it can be concluded that due to the slight difference in fuel density, the mass flow rate, the vapor spray penetration and the spray angle can be considered similar for all fuels. ABE20 presents a shorter liquid length compared to other fuels due to its highest volatility, which favors the vaporization process. Moreover, its ability of auto-ignition (cetane number) is expected higher than the other alcohol blends, its lift-off length and ignition delay are also closer to pure n-Do100 for all ambient conditions. As a result, ABE20 has a high possibility to be used as Diesel substitute fuel. In overview, the linear relationship between the lift-off length and ignition delay for all conditions is verified for all fuels even if their oxygen content is different. The lift-off length is not only strongly linked to the auto-ignition ability of the fuel but also to the oxygen

content in fuel. For the effect of alcohol in the blend, the increase of butanol and the addition of ethanol in blends increase the LL due to the cooling effect from the latent heat of vaporization. Increasing of alcohol quantity in the blend induces the longer LOL and ID, due to the lower ability of auto-ignition and higher oxygen content. Due to the presence of Acetone in ABE, the competition between all properties of fuel components of the mixture provides a different behaviors of ABE spray.

Previously, ABE20 presented a high opportunity to use as fuel in CI engine due to a similar the spray and combustion characteristics with conventional surrogate diesel fuel, n-dodecane. According to the suggestion of Wu et al. [13], the appropriate ratio of ABE for CI engine is between 20%v and 50%v, therefore, the various volume fractions of ABE in 20%v, 30%v, 40%v and 50%v blended with n-dodecane were investigated in the spray and combustion characterizations. The result showed that even if the mass flow rate of ABE blends increases with ABE ratio in the blend as increasing the fuel density, their liquid length slightly decreases due to higher volatility enhancing the vaporization process. While only a small difference in vapor spray characteristics (penetration and angle) was observed for all blends as slight different fuel density. In the combustion process, the blends with higher contents of ABE need more time to ignite inducing longer lift-off length due to the lower ability of auto-ignition and increasing of the oxygen concentration, which is the major characteristic to improve the fuel-air mixture and lower NO_x and soot. Therefore, ABE blends can certainly be considered a good surrogate for any future advanced combustion modes (HCCI, PCCI, LTC, etc.). Finally, in Diesel standards conditions, this study allows to confirm the conclusion provided by Wu et al. [13] but for different conditions. Due to its similar combustion characteristics (i.e., ignition delay and lift-off-length) with n-dodecane, ABE20 can be used as Diesel substitute fuel with minor engine modification.

6.2 Perspective

Although ABE20 can be considered as one new alternative fuel for CI engine due to similar spray and combustion characteristics with n-dodecane at the standard ECN Spray-A conditions, the impact of the ABE in fuel has to be characterized in terms of soot production and oxidation in the same experimental set-up in comparison to diesel surrogate fuel and also butanol blends.

From the experimental results, a shorter liquid length of ABE blends was observed, expected by the high volatility enhancing on atomization and vaporization process. However, there is no simulation model or quantitative measurement to explicitly explain these complex phenomena. Even if the scaling-law simulation model was used to explain them, only single component fuel was taken into account due to the lack information of some fuel properties to evaluate the LL for the multi-component fuels like multi-alcohol and ABE blends, i.e., boiling point, vapor pressure, latent heat of vaporization etc. Therefore, the quantitative and accurate measurement of fuel properties for the blending fuels are needed for future research, which is not only useful to understand better these behavior but also important to improve the simulation model itself.

The result showed that ABE blends can promote the combustion process as they induced shorter ignition delay and lift-off length when compared with other alcohol blends at the same blending ratio. Although this trend was explained by assuming cetane number evolution as a function of the blend and also with the determination of the pre-exponential constant and the apparent activation energy of the auto-ignition delay empirical correlation, the knowledge of cetane number is necessary to better identify the effect on ignition delay and lift-off length.

Some fuel properties, such as the latent heat of vaporization were expected to affect in spray and combustion process due to inducing the cooling effect leads to reduce the local ambient temperature, especially for alcohol blends presenting the high latent heat vaporization. However, up to now, there is no quantitative measurement to identify this effect on combustion parameters. Furthermore, the current empirical correlations for evaluating combustion parameters take into account only ambient parameters. Therefore, the empirical correlation

could be improved by taking into account some fuel properties: cetane number, latent heat vaporization, vapor pressure, etc.

In order to complement perspective of the use of ABE blends as biofuel for CI engine, other studies based on engine performance and emissions as a function of the engine operating modes have to be investigated in full range of engine operations and also advanced combustion modes.

Last, as NOSE achieved the standard condition of ECN Spray-A and can operate in wide range of ambient conditions, with a maximum ambient pressure of 100 bar and temperature of 1000 K. Therefore, some experiments can be done to extend to other targets condition of ECN and other CI conditions such as ECN Spray-B, Spray-C, Spray-D and multiple injections. Moreover, one major advantage of NOSE is the control of the species introduced inside the combustion chamber prior to injection, unlike in the case of Constant-Volume Preburn (CVP), which presents a certain amount of residual gases from the incomplete combustion products during the pre-combustion phase. Therefore, the effect of these different combustion products (such as H_2O , CO_2 , CO , $NO...$) in the ambient gases has to be studied to assess their impact on combustion development and soot production/oxidation. This could be important in the context of ECN as it can provide new types of data to improve the simulation.

APPENDIX A

ENGINEERING DRAWING OF NOSE

A.1 Engineering Drawing and Picture of NOSE

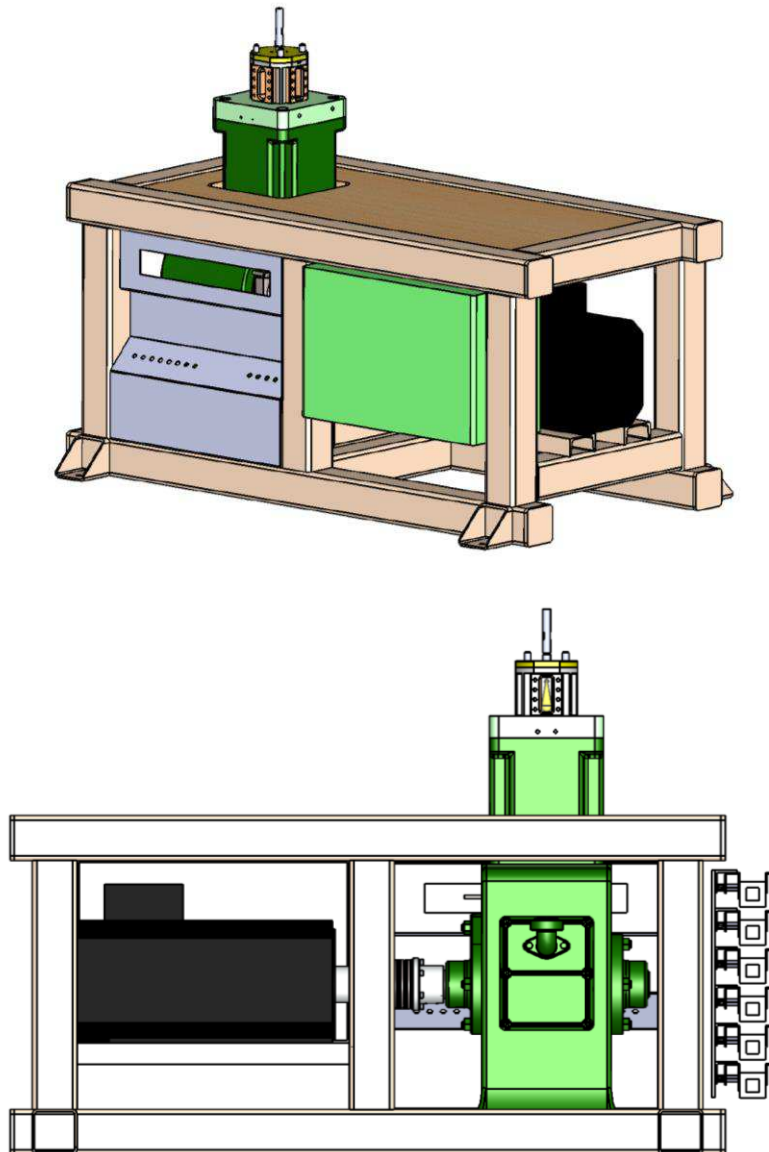
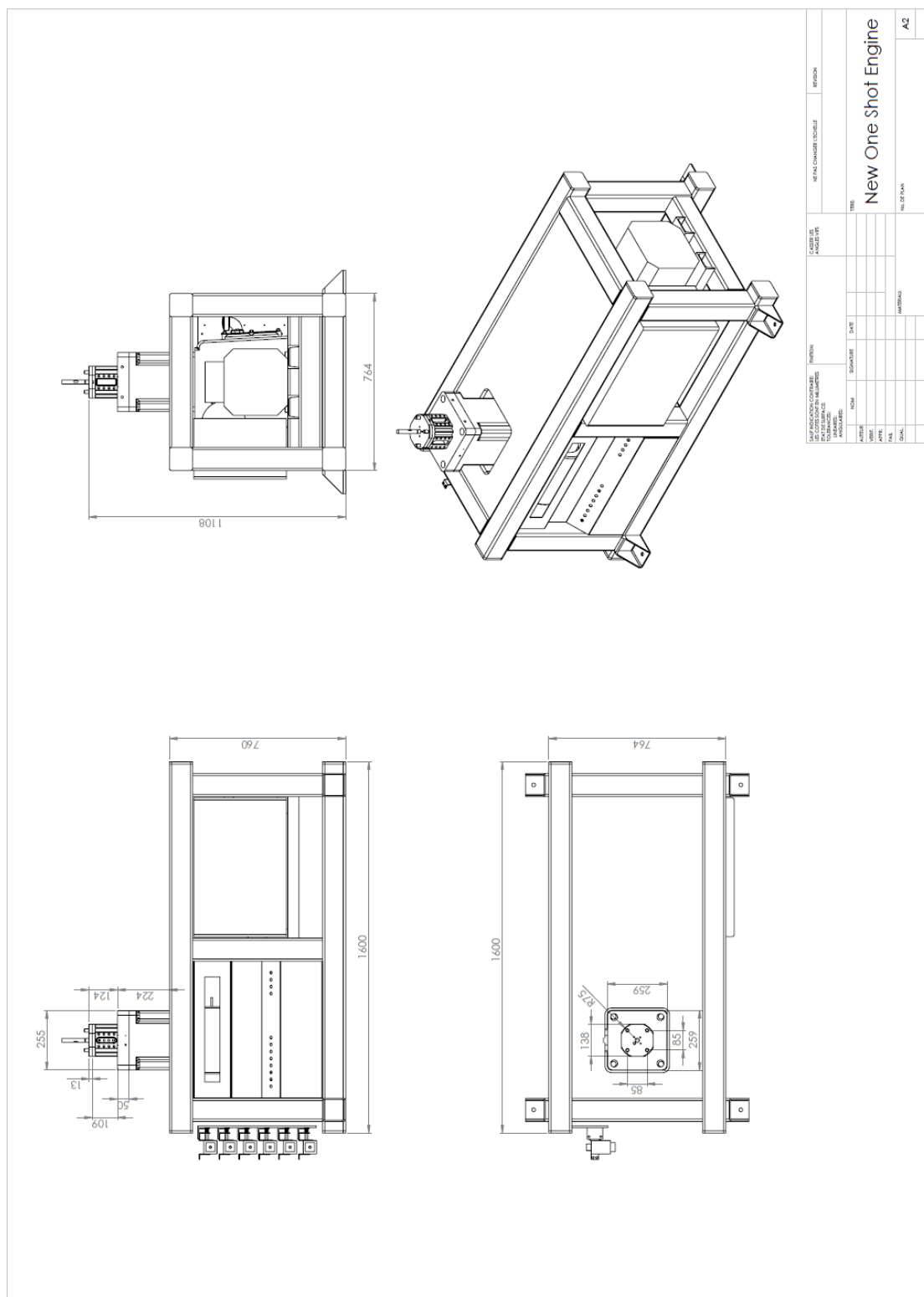


Figure A-1 Three-dimensional drawing of the NOSE.



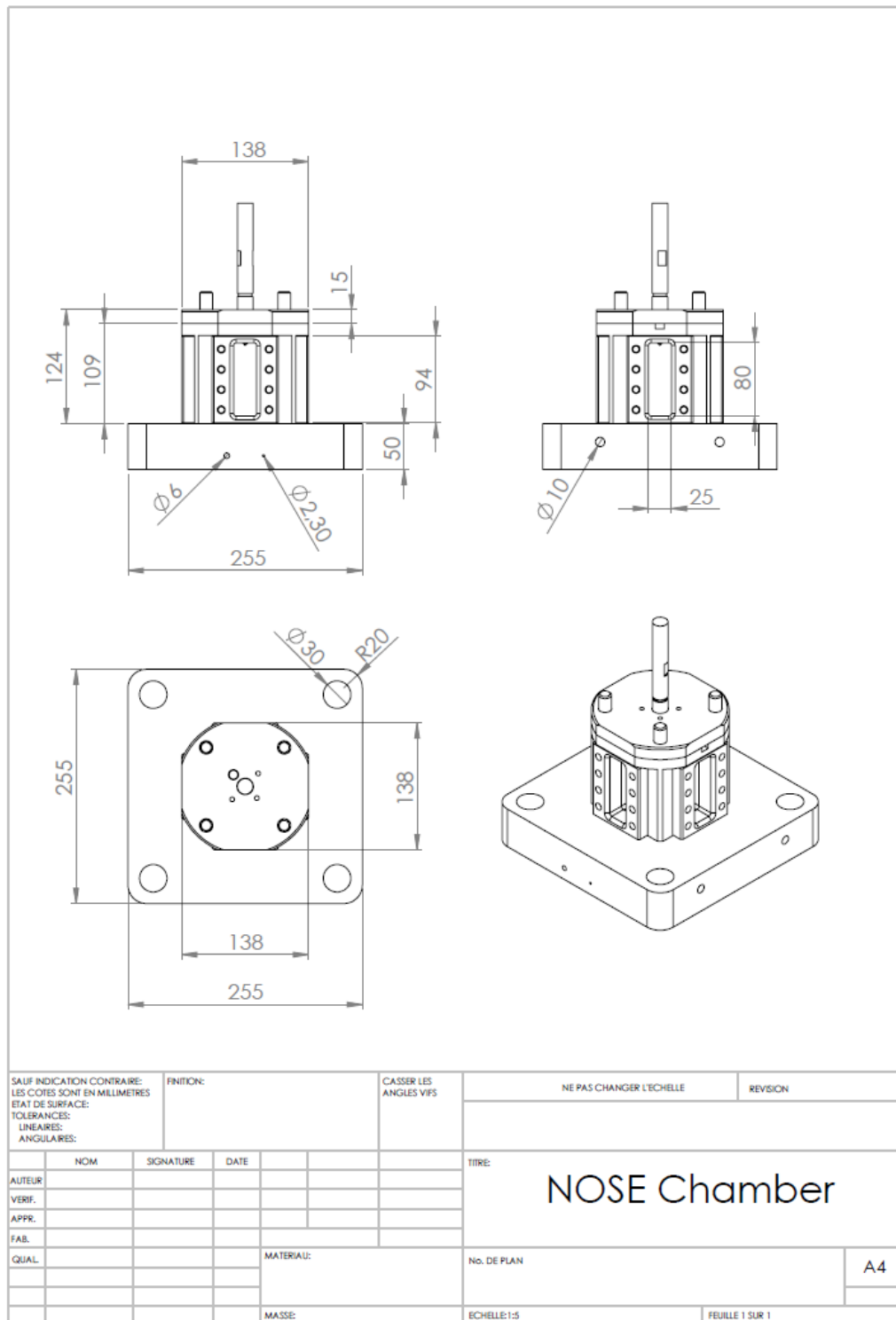


Figure A-3 Two-dimensional drawing of the NOSE chamber

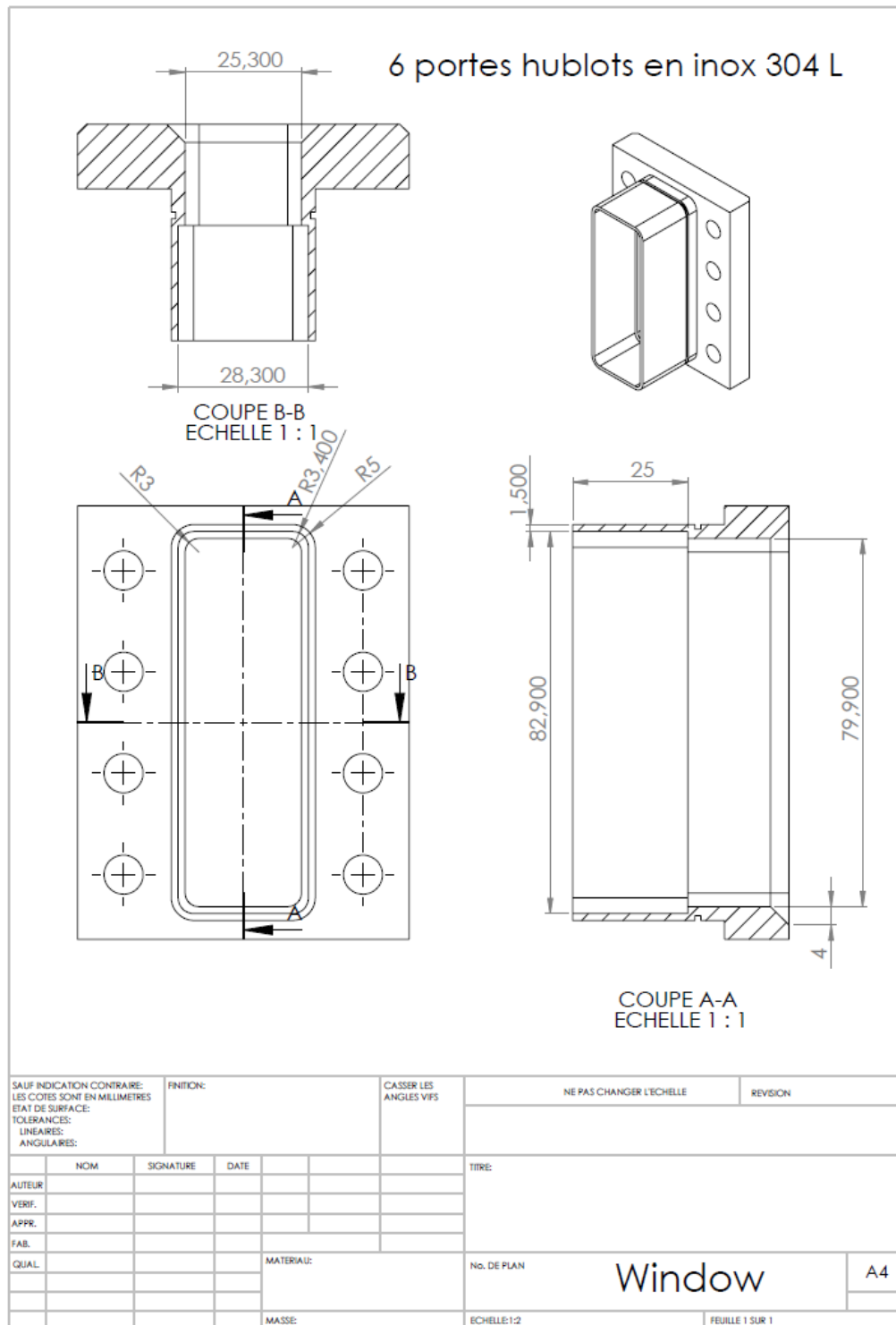


Figure A-4 Two-dimensional drawing of the optical window.

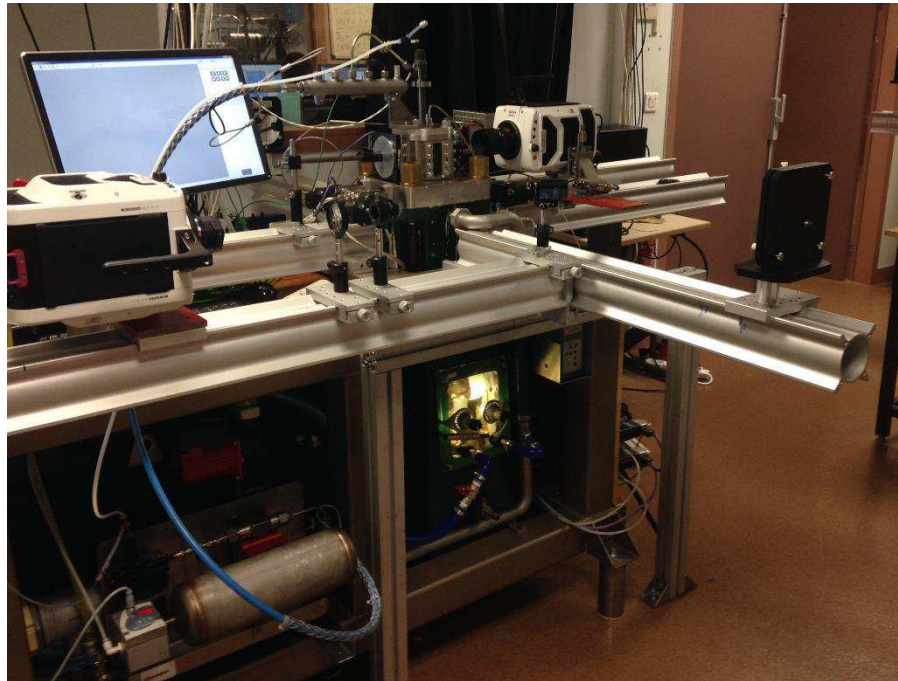


Figure A-5 Overview picture of NOSE set up for the non-reactive condition.

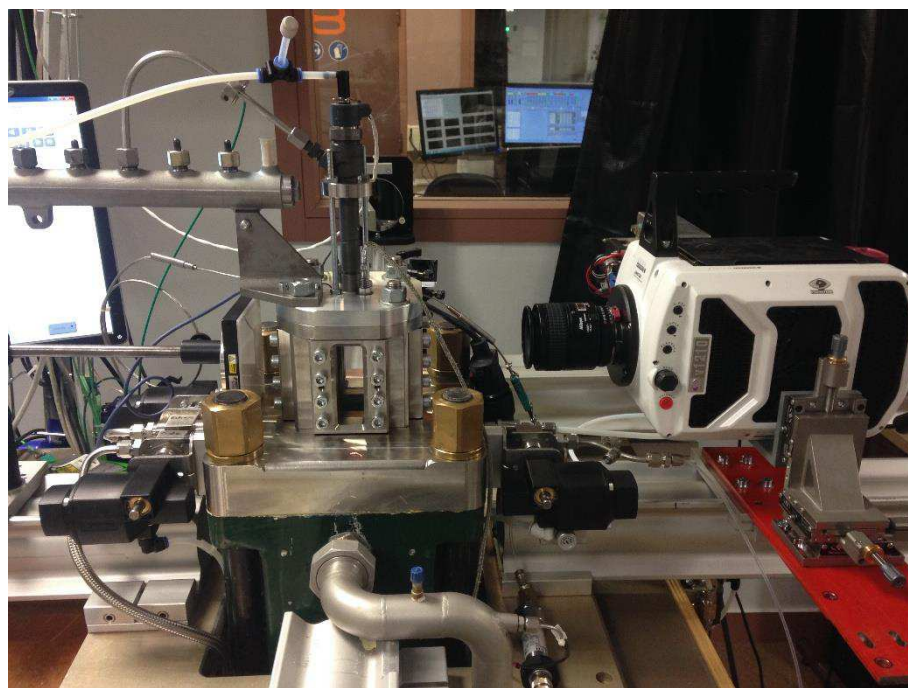


Figure A-6 Picture of NOSE chamber set up for the Diffused Back-Illumination (DBI).

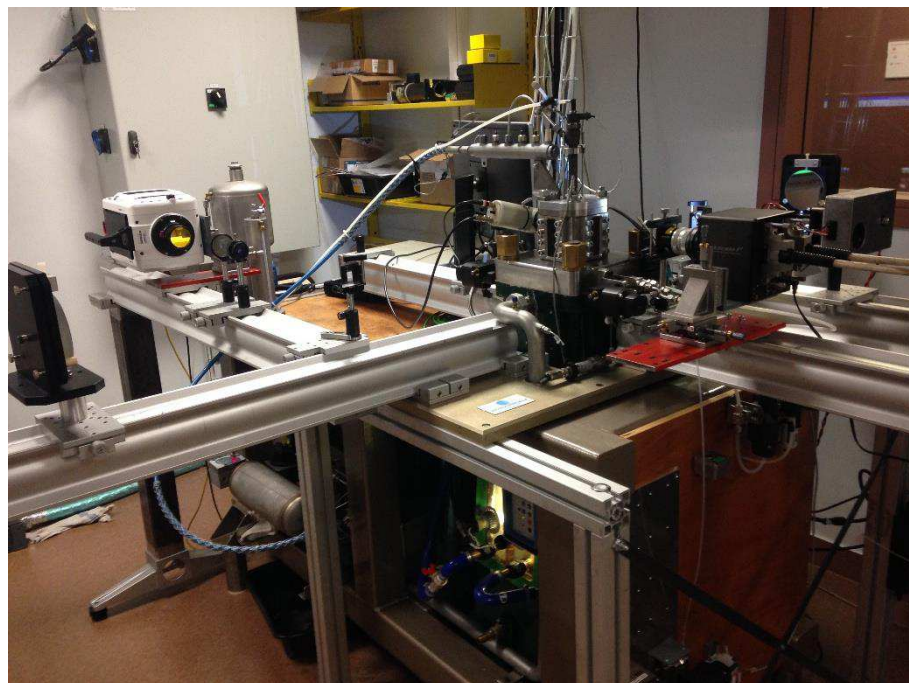


Figure A-7 Overview picture of NOSE set up for the reactive condition.

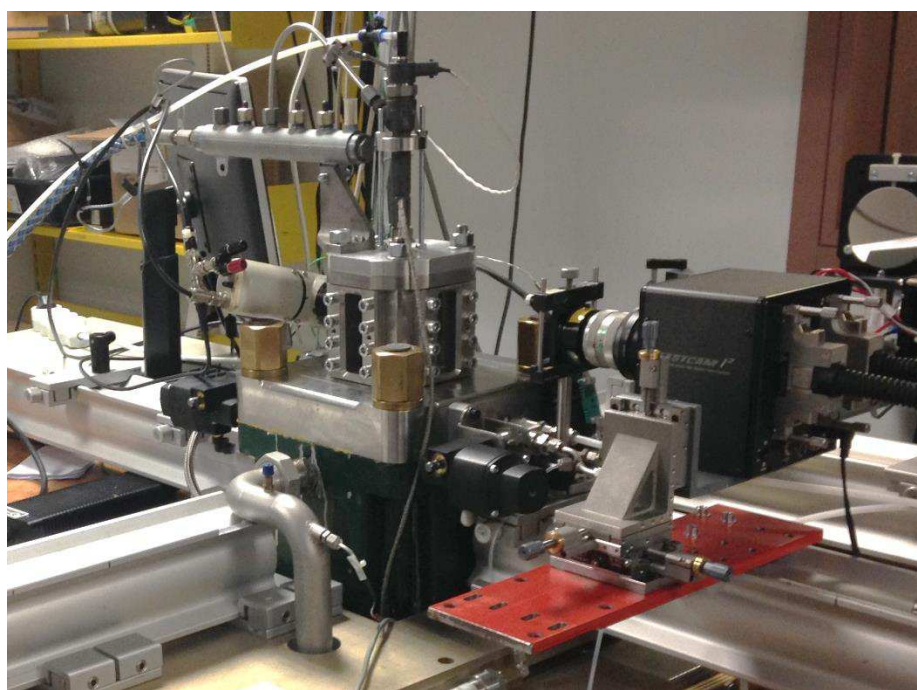


Figure A-8 Picture of NOSE chamber set up for the OH* Chemiluminescence.

A.2 Specification of Motor and Driver

A.2.1 Specification of the brushless DC motor PHASE Automation U31340

Technical Data Summary

Motor Type	MotorCode = "U3 1340.15.3"
Document	DocNum = "Preliminary - for evaluation purpose only"

Reference data (referred to coolant 40 C, copper 120 C)

<u>DC bus setting</u>	Vdcbus = 537·volt
<u>Series inductance</u>	Lseries = 0·mH

Nominal torque, cont. duty S1, 1 rpm, coil at 130 C	C0 = 434·N·m
S6 duty torque, 40% duty, 1 rpm, coil at 130 C, 10 min	C0S6 = 685·N·m
Knee speed	wknee1 = 1498·rpm
Max speed	$\omega 1 = 1.5 \times 10^3 \cdot \text{rpm}$
Nominal Power, S1, wknee	Mpower(wknee1) = 62.96·kW
Nominal Power, S6 10 minutes, wknee	MpowerS6(wkneeS6) = 93.91·kW
Power at max speed	Mpower($\omega 1$) = 63.01·kW
Absolute max torque	Cul = 1175·N·m
Motor constant	$\text{Mcst} = 13.8 \cdot \text{N} \cdot \frac{\text{m}}{\sqrt{\text{watt}}}$

Physical data:

Maximum speed	$W_{\text{max}} := 300 \cdot \text{rad} \cdot \text{sec}^{-1}$
Rotor inertia	$J_{\text{rot}} = 0.0698 \text{ kg} \cdot \text{m}^2$
Acceleration at peak torque	$A_{\text{pk}} = 1.6847 \times 10^4 \text{ s}^{-2}$
Max. shock on motor, any direction	Shk := 5·g
Max. vibration level on motor, any direction	Vlevel := 2·g
Motor mass	Mstat = 90 kg
Airgap, mechanical	Agap = 0.8·mm
Maximum inner rotor diameter	Diamin = 107·mm
Outer rotor diameter	Diamax = 139.2·mm
Stack length	Stkl = 400·mm
Stator diameter, including outer sleeve	Dout = 250·mm
Overall stator length	Stlength = 496·mm
Insulation class	Class H
Cooling	Fluid cooling

Thermal data:

Motor loss at S1 torque, 1 rpm
Motor loss at S1 torque max speed
No load loss at maximum speed
Thermal impedance, copper to coolant
Thermal capacity
Thermal time constant
Threshold of built-in PTC
Max. air temperature

$\text{Loss}(1\text{-rpm}) = 1.71\text{-kW}$
 $\text{Loss}(\omega_1) = 1.77\text{-kW}$
 $\text{Loss0load}(\omega_1) = 0.31\text{-kW}$
 $R_{th} = 0.0436\text{-K}\cdot\text{watt}^{-1}$
 $C_{th} = 3.7872 \times 10^4\text{-joule}\cdot\text{K}^{-1}$
 $\tau_a = 2 \times 10^3\text{ s}$
 $\text{PTCt} := 130\text{-K}$
 $\text{Intemp} := 40\text{ }^\circ\text{C}$

Electrical data, each drive:

Pole number
Connection
Back EMF between phases
Torque constant, 0 deflux angle
Temperature coefficient of back EMF and Kt
Winding resistance, 20 C
Winding inductance
Nominal RMS current, 1 rpm, S1
Max. current S6 40% 1 rpm, 10 min
Frequency at wmax
Nominal voltage at >=knee1 speed
Efficiency at knee1 speed
Peak current at Cul
Torque rise time at Vmax
No load current a w1
Deflux initial speed at no load
Current limit setting at w1

$P_n = 8$
Wye
 $\text{EMF} = 2.3\text{-volt}\cdot\text{sec}$
 $K_t = 4\text{-N}\cdot\text{m}\cdot\text{amp}^{-1}$
 $D_{ke}/D_t = -0.09\%/K$
 $R_w = 0.05\text{-ohm}$
 $L_c = 1.7\text{-mH}$
 $\text{Currentlim}\left(\frac{1\text{-rad}}{\text{sec}}\right) = 121.9218\text{-amp}$
 $\text{MaxiS6} = 193\text{-amp}$
 $F_{n1} = 100\text{-Hz}$
 $V_{nom} = 381\text{-volt}$
 $\text{Efficiency}(w_{knee1}) = 0.97$
 $C_{nonlin} = 313\text{-amp}$
 $\text{Trise} = 1.3 \times 10^3\text{-N}\cdot\frac{\text{m}}{\text{msec}}$
 $I_{dnl}(\omega_1) = 0\text{-amp}$
 $w_{initdefl} = 166\text{ s}^{-1}$
 $\text{Currentlim}(\omega_1) = 113\text{-amp}$

A.2.2 Specification of the electric driver motor AxM300-400

Test conditions, where not differently specified:
VDC=700V, VAC=400V, cooling water temp. = 20°C

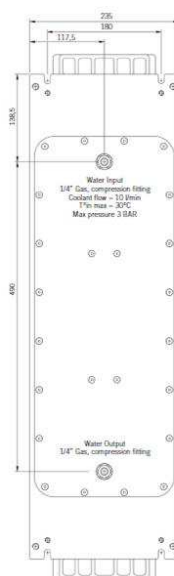
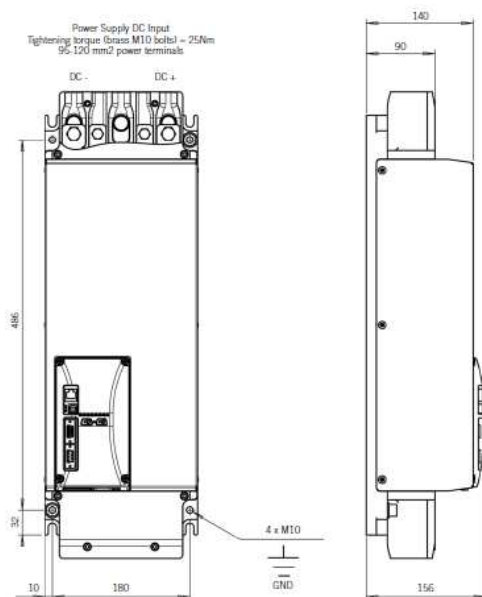
DC Side	AxW 250.330.6	AxW 300.400.6	Unit
Max DC Power	223	228	kW
Absolute MAX DC Voltage	950		Vdc
DC Voltage Range (VDC)	0 - 900		Vdc
Max DC Current (IDC)	245	297	Arms
Power Terminal Dimension	95 - 120		mm2

AC Side	AxW 250.330.6	AxW 300.400.6	Unit
Max AC Power	217	280	kW
MAX AC Voltage (VAC)	(Vac / sqrt(2)) - 10%		
Max AC Current	330	400	Arms
Max AC Frequency	1,2		kHz
Ripple Current Frequency	16		kHz
Power Terminal Dimension	95 - 120		mm2

Performance	AxW 250.330.6	AxW 300.400.6	Unit
Efficiency	97,4 (*)		%
Water Cooling Temp. Range	18 - 60 (!)		°C
Nominal Coolant Flow	10	15	l/min
Water In / Out Interface	1/4" Gas NPT		
Pressure Drop in Cooling Circuit	0.5		bar
Max Pressure in Cooling Circuit	5		bar
Environment Temperature	0 - 40		°C

(*) – when the Drive is supplying 100KW of output power.

(*)! CAUTION: Never overcool in order to avoid condensation; see Curves referred to
Vac = 400V



APPENDIX B

CORRECTIVE AMBIENT CONDITION

B.1 Corrective ambient gas temperature

To confirm that NOSE can reach ECN, it needs to characterize the ambient gas temperature respected to the requirements of ECN. For this reason, the fine-wire thermocouples (13 μm and 25 μm), type K, were used to measure hot gas temperature in the middle plane of the chamber in order to investigate the distribution of ambient temperature inside the chamber, as seen in **Figure B-1**.

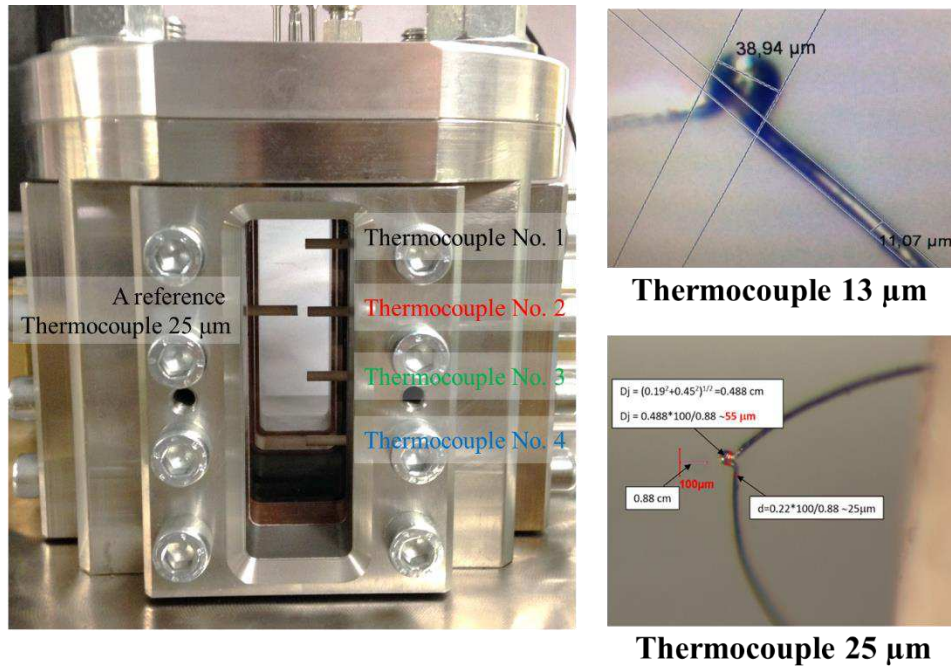


Figure B-1 Wire-fine thermocouples: (a) a photograph of the local position to characterize the ambient temperature inside the NOSE chamber, (b) the zoom images of 13 μm and 25 μm thermocouples obtained by microscope.

Although a fine-wire thermocouple has a fast response time, heat transfer between bead thermocouple, hot gases and cylinder walls has an effect on the precision of the measuring gas temperature. Therefore, the gas temperature has to be corrected by applied energy balance equation at the location of bead thermocouple, composed of the conductive, convective and radiative heat transfer, [142], [143] as seen in **Figure B-2** and **Eq. B-1** to **Eq. B-3**.

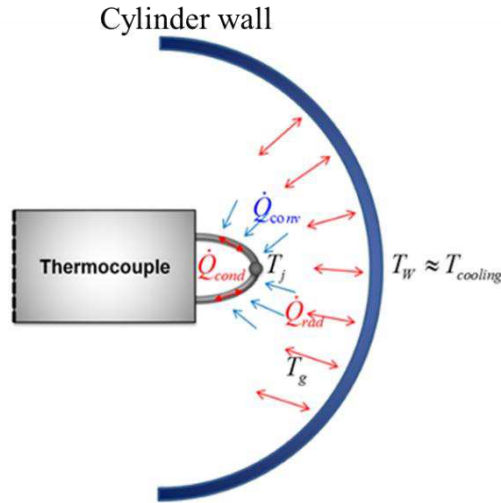


Figure B-2 Schematic diagram of the energy balance equation.

$$\dot{Q}_{store} = \dot{Q}_{conv} + \dot{Q}_{cond} + \dot{Q}_{rad} \quad \text{Eq. B-1}$$

$$\rho_b C_b V_b \frac{dT_{ms}}{dt} = h A_{sr} (T_c - T_{ms}) - \frac{k A_{cr}}{L} \Delta T - \epsilon \sigma A_{sr} (T_{ms}^4 - T_w^4) \quad \text{Eq. B-2}$$

$$T_{cor} = T_{ms} + \tau \frac{dT_{ms}}{dt} + \frac{k A_{cr}}{L A_{sr}} \Delta T + \frac{\epsilon \sigma}{h} (T_{ms}^4 - T_w^4) \quad \text{Eq. B-3}$$

where $\dot{Q}_{store}$ is heat store in the thermocouple junction. In term on the left hand side, $\dot{Q}_{conv}$ presents convective heat transfer between junction and hot gas inside the chamber, while $\dot{Q}_{cond}$ is a term of conduction heat transfer across thermocouple. In the last term, $\dot{Q}_{rad}$ presents the radiative heat transfer between the junction and surface cylinder wall. For T_{cor} , T_{ms} and T_w are

the corrected temperature [K], measured temperature at the bead [K] and wall or cooling temperature [K], respectively. While ϵ , σ and h are the emissivity of the bead thermocouple [-], the Stefan-Boltzmann constant, 5.6703×10^{-8} [W.m⁻².K⁻⁴] and the heat transfer coefficient [W.m⁻².K⁻¹]. For subscript b denotes the bead thermocouple, ρ the density [kg.m⁻³], C_b the specific heat density [J.kg⁻¹.K⁻¹], V the volume [m]. A_{sr} , A_{cr} and k are the surface area of bead thermocouple, cross section area of wire thermocouple and the thermal conductivity of gas [W.m⁻¹.K⁻¹].

Time constant of thermocouple

In second term of **Eq. B-3**, the time constant of thermocouple (τ) is respond time of thermocouple to sensitively for changing temperature, which it is not only calculates by properties of thermocouple junction but also fluid around junction are considered as seen in **Eq. B-4**:

$$\tau = \frac{\rho_j C_j V_j}{h A_{sr}} = \frac{\rho_j C_j L_c}{n_c h} \quad \text{Eq. B-4}$$

If the physical properties of junction and the fluid are kept constant regardless of temperature [5], therefore time constant is determined by convective heat transfer coefficient (h) which depends on the flow conditions and the thermos-physical properties of fluid. Moreover, time constant depends on geometry of junction of thermocouple, which defines in term of characteristic diameter (L_c), it is the ratio of volume and surface area of thermocouple junction and n_c is a characteristic number.

In this study, Dupont's correlation [67] recommended by ECN was used to determine the time constant, the time constant for wire (τ_w) and bead (τ_b) of thermocouple are presented in **Eq. B-5** and **Eq. B-6**. The Nussult number (Nu) defined by Kramers's correlation [144] for the cylindrical and spherical shape are shown in **Eq. B-7** and **Eq. B-8**. As seen in **Figure B-1** (right), the shape of the bead thermocouple is similar to a spherical shape, therefore, the time constant and Nussult number of the spherical shape was considered to apply in this work as presented in **Eq. B-6** and **Eq. B-8**.

$$\text{For the thermocouple wire: } \tau_w = \frac{\rho_w \cdot C_w \cdot d_w^2}{4Nu_w \cdot k} \quad \text{Eq. B-5}$$

$$\text{For the thermocouple bead: } \tau_b = \frac{\rho_w \cdot C_w \cdot d_b^2 [1 + 0.5(d_w^2/d_b^2)]}{6Nu_b \cdot k} \quad \text{Eq. B-6}$$

$$\text{For the thermocouple wire: } Nu_w = 0.42Pr^{0.2} + 0.57Pr^{0.33}Re^{0.5} \quad \text{Eq. B-7}$$

$$\text{For the thermocouple bead: } Nu_b = 2 + 1.3Pr^{0.15} + 0.66Pr^{0.31}Re^{0.5} \quad \text{Eq. B-8}$$

Reynolds Number (Re) is defined in equation **Eq. B-9**, where ρ and μ are density and dynamic viscosity of the gas. U is an average velocity of the gas inside the chamber, estimated around 0.1 m/s as obtained by PIV measurement in **Chapter 2**. d_b is diameter of the bead thermocouple that immersed in fluid, which is 39 μm for the 13 μm thermocouple as presented in **Figure B-1** (right-top).

Prandtl Number (Pr) is defined in equation **Eq. B-10**, where ν , α , C_p and k are kinematic viscosity, thermal diffusivity, specific heat and thermal conductivity of working fluid [143], respectively.

$$Re = \frac{\rho U d_L}{\mu} \quad \text{Eq. B-9}$$

$$Pr = \frac{\nu}{\alpha} = \frac{\mu C_p}{k} \quad \text{Eq. B-10}$$

Conductive heat transfer

The third term of **Eq. B-3** presents the conductive heat transfer across thermocouple, it can be neglect the term of conductive heat transfer as the result of the thermocouple diameter is too small and leading to the temperature gradient of throughout wire is uniform. It can explain by Biot Number (Bi) of lump system analysis in **Eq. B-10** [143]. A small Bi number represent small resistance to heat conduction and thus small temperature gradients with the thermocouple wire. Thus, when $Bi < 0.1$, the variation of temperature with location within the body is slight and can reasonably be approximated as being uniform. From physical properties of the

thermocouple can determine the Bi about 0.00129, less than 0.1. Therefore, it can be concluded that the temperature gradient throughout wire is uniform and conductive term of **Eq. B-3** can be neglected. The corrected gas temperature equation can be rewritten by **Eq. B-11** for the spherical shape of bead thermocouple.

$$Bi = \frac{hL_c}{k} \quad \text{Eq. B-10}$$

$$T_{cor} = T_{ms} + \left(\frac{\rho_w \cdot C_w \cdot d_b^2 [1 + 0.5(d_w^2/d_b^2)]}{6Nu_b \cdot k} \right) \frac{dT_{ms}}{dt} + \frac{\epsilon\sigma}{h} (T_{ms}^4 - T_w^4) \quad \text{Eq. B-11}$$

Radiation heat transfer

The last term in of **Eq. B-11**, the radiation heat exchanged between the thermocouple junction and cylinder wall are presented. The temperature of cylinder wall can be approximated to be cooling temperature, while the emissivity (ϵ) of junction is difficult to define because there is no specification from the producer. However, the type K thermocouple normally made from two materials between Chromal (oxidized) and Alumel (oxidized) which have emissivity about 0.6-0.85 and 0.6, respectively, thus this report approximates emissivity value at 0.6.

B.2 Adiabatic ambient temperature

According to the first law of thermodynamics, the change in internal energy (dU) to the work (dW) done by the heat (dQ) added to it. An adiabatic process is one in which no heat ($dQ = 0$) is gained or lost by the system, therefore, the first law can rearranged by **Eq. B-12**.

$$dU = dW \quad \text{Eq. B-12}$$

$$nC_v dT = -PdV \quad \text{Eq. B-13}$$

By applying, the temperature from real gas law equation of the Van der Waal's equation (**Eq. B-13**) and $\frac{C_v}{R_u} = \frac{1}{\gamma-1}$, the adiabatic pressure (P_{adb}) can be derived in equation **Eq. B-14**.

$$T = \frac{(P + \frac{an^2}{V^2})(V - nb)}{nR_u} \quad \text{Eq. B-13}$$

$$P_{adb(i)} \left[\frac{1}{dV} + \frac{\gamma}{V - nb} \right] = \frac{2n^3ab}{V^3(V - nb)} + \frac{P_{adb(i-1)}}{dV} \quad \text{Eq. B-14}$$

Finally, the adiabatic temperature (T_{adb}) concluded real gas and combined effect of compressibility can be defined in **Eq. B-15**.

$$T_{adb} = \frac{P_{adb}V}{nR_uZ} \quad \text{Eq. B-15}$$

Where Z is the compressibility factor from Van de Waals equation can be written as **Eq. B-16**

$$Z = \frac{V_m}{V_m - b} - \frac{a}{RTV_m} \quad \text{Eq. B-16}$$

The a and b are the Van der Waals constant of gas, which are 1.352 and 0.0387 for Nitrogen in example. V_m is molar volume of the gas.

B.3 Bulk Temperature

Normally, the bulk temperature can be derived by using cylinder pressure data from piëzo-electric sensor and perfect gas theory. In this study, a well-known the Van der Waals's gas law is used to calculate the bulk temperature in order to take into account on the real gas. The main reason to make different between perfect gas and real gas is the postulate of the kinetic molecular theory of perfect gas ignore the volume occupied by the molecules of a gas and the interaction between molecules. The Van der Waal's equation corrected the term of real volume of gas by nb and term of interaction between particles by $\frac{an^2}{V^2}$, it can summary in **Eq. B-17**,

$$T_{bulk} = \frac{(P + \frac{an^2}{V^2})(V - nb)}{nR_u}$$

Eq. B-17

where constant value a and b of N_2 are 1.352 and 0.0387 and R_u is universal gas constant.

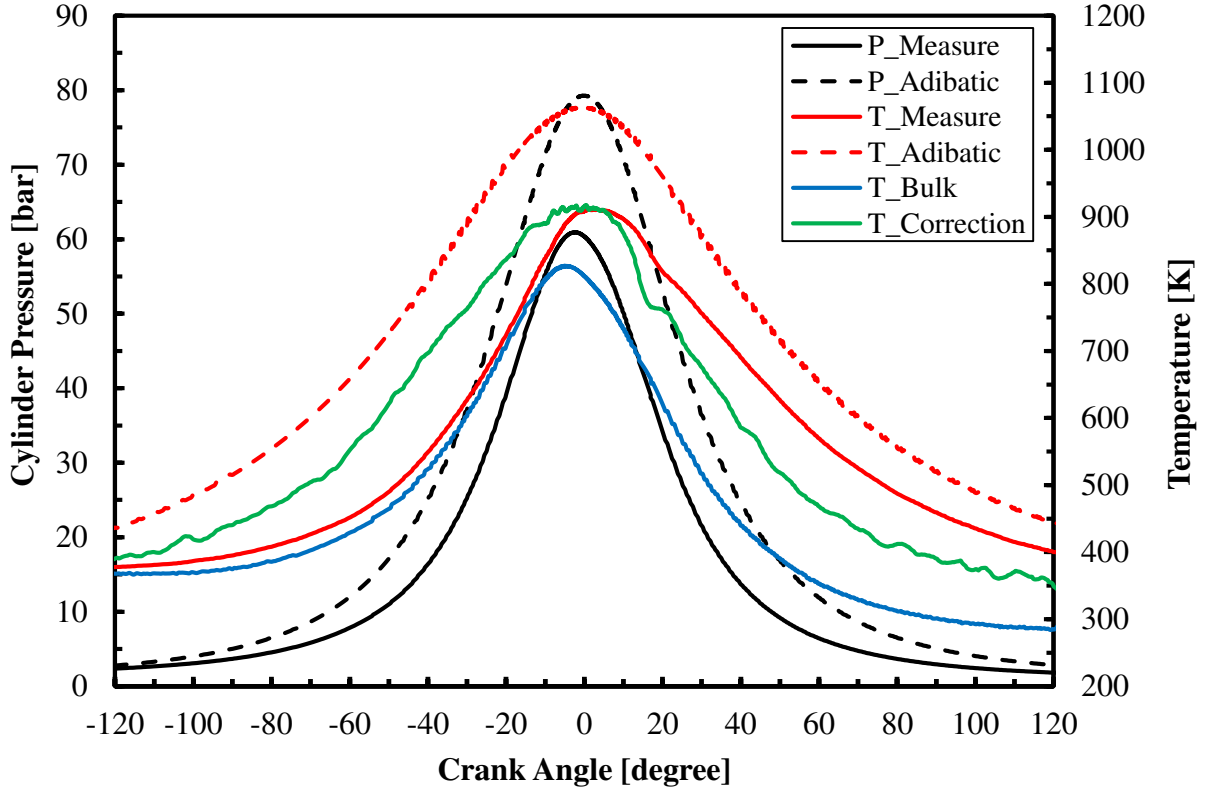


Figure B-3 Thermodynamic ambient condition of NOSE during the compression stroke.

Figure B-3 presents a thermodynamic ambient condition of the ECN Spray-A in reactive condition (900 K, 60 bar and 22.8 kg/m³), pressure and temperature, measured inside the combustion chamber during compression stroke. It can be seen that the heat loss during the compression process can be observed by the difference of pressure and temperature between the measurement value and calculation value of adiabatic compression process, calculated by **Eq. B-14** and **Eq. B-15** for pressure and temperature, respectively. While a green line presents the corrective temperature from **Eq. B-11**. As presented in **Chapter 2**,

- During the compression stroke, the corrected gas temperature (T_{cor}) is dominated by convective heat transfer from hot gases to the bead of thermocouple, because there are highly different rates of temperature ($\frac{dT_{TC}}{dt}$), as seen in a dotted green line of **Figure B-4**.
- Around TDC, there is a slight exchange, as the radiative heat transfer is about 3-5 K between hot gases inside chamber and wall temperatures, as seen in a dot-dash green line of **Figure B-4**.
- During expansion stroke, the convective heat transfer is also dominated, but heat is transferred from the bead thermocouple to gases lead to T_{cor} in this period lower than T_{ms} .

The time constant (τ) of thermocouple for whole cycle is around 3.0 to 8.4, which is lowest at around TDC due to the lowest speed of piston movement.

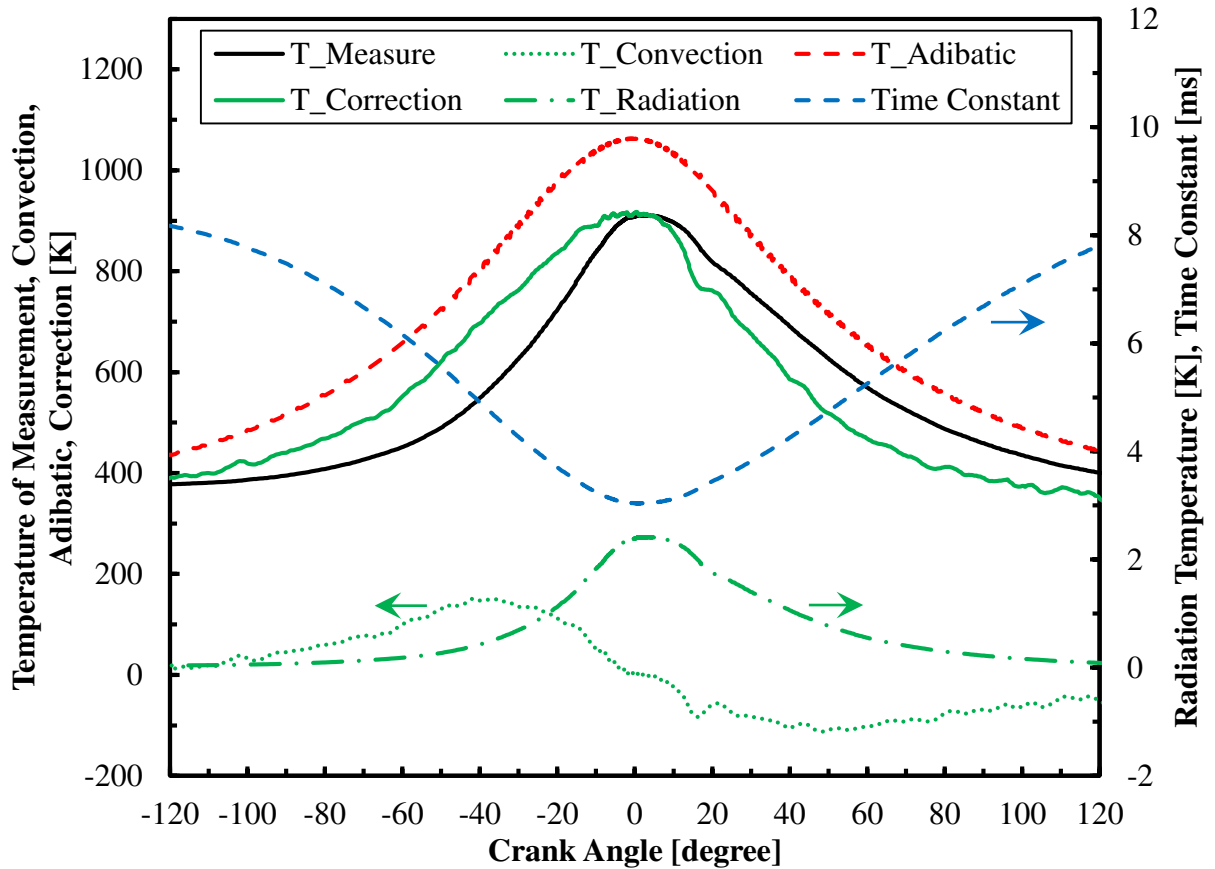


Figure B-4 Thermodynamic ambient condition of NOSE during compression stroke.

B.4 Changing Compression Ratio

The compression ratio (CR) can be changed by adjusting the metallic plate at the piston base, changing the volumetric ratio of compression, as presented in **Chapter 2**. As seen in **Figure A-9 (a)**, after removing the cylinder head of NOSE the piston head can be observed. Then, remove the piston head and change the metallic plate as illustrated in **Figure A-9 (b)**, the thickness of the metallic plate related to compression ratio presents in **Table A-1**.

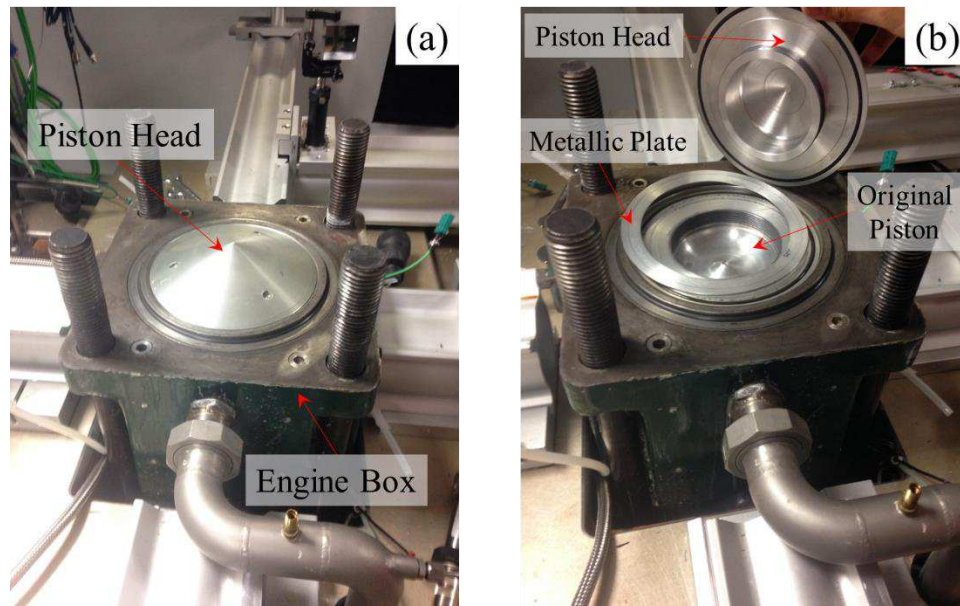


Figure A-9 Changing compression ratio of the NOSE

Table A-1 The compression ratio (CR) in different thickness of metallic plate.

Thickness of Metallic plate [mm]	Volume at BDC [cm ³]	Volume at TDC [cm ³]	Compression Ratio (CR) [-]
4.00	3601.6	240.4	15.0
2.55	3629.8	268.7	13.5
1.55	3648.7	287.5	12.7
1.23	3658.2	297.0	12.3

APPENDIX C

DETERMINATION OF TRANSFER NUMBER (B)

According to the Siebers's the liquid length scaling [34]. It is derived by solving mass, momentum and energy balances for the axial location at which fuel vaporization is complete in the idealized spray model. The transfer number (B) is defined in term of the fuel and ambient gas properties, the initial fuel and ambient gas conditions: the ambient gas temperature (T_a) and pressure (P_a) and fuel temperature (T_f) and an unknown parameter the steady-state value of surface temperature (T_s), as presented in **Eq. C-1**. (see more details of derivation in [34])

$$B = \frac{Z_a(T_s, P_a - P_s) \cdot P_s \cdot M_f}{Z_f(T_s, P_s) \cdot [P_a - P_s] \cdot M_a} = \frac{h_a(T_a, P_a) - h_a(T_s, P_a - P_s)}{h_f(T_s) - h_f(T_f, P_a)} \quad \text{Eq. C-1}$$

The unknown, T_s , can be solved for iteratively given the fuel and ambient gas properties and initial fuel and initial fuel and ambient gas conditions. Once determined, T_s defines B , as well as the pressure, temperature and enthalpies of the fuel and ambient gas at the liquid length location. The term B is analogous to the mass and thermal transfer numbers used in droplet vaporization studies [139], called “Graphic Method”.

The graphic method is based on the evaporation theory of fuel droplet, which assumes a pure fuel droplet is suddenly immersed in ambient hot gases, the mass transfer number (B_M) and the heat transfer number (B_T) between the droplet and ambient hot gases have to be equal as the evaporation rate is constant. The basic idea of this method is to plot B_M and B_T evolution versus surface temperature, T_s , in a temperature range below the normal fuel boiling temperature value. The intersection of the two curves provides B and T_s values, for the steady-state condition. In this section, the procedures to determine B and T_s by the graphic method are briefly described by following steps:

- 1) Select a starting value of T_s , it should be lower than the boiling point (T_b) of fuel.
- 2) Calculate a mass transfer number (B_M) by

$$B_M = \frac{Y_{f,s}}{1 - Y_{f,s}} \quad \text{Eq. C-2}$$

The fuel mass factor ($Y_{f,s}$) at droplet surface at T_s can be estimated by

$$Y_{f,s} = \frac{P_{f,s} \cdot M_f}{P_{f,s} \cdot M_f + (P - P_{f,s})M_a} = \left[1 + \left(\frac{P}{P_{f,s}} - 1 \right) \frac{M_a}{M_f} \right]^{-1} \quad \text{Eq. C-3}$$

where M_a and M_f are the molecular weights of fue and air, respectively and P is the ambient pressure. For the vapor pressure of fuel ($P_{f,s}$) at T_s can be determined by using Antoine equation [145] as:

$$\log_{10}(P_{f,s}) = a - \frac{b}{T_s - c} \quad \text{Eq. C-4}$$

where value of a and b for several hydrocarbon fuels (see in [145]).

- 3) At the steady-state condition, the mass transfer number (B_M) and heat transfer number (B_T) are equilibrium ($B_M = B_T = B$), therefore, B_T calculated by,

$$B_T = \frac{C_{p,g}(T_a - T_s)}{L_v} \quad \text{Eq. C-5}$$

where L_v is the latent heat of fuel vaporization corresponding to the T_s . The $C_{p,g}$ is the specific heat of gas at constant pressure at the reference temperature (T_r).

3.1 Determination of $C_{p,g}$

To determine the averaged gas properties i.e. $C_{p,g}$, the one-third rule of Sparrow and Gregg is recommended to apply in this method [139], the $C_{p,g}$ is evaluated at the following reference temperature and composition:

$$C_{p,g} = Y_{a,r}(C_{p,a} \text{ at } T_r) + Y_{f,r}(C_{p,v} \text{ at } T_r) \quad \text{Eq. C-6}$$

$$T_r = T_s + \frac{T_a - T_s}{3} \quad \text{Eq. C-7}$$

$Y_{a,r}$ and $Y_{f,r}$ are the mass fraction of ambient gas and fuel vapor at the reference temperature (T_r) calculated from **Eq. C-7**. For $C_{p,a}$ and $C_{p,v}$ are the specific heat ratio of ambient gas and fuel vapor at T_r .

$$Y_{f,r} = \frac{2}{3} Y_{f,s} \quad \text{Eq. C-8}$$

$$Y_{a,r} = 1 - Y_{f,r} = 1 - \frac{2}{3} Y_{f,s} \quad \text{Eq. C-9}$$

The variation of specific heat of hydrocarbon fuel vapor with temperature is described by the relationship,

$$C_{p,v} = (363 + 0.467T)(5 - 0.001\rho_{f_0}) \quad \text{Eq. C-10}$$

where ρ_{f_0} is the fuel density at a temperature of 288.6 K. While the specific heat of ambient gas ($C_{p,a}$), i.e. Nitrogen, Oxygen, etc. can be found in the NIST chemistry webbook (<https://webbook.nist.gov/chemistry/>).

3.2 The latent heat of vaporization (L_v) is given by Watson [146] as

$$L_v = L_{T_b} \left(\frac{T_{cr} - T_s}{T_{cr} - T_b} \right) \quad \text{Eq. C-11}$$

where L_{T_b} , T_{cr} and T_b are the latent heat of vaporization at boiling point, critical temperature and boiling point, respectively. Due to the lack of data L_{T_b} , T_{cr} and T_b for blends fuel (ABE blends and alcohol blends) these data is estimated from the mass fraction of single-component fuels.

- 4) After calculation, the value of B_M and B_T is compared. If $B_M < B_T$, that mean the selected T_s in first step is too low, therefore, T_s would be increased.
- 5) Repeat calculation from 1) – 4) by increasing T_s until reaching the equilibrium point that $B_M = B_T$, as seen in **Figure C-1**.

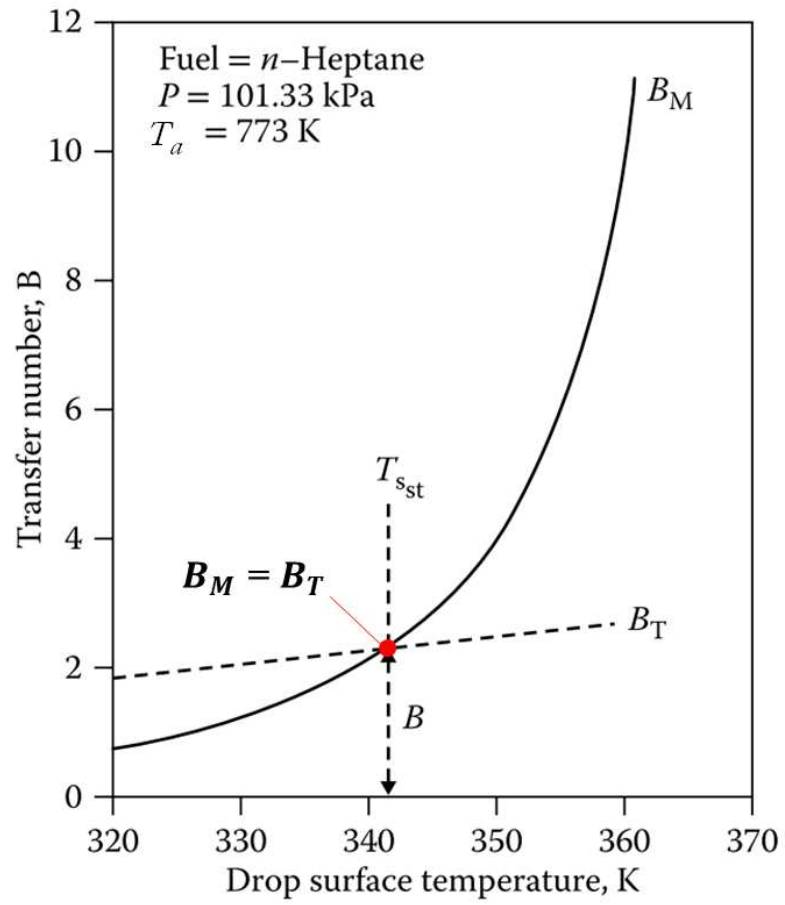


Figure C-1 Variation of B_M and B_T with drop surface temperature [139].

BIBLIOGRAPHY

- [1] U.S. Energy Information Administration. International Energy Outlook 2017 n.d. <https://www.eia.gov/outlooks/ieo/> (accessed June 26, 2018).
- [2] Miller JD, Façanha C. The State Of Clean Transport Policy a 2014 Synthesis of Vehicle and fuel policy developments. 2014.
- [3] IRENA. IRENA Work on Bioenergy for Sustainable Development: Accomplishments and Findings 2014-2017. 2017.
- [4] Kumar S, Cho JH, Park J, Moon I. Advances in Diesel-Alcohol Blends and Their Effects on the Performance and Emissions of Diesel Engines. *Renew Sustain Energy Rev* 2013;22:46–72. doi:10.1016/j.rser.2013.01.017.
- [5] Jin C, Yao M, Liu H, Lee CFF, Ji J. Progress in the Production and Application of n-Butanol as a Biofuel. *Renew Sustain Energy Rev* 2011;15:4080–106. doi:10.1016/j.rser.2011.06.001.
- [6] Kumar BR, Saravanan S, Rana D, Nagendran A. A comparative analysis on combustion and emissions of some next generation higher-alcohol / diesel blends in a direct-injection diesel engine. *Energy Convers Manag* 2016;119:246–56. doi:10.1016/j.enconman.2016.04.053.
- [7] Liu H, Bi X, Huo M, Lee CFF, Yao M. Soot Emissions of Various Oxygenated Biofuels in Conventional Diesel Combustion and Low-Temperature Combustion Conditions. *Energy and Fuels* 2012;26:1900–11. doi:10.1021/ef201720d.
- [8] Irimescu A, Marchitto L, Merola SS, Tornatore C, Valentino G. Combustion process investigations in an optically accessible DISI engine fuelled with n-butanol during part load operation. *Renew Energy* 2015;77:363–76. doi:10.1016/j.renene.2014.12.029.
- [9] Valentino G, Merola S, Marchitto L, Tornatore C. Butanol-Diesel Blend Spray Combustion Investigation by UV-Visible Flame Emission in a Prototype Single Cylinder

- Compression Ignition Engine. SAE Int J Engines 2015;8:2015-24–2435. doi:10.4271/2015-24-2435.
- [10] Wu H, Nithyanandan K, Zhou N, Lee TH, Lee CFF, Zhang C. Impacts of acetone on the spray combustion of Acetone-Butanol-Ethanol (ABE)-Diesel blends under low ambient temperature. Fuel 2015;142:109–16. doi:10.1016/j.fuel.2014.10.009.
- [11] Chang YC, Lee WJ, Lin SL, Wang LC. Green energy: Water-Containing Acetone-Butanol-Ethanol Diesel Blends Fueled in Diesel Engines. Appl Energy 2013;109:182–91. doi:10.1016/j.apenergy.2013.03.086.
- [12] Karimi K, Tabatabaei M, Horváth IS, Kumar R. Recent Trends in Acetone, Butanol, and Ethanol (ABE) Production. Biofuel Res J 2015;8:301–8. doi:10.18331/BRJ2015.2.4.4.
- [13] Wu H, Nithyanandan K, Zhang J, Lin Y, Lee TH, Lee CF, et al. Impacts of Acetone–Butanol–Ethanol (ABE) Ratio on Spray and Combustion Characteristics of ABE–Diesel Blends. Appl Energy 2015;149:367–78. doi:10.1016/j.apenergy.2014.11.053.
- [14] Chang YC, Lee WJ, Wu TS, Wu CY, Chen SJ. Use of Water Containing Acetone-Butanol-Ethanol for NO_x-PM (Nitrogen Oxide-Particulate Matter) Trade-Off in the Diesel Engine Fueled with Biodiesel. Energy 2014;64:678–87. doi:10.1016/j.energy.2013.10.077.
- [15] Wu H, Nithyanandan K, Lee TH, Lee CF, Zhang C. Spray and Combustion Characteristics of Neat Acetone-Butanol-Ethanol, n -Butanol, and Diesel in a Constant Volume Chamber. Energy & Fuels 2014;28:6380–91. doi:10.1021/ef5013819.
- [16] Wu H, Huo M, Zhou N, Nithyanandan K, Lee C-F, Zhang C, et al. An Experimental Investigation of the Combustion Characteristics of Acetone-Butanol-Ethanol-Diesel Blends with Different ABE Component Ratios in a Constant Volume Chamber. SAE Tech Pap 2014-01-1452. doi:10.4271/2014-01-1452.
- [17] IPCC. Summary for Policymakers. In: Intergovernmental Panel on Climate Change, editor. Clim. Chang. 2013 - Phys. Sci. Basis, Cambridge: Cambridge University Press; 2013, p. 1–30. doi:10.1017/CBO9781107415324.004.
- [18] UNFCCC. Conference of the Parties (COP). Paris Climate Change Conference-

November 2015, COP 21. Adopt Paris Agreement Propos by Pres 2015;21932:32. doi:FCCC/CP/2015/L.9/Rev.1.

- [19] Rogelj J, Den Elzen M, Höhne N, Fransen T, Fekete H, Winkler H, et al. Paris Agreement Climate Proposals Need a Boost to Keep Warming Well below 2 °C. *Nature* 2016;534:631–9. doi:10.1038/nature18307.
- [20] IPCC. Summary for policymakers. *Clim. Chang.* 2014 Impacts, Adapt. Vulnerability. Part A Glob. Sect. Asp. Contrib. Work. Gr. II to Fifth Assess. Rep. Intergov. Panel Clim. Chang., Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, pp. 1-32.; 2014, p. 1–32.
- [21] Energy Information Administration (EIA). Transportation Sector Energy Consumption. *Int. Energy Outlook 2016*, 2016, p. 127–37.
- [22] Ritchie H, Roser M. CO2 and other Greenhouse Gas Emissions. OurWorldInDataOrg 2015:1–32. <https://ourworldindata.org/co2-and-other-greenhouse-gas-emissions> (accessed June 25, 2018).
- [23] International Council on Clean Transportation. Passenger car CO2 emissions and fuel consumption, normalized to NEDC n.d.:2020. <https://www.theicct.org/chart-library-passenger-vehicle-fuel-economy> (accessed June 27, 2018).
- [24] The International Renewable Energy Agency (IRENA). *REmap 2030* 2011:6. doi:10.1080/000164702753671623.
- [25] The International Renewable Energy Agency (IRENA). *The Renewable Route To Sustainable Transport*. 2016.
- [26] No SY. A Review on Spray Characteristics of Bioethanol and Its Blended Fuels in CI Engines. *J ILASS-KOREA* 2015;19:1–8.
- [27] Park SH, Kim HJ, Lee CS. Effect of Multiple Injection Strategies on Combustion and Emission Characteristics in a Diesel Engine. *Energy & Fuels* 2016;acs.energyfuels.5b02121. doi:10.1021/acs.energyfuels.5b02121.
- [28] Mendez S, Thirouard B. Using Multiple Injection Strategies in Diesel Combustion: Potential to Improve Emissions, Noise and Fuel Economy Trade-Off in Low CR Engines.

- SAE Int J Fuels Lubr 2008;1:2008-01-1329. doi:10.4271/2008-01-1329.
- [29] Hiroyasu H, Arai M. Structures of Fuel Sprays in Diesel Engines. SAE Tech. Pap. Ser., 1990:900475. doi:10.4271/900475.
 - [30] Soid SN, Zainal ZA. Spray and combustion characterization for internal combustion engines using optical measuring techniques - A review. Energy 2011;36:724–41. doi:10.1016/j.energy.2010.11.022.
 - [31] Fansler TD, Parrish SE. Spray measurement technology: A review. Meas Sci Technol 2015;26:12002. doi:10.1088/0957-0233/26/1/012002.
 - [32] Dec JE. A Conceptual Model of DI Diesel Combustion Based on Laser-Sheet Imaging. SAE Tech Pap 1997:970873. doi:10.4271/970873.
 - [33] Hattori H, Narumiya K, Tsue M, Kadota T. Analysis of Initial Breakup Mechanism of Diesel Spray Injected into High-Pressure Ambience. SAE Pap 2004-01-0528. doi:10.4271/2004-01-0528.
 - [34] Siebers DL. Scaling Liquid-Phase Fuel Penetration in Diesel Sprays Based on Mixing-Limited Vaporization. SAE Pap 1999-01-0528. doi:10.4271/1999-01-0528.
 - [35] Siebers DL. Liquid-Phase Fuel Penetration in Diesel Sprays 1998: 980809. doi:10.4271/980809.
 - [36] Musculus MPB, Miles PC, Pickett LM. Conceptual models for partially premixed low-temperature diesel combustion. vol. 39. Elsevier Ltd; 2013. doi:10.1016/j.pecs.2012.09.001.
 - [37] Desantes JM, Benajes J, Molina S, González CA. The Modification of the Fuel Injection Rate in Heavy-Duty Diesel Engines. Part 1: Effects on Engine Performance and Emissions. Appl Therm Eng 2004;24:2701–14. doi:10.1016/j.applthermaleng.2004.05.003.
 - [38] Wang Z, Wyszynski ML, Xu H, Abdullah NR, Piaszyk J. Fuel Injection and Combustion Study by the Combination of Mass Flow Rate and Heat Release Rate with Single and Multiple Injection Strategies. Fuel Process Technol 2015;132:118–32. doi:10.1016/j.fuproc.2014.11.024.

- [39] Glenn R. Bower and David E. Foster. A Comparison of the Bosch and Zuech Rate of Injection Meters. SAE Tech Pap 1991: 910724. doi:10.4271/910724.
- [40] Tanabe K, Kohketsu S, Mori K, Kawai K. Innovative Injection Rate Control with Next Generation Common Rail Fuel Injection System. FISITA World Automot Congr Seoul, Pap F2000A055 2000;286.
- [41] Payri R, Gimeno J, Bardi M, Plazas A. Effect of Injection Rate Shaping Over Diesel Spray Development in Non Reacting Evaporative Conditions. ASME 2012 Intern. Combust. Engine Div. Spring Tech. Conf., ASME; 2012, p. 347. doi:10.1115/ICES2012-81206.
- [42] Han C, Yuan C, He Y, Liu Y. Effect of Fuel Injection Rate Shapes on Mixture Formation and Combustion Characteristic in a Free-Piston Diesel Engine Generator. Adv Mech Eng 2018;10:1–11. doi:10.1177/1687814018775242.
- [43] Ikegami M, Nakatani K, Tanaka S, Yamane K. Fuel Injection Rate Shaping and Its Effect on Exhaust Emissions in a Direct-Injection Diesel Engine Using a Spool Acceleration Type Injection System. SAE Tech. Pap. 970347, 1997. doi:10.4271/970347.
- [44] Higgins BS, Mueller CJ, Siebers DL. Measurements of Fuel Effects on Liquid-Phase Penetration in DI Sprays. SAE Trans 1999-01-0519. doi:10.4271/1999-01-0519.
- [45] Bardi M, Payri R, Malbec LM, Bruneaux G, Pickett LM, Manin J, et al. Engine Combustion Network: Comparison of Spray Development, Vaporization, and Combustion in Different Combustion Vessels. At Sprays 2012;22:807–42. doi:10.1615/AtomizSpr.2013005837.
- [46] Payri R, Gimeno J, Bardi M, Plazas AH. Study Liquid Length Penetration Results Obtained with a Direct Acting Piezo Electric Injector. Appl Energy 2013;106:152–62. doi:10.1016/j.apenergy.2013.01.027.
- [47] Payri R, Gimeno J, Bracho G, Vaquerizo D. Study of Liquid and Vapor Phase Behavior on Diesel Sprays for Heavy Duty Engine Nozzles. Appl Therm Eng 2016;107:365–78. doi:10.1016/j.applthermaleng.2016.06.159.
- [48] Desantes JM, Payri R, Pastor JM, Gimeno J. Experimental Characterization of Internal

Nozzle Flow and Diesel Spray Behavior. Part I: Nonevaporative Conditions. *At Sprays* 2005;15:489–516. doi:10.1615/AtomizSpr.v15.i5.20.

- [49] Naber JD, Siebers DL. Effects of Gas Density and Vaporization on Penetration and Dispersion of Diesel Sprays. *SAE Pap* 1996: 960034. doi:10.4271/960034.
- [50] Dernotte J, Hespel C, Houille S, Foucher F, Mounaim-Rousselle C. Influence of Fuel Properties on the Diesel Injection Process in Nonvaporizing Conditions. *At Sprays* 2012;22:461–92. doi:10.1615/AtomizSpr.2012004401.
- [51] Payri R, Gimeno J, Viera JP, Plazas AH. Needle Lift Profile Influence on the Vapor Phase Penetration for a Prototype Diesel Direct Acting Piezoelectric Injector. *Fuel* 2013;113:257–65. doi:10.1016/j.fuel.2013.05.057.
- [52] Payri R, García-Oliver JM, Bardi M, Manin J. Fuel Temperature Influence on Diesel Sprays in Inert and Reacting Conditions. *Appl Therm Eng* 2012;35:185–95. doi:10.1016/j.applthermaleng.2011.10.027.
- [53] Kook S, Pickett LM. Liquid Length and Vapor Penetration of Conventional, Fischer-Tropsch, Coal-Derived, and Surrogate Fuel Sprays at High-Temperature and High-Pressure Ambient Conditions. *Fuel* 2012;93:539–48. doi:10.1016/j.fuel.2011.10.004.
- [54] Stanton DW, Lippert AM, Reitz RD, Rutland C. Influence of Spray-Wall Interaction and Fuel Films on Cold Starting in Direct Injection Diesel Engines. *SAE Tech. Pap.*, 1998: 982584. doi:10.4271/982584.
- [55] Li K, Nishida K, Ogata Y, Shi B. Effect of Flat-Wall Impingement on Diesel Spray Combustion. *Proc Inst Mech Eng Part D J Automob Eng* 2015;229:535–49. doi:10.1177/0954407014547242.
- [56] J. Kashdan SM and GB. An Investigation of Unburned Hydrocarbon Emissions in Wall Guided, Low Temperature Diesel Combustion. *Oil Gas Sci Technol* 2008;63:433–59. doi:10.2516/ogst:2008018.
- [57] Som S, Ramirez AI, Longman DE, Aggarwal SK. Effect of Nozzle Orifice Geometry on Spray, Combustion, and Emission Characteristics under Diesel Engine Conditions. *Fuel* 2011;90:1267–76. doi:10.1016/j.fuel.2010.10.048.

- [58] Dernet J, Hespel C, Foucher F, Houillé S, Mounaïm-Rousselle C. Influence of Physical Fuel Properties on the Injection Rate in a Diesel Injector. *Fuel* 2012;96:153–60. doi:10.1016/j.fuel.2011.11.073.
- [59] Kastengren AL, Tilocco FZ, Powell CF, Manin J, Pickett LM, Payri R, et al. Engine Combustion Network (ECN): Measurements of Nozzle Geometry and Hydraulic Behavior. *Atomiz Sprays* 2012;22:1011–52. doi:10.1615/AtomizSpr.2013006309.
- [60] Blessing M, König G, Krüger C, Michels U, Schwarz V. Analysis of Flow and Cavitation Phenomena in Diesel Injection Nozzles and Its Effects on Spray and Mixture Formation 2003. doi:10.4271/2003-01-1358.
- [61] Musculus MPB, Kattke K. Entrainment Waves in Diesel Jets. *SAE Int J Engines* 2009-01-1355. doi:10.4271/2009-01-1355.
- [62] Pastor J, Garcia-Oliver JM, Garcia A, Nareddy VR. Characterization of Spray Evaporation and Mixing Using Blends of Commercial Gasoline and Diesel Fuels in Engine-Like Conditions 2017. doi:10.4271/2017-01-0843.
- [63] Pickett LM, Kook S, Williams TC. Visualization of Diesel Spray Penetration, Cool-Flame, Ignition, High-Temperature Combustion, and Soot Formation Using High-Speed Imaging. *SAE Int J Engines* 2009-01-0658. doi:10.4271/2009-01-0658.
- [64] Higgins B, Siebers D, Aradi A. Diesel-Spray Ignition and Premixed-Burn Behavior SAE Tech. Pap., 2000-01-0940. doi:10.4271/2000-01-0940.
- [65] Lapuerta M, Sanz-Argent J, Raine RR. Ignition Characteristics of Diesel Fuel in a Constant Volume Bomb Under Diesel-Like Conditions. Effect of the Operation Parameters. *Energy and Fuels* 2014;28:5445–54. doi:10.1021/ef500535j.
- [66] Lapuerta M, Hernández JJ, Fernández-Rodríguez D, Cova-Bonillo A. Autoignition of blends of n-butanol and ethanol with diesel or biodiesel fuels in a constant-volume combustion chamber. *Energy* 2017;118:613–21. doi:10.1016/j.energy.2016.10.090.
- [67] Meijer M, Galle J, Somers LMT, Griensven JG., Verhelst S. High-Speed Characterization of ECN Spray A Using Various Diagnostic Techniques. *SAE Int J Engines* 2013-01-1616. doi:10.4271/2013-01-1616.

- [68] Donkerbroek AJ, Boot MD, Luijten CCM, Dam NJ, ter Meulen JJ. Flame Lift-Off Length and Soot Production of Oxygenated Fuels in Relation with Ignition Delay in a DI Heavy-Duty Diesel Engine. *Combust Flame* 2011;158:525–38. doi:10.1016/j.combustflame.2010.10.003.
- [69] Pickett LM, Siebers DL, Idicheria CA. Relationship Between Ignition Processes and the Lift-Off Length of Diesel Fuel Jets. SAE Tech Pap 2005-01-3843. doi:10.4271/2005-01-3843.
- [70] Zheng Z, Badawy T, Henein N, Sattler E. Investigation of Physical and Chemical Delay Periods of Different Fuels in the Ignition Quality Tester. *J Eng Gas Turbines Power* 2013;135:061501. doi:10.1115/1.4023607.
- [71] Manin J, Skeen S, Pickett L, Kurtz E, Anderson JE. Effects of Oxygenated Fuels on Combustion and Soot Formation/Oxidation Processes. *SAE Int J Fuels Lubr* 2014-01-2657. doi:10.4271/2014-01-2657.
- [72] Payri R, Salvador FJ, Gimeno J, de la Morena J. Effects of Nozzle Geometry on Direct Injection Diesel Engine Combustion Process. *Appl Therm Eng* 2009;29:2051–60. doi:10.1016/j.applthermaleng.2008.10.009.
- [73] Siebers DL, Higgins B, Pickett L. Flame Lift-Off on Direct-Injection Diesel Fuel Jets: Oxygen Concentration Effects 2002. doi:10.4271/2002-01-0890.
- [74] Payri R, Salvador FJ, Manin J, Viera A. Diesel Ignition Delay and Lift-Off Length Through Different Methodologies Using a Multi-Hole Injector. *Appl Energy* 2016;162:541–50. doi:10.1016/j.apenergy.2015.10.118.
- [75] Ito T, Kitamura T. Effects of Flame Lift-Off and Flame Temperature on Soot Formation in Oxygenated Fuel Sprays. SAE Tech Pap 2003-01-0073. doi:10.4271/2003-01-0073.
- [76] Siebers DL, Higgins B. Flame Lift-Off on Direct-Injection Diesel Sprays Under Quiescent Conditions. SAE Tech Pap 2001-01-0530. doi:10.4271/2001-01-0530.
- [77] Musculus MP, Dec JE, Tree DR. Effects of Fuel Parameters and Diffusion Flame Lift-Off on Soot Formation in a Heavy-Duty DI Diesel Engine In-Cylinder Diesel Particulates and NO_x Control. SAE Trans 2002-01-0889. doi:10.4271/2002-01-0889.

- [78] Kumfer BM, Skeen SA, Axelbaum RL. Soot inception limits in laminar diffusion flames with application to oxy-fuel combustion. *Combust Flame* 2008;154:546–56. doi:10.1016/j.combustflame.2008.03.008.
- [79] Peters N. *Turbulent Combustion*. Cambridge: Cambridge University Press; 2000. doi:10.1017/CBO9780511612701.
- [80] Lapuerta M, García-Contreras R, Campos-Fernández J, Dorado MP. Stability, lubricity, viscosity, and cold-flow properties of alcohol-diesel blends. *Energy and Fuels* 2010;24:4497–502. doi:10.1021/ef100498u.
- [81] Valentino G, Corcione FE, Iannuzzi SE, Serra S. Experimental Study on Performance and Emissions of a High Speed Diesel Engine Fuelled with n-Butanol Diesel Blends under Premixed Low Temperature Combustion. *Fuel* 2012;92:295–307. doi:10.1016/j.fuel.2011.07.035.
- [82] Wu M, Wang M, Liu J, Huo H. Review : Bioseparations and Assessment of Potential Life-Cycle Energy and Greenhouse Gas Emission Effects. *Biotechnol Prog* 2008;1204–14. doi:10.1021/bp.71.
- [83] Tuner M. Review and Benchmarking of Alternative Fuels in Conventional and Advanced Engine Concepts with Emphasis on Efficiency, CO₂, and Regulated Emissions. SAE Tech Pap 2016-01-0882. doi:10.4271/2016-01-0882.
- [84] Rakopoulos DC, Rakopoulos CD, Giakoumis EG, Dimaratos AM, Kyritsis DC. Effects of Butanol-Diesel Fuel Blends on the Performance and Emissions of a High-Speed DI Diesel Engine. *Energy Convers Manag* 2010;51:1989–97. doi:10.1016/j.enconman.2010.02.032.
- [85] Chen Z, Wu Z, Liu J, Lee C. Combustion and Emissions Characteristics of High n-Butanol/Diesel Ratio Blend in a Heavy-Duty Diesel Engine and EGR Impact. *Energy Convers Manag* 2014;78:787–95. doi:10.1016/j.enconman.2013.11.037.
- [86] Saisirirat P, Togbé C, Chanchaona S, Foucher F, Mounaïm-Rousselle C, Dagaut P. Auto-ignition and combustion characteristics in HCCI and JSR using 1-butanol/n-heptane and ethanol/n-heptane blends. *Proc Combust Inst* 2011;33:3007–14. doi:10.1016/j.proci.2010.07.016.

- [87] No SY. Application of Biobutanol in Advanced CI Engines - A Review. *Fuel* 2016;183:641–58. doi:10.1016/j.fuel.2016.06.121.
- [88] Saisirirat P, Foucher F, Chanchaona S, Mounaïm-Rousselle C. Effects of Ethanol, n-Butanol — n-Heptane Blended on Low Temperature Heat Release and HRR Phasing in Diesel-HCCI. *SAE Tech. Pap.* 2009-24-0094, 2009, p. doi:10.4271/2009-24-0094.
- [89] Miers SA, Carlson RW, McConnell SS, Ng HK, Wallner T, Esper JL. Drive Cycle Analysis of Butanol/Diesel Blends in a Light-Duty Vehicle. *SAE Pap* 2008-01-2381. doi:10.4271/2008-01-2381.
- [90] Marchitto L, Merola SS, Tornatore C, Valentino G. An Experimental Investigation of Alcohol/Diesel Fuel Blends on Combustion and Emissions in a Single-Cylinder Compression Ignition Engine. *SAE Tech Pap* 2003-01-0345. doi:10.4271/2003-01-0345.
- [91] Mo J, Tang C, Li J, Guan L, Huang Z. Experimental Investigation on the Effect of n-Butanol Blending on Spray Characteristics of Soybean Biodiesel in a Common-Rail Fuel Injection System. *Fuel* 2016;182:391–401. doi:10.1016/j.fuel.2016.05.109.
- [92] Liu Y, Li J, Jin C. Fuel Spray and Combustion Characteristics of Butanol Blends in a Constant Volume Combustion Chamber. *Energy Convers Manag* 2015;105:1059–69. doi:10.1016/j.enconman.2015.08.047.
- [93] Xue C, Zhao XQ, Liu CG, Chen LJ, Bai FW. Prospective and Development of Butanol as an Advanced Biofuel. *Biotechnol Adv* 2013;31:1575–84. doi:10.1016/j.biotechadv.2013.08.004.
- [94] Sarchami T, Munch G, Johnson E, Kießlich S, Rehmann L. A Review of Process-Design Challenges for Industrial Fermentation of Butanol from Crude Glycerol by Non-Biphasic *Clostridium pasteurianum*. *Fermentation* 2016;2:13. doi:10.3390/fermentation2020013.
- [95] Ndaba B, Chiyanzu I, Marx S. N-Butanol Derived from Biochemical and Chemical Routes: A Review. *Biotechnol Reports* 2015;8:1–9. doi:10.1016/j.btre.2015.08.001.
- [96] Kurkijärvi A, Lehtonen J, Linnekoski J. Novel Dual Extraction Process for Acetone-Butanol-Ethanol Fermentation. *Sep Purif Technol* 2014;124:18–25. doi:10.1016/j.seppur.2014.01.007.

- [97] Pfromm PH, Amanor-Boadu V, Nelson R, Vadlani P, Madl R. Bio-Butanol vs. Bio-Ethanol: A Technical and Economic Assessment for Corn and Switchgrass Fermented by Yeast or *Clostridium Acetobutylicum*. *Biomass and Bioenergy* 2010;34:515–24. doi:10.1016/j.biombioe.2009.12.017.
- [98] Lee T, Lin Y, Wu H, Meng L, Hansen A, Lee CF. Characterization Spray and Combustion Processes of Acetone-Butanol-Ethanol (ABE) in a Constant Volume Chamber. *SAE Tech Pap* 2015-01-0919. doi:10.4271/2015-01-0919.
- [99] Pickett LM, Genzale CL, Bruneaux G, Malbec L-M, Hermant L, Christiansen C, et al. Comparison of Diesel Spray Combustion in Different High-Temperature, High-Pressure Facilities. *SAE Int J Engines* 2010-01-2106. doi:10.4271/2010-01-2106.
- [100] Meijer M, Somers B, Johnson J, Naber J, Lee S-Y, Malbec LM, et al. Engine Combustion Network (ECN): Characterization and Comparison of Boundary Condition for Different Combustion Vessels. *At Sprays* 2012;22:777–806. doi:10.1615/AtomizSpr.2012006083.
- [101] Baert RSG, Frijters PJM, Somers B, Luijten CCM, de Boer W. Design and Operation of a High Pressure, High Temperature Cell for HD Diesel Spray Diagnostics: Guidelines and Results. *SAE Pap.* 2009-01-0649, vol. 4970, 2009. doi:10.4271/2009-01-0649.
- [102] Bermúdez V, Garcia JM, Juliá E, Martínez S. Engine with Optically Accessible Cylinder Head: A Research Tool for Injection and Combustion Processes. *SAE Tech Pap Ser* 2003-01-1110. doi:10.4271/2003-01-1110.
- [103] Malbec L-M, Egúsqiza J, Bruneaux G, Meijer M. Characterization of a Set of ECN Spray A Injectors: Nozzle to Nozzle Variations and Effect on Spray Characteristics. *SAE Int J Engines* 2013-24-0037. doi:10.4271/2013-24-0037.
- [104] Verhoeven D, Vanhemelryck J-L, Baritaud T. Macroscopic and Ignition Characteristics of High-Pressure Sprays of Single-Component Fuels 1998. doi:10.4271/981069.
- [105] Nesbitt JE, Johnson SE, Pickett LM, Siebers DL, Lee SY, Naber JD. Minor Species Production from Lean Premixed Combustion and Their Impact on Autoignition of Diesel Surrogates. *Energy and Fuels* 2011;25:926–36. doi:10.1021/ef101411f.
- [106] Pei Y, Davis MJ, Pickett LM, Som S. Engine Combustion Network (ECN): Global

- sensitivity analysis of Spray A for different combustion vessels. *Combust Flame* 2015;162:2337–47. doi:10.1016/j.combustflame.2015.01.024.
- [107] Teini PD, Karwat DMA, Atreya A. The Effect of CO₂/H₂O on the Formation of Soot Particles in the Homogeneous Environment of a Rapid Compression Facility. *Combust Flame* 2012;159:1090–9. doi:10.1016/j.combustflame.2011.10.002.
- [108] Bardi M, Bruneaux G, Malbec L. Study of ECN Injectors' Behavior Repeatability with Focus on Aging Effect and Soot Fluctuations. SAE Tech. Pap., 2016-01-0845. doi:10.4271/2016-01-0845.
- [109] Johnson S, Nesbitt J, Lee S, Naber JD. Premixed Combustion for Acetylene-Hydrogen Fuel Mixtures used in a Constant Volume Combustion Vessel for Thermodynamic State Generation. *J KONES Powertrain Transp* 2009;16:199–208.
- [110] Payri R, Garcia-Oliver JM, Manin J, Bardi M. Fuel Temperature Influence on Diesel Sprays in Reacting Conditions. *ILASS-Americas 23rd Annu. Conf. Liq. At. Spray Syst.*, Ventura, CA: 2011.
- [111] Pei Y, Hawkes ER, Kook S, Goldin GM, Lu T. Modelling n-dodecane spray and combustion with the transported probability density function method. *Combust Flame* 2015;162:2006–19. doi:10.1016/j.combustflame.2014.12.019.
- [112] Kennaird DA, Crua C, Lacoste J, Heikal MR, Gold MR, Jackson NS. In-Cylinder Penetration and Break-Up of Diesel Sprays Using a Common-Rail Injection System 2002. doi:10.4271/2002-01-1626.
- [113] Crua C. Combustion Processes in a Diesel Engine. PhD Thesis 2002:271.
- [114] Pastor J, Garcia-Oliver JM, Garcia A, Zhong W, Micó C, Xuan T. An Experimental Study on Diesel Spray Injection into a Non-Quiescent Chamber. *SAE Int J Fuels Lubr* 2017-01-0850. doi:10.4271/2017-01-0850.
- [115] Nilaphai O, Hespel C, Moreau B, Contino F, Bourgeois N, Chanchaona S, et al. New High-Pressure and High-Temperature Chamber for Diesel Spray Characterization. *ILASS – Eur. 2016, Brighton UK: 2016*, p. 4–5.
- [116] Nilaphai O, Ajrouche H, Hespel C, Moreau B, Chanchaona S, Foucher F, et al. Spray and

Combustion Characterizations of Acetone - Butanol - Ethanol (ABE) blend at High - Pressure and High - Temperature Conditions. 28th Conf Liq At Spray Syst ILASS–Europe 2017, 6-8 Sept 2017 2017:1–8.

- [117] Nilaphai O, Hespel C, Chanchaona S, Mounaïm-Rousselle C. Spray and Combustion Characterization of the Alcohol Blends in the High-Pressure High-Temperature Conditions. ILASS–Asia 2017 Oct. 18-21, 2017, Jeju, Korea Spray, Jeju, Korea Spray: ILASS–Asia 2017 Oct. 18-21, 2017, Jeju, Korea Spray; 2017, p. Oct. 18-21, 2017.
- [118] Nilaphai O, Hespel C, Chanchaona S, Mounaïm-Rousselle C. Spray and Combustion Characterizations of ABE/Dodecane Blend in Comparison to Alcohol/Dodecane Blends at High-Pressure and High-Temperature Conditions. Fuel 2018;225:542–53. doi:10.1016/j.fuel.2018.03.184.
- [119] Chiboub I, Ajrouche H, Nilaphai O, Dozias S, Moreau B, Hespel C, et al. X-Ray Diagnostics of Dodecane Jet in Spray A Conditions Using the New One Shot Engine (NOSE). 28th Conf. Liq. At. Spray Syst. ILASS–Europe 2017, 6-8 Sept. 2017, 2017, p. 1–8.
- [120] Ajrouche H, Nilaphai O, Moreau B, Hespel C, Foucher F, Mounaïm-Rousselle C. Engine Combustion Network (ECN): Characterization and comparison of Diesel spray combustion in New High-Pressure and High-Temperature Chamber. ILASS–Asia 2017 Oct. 18-21, 2017, Jeju, Korea Spray, 2017.
- [121] Bosch W. The Fuel Rate Indicator: A New Measuring Instrument For Display of the Characteristics of Individual Injection. SAE 1966: 660749. doi:10.4271/660749.
- [122] Pickett LM, Genzale CL, Manin J, Malbec L-M, Hermant L. Measurement Uncertainty of Liquid Penetration in Evaporating Diesel Sprays. ILASS Am. 23rd Annu. Conf. Liq. At. Spray Syst., Ventura, CA: 2011.
- [123] Laboratories SN. Engine Combustion Network (ECN) n.d. <https://ecn.sandia.gov/> (accessed March 14, 2017).
- [124] M. Meijer, L-M. Malbec, G. Bruneaux” LMTS. Engine Combustion Network: “Spray A” basic measurements and advanced diagnostics. ICLASS 2012, 12th Int. Conf. Liq. At. Spray Syst., Heidelberg, Germany: 2012.

- [125] Settles GS. Schlieren and Shadowgraph Techniques; Visualizing Phenomena in Transparent Media. Springer; 2001. doi:10.1007/978-3-642-56640-0.
- [126] Payri R, García-Oliver JM, Xuan T, Bardi M. A study on diesel spray tip penetration and radial expansion under reacting conditions. *Appl Therm Eng* 2015;90:619–29. doi:10.1016/j.applthermaleng.2015.07.042.
- [127] Panigrahi PK, Muralidhar K. Schlieren and Shadowgraph Methods in Heat and Mass Transfer. *Therm Eng Appl Sci* 2012;2:139. doi:10.1007/978-1-4614-4535-7.
- [128] Pastor JV, Payri R, Garcia-Oliver JM, Nerva J-G. Schlieren Measurements of the ECN-Spray a Penetration under Inert and Reacting Conditions. *SAE Tech Pap* 2012-01-0456. doi:10.4271/2012-01-0456.
- [129] Pastor J V., Payri R, Garcia-Oliver JM, Briceño FJ. Schlieren Methodology for the Analysis of Transient Diesel Flame Evolution. *SAE Int J Engines* 2013-24-0041. doi:10.4271/2013-24-0041.
- [130] Jung Y, Manin J, Skeen S, Pickett LM. Measurement of Liquid and Vapor Penetration of Diesel Sprays with a Variation in Spreading Angle, 2015. doi:10.4271/2015-01-0946.
- [131] Gaydon AG. *The Spectroscopy of Flames*. Dordrecht: Springer Netherlands; 1974. doi:10.1007/978-94-009-5720-6.
- [132] Heywood JB. *Internal Combustion Engine Fundamentals* 1988.
- [133] Dec JE, Espey C. Chemiluminescence Imaging of Autoignition in a DI Diesel Engine. *SAE Tech. Pap.* 982685, 1998. doi:10.4271/982685.
- [134] Benajes J, Payri R, Bardi M, Martí-Aldaraví P. Experimental characterization of diesel ignition and lift-off length using a single-hole ECN injector. *Appl Therm Eng* 2013;58:554–63. doi:10.1016/j.applthermaleng.2013.04.044.
- [135] Kreith F. *The CRC Handbook of Thermal Engineering*. Springer Science & Business Media; 2000.
- [136] Murphy MJ, Taylor JD, McCormick RL. Compendium of Experimental Cetane Number Data. *Natl Renew Energy Lab* 2004;1–48. doi:10.2172/1086353.

- [137] National Center for Biotechnology Information. Open Chemistry Database n.d. <https://www.nih.gov/> (accessed March 14, 2017).
- [138] The Editors of Encyclopedia Britannica. Latent Heat. *Encycl Br* 2014;25–8.
- [139] Arrowsmith A. Atomization and Sprays. vol. 45. 1990. doi:10.1016/0009-2509(90)87140-N.
- [140] Cao W, Li J, Lue L. Study on the Ignition Behavior and Kinetics of Combustion of Biomass. *Energy Procedia* 2017;142:136–41. doi:10.1016/j.egypro.2017.12.022.
- [141] Nilaphai O, Hespel C, Chanchaona S, Mounaïm-Rousselle C. Spray and Combustion Characterizations of ABE / Dodecane Blend in Comparison to Alcohol / Dodecane Blends at High-Pressure and High- Temperature Conditions. *Fuel* 2018;225:542–53. doi:10.1016/j.fuel.2018.03.184.
- [142] Cengel YA, Boles MA. *Thermodynamics: An Engineering Approach*. 5th ed. Tata McGraw-Hill; 2006.
- [143] Cengel YA. *Heat Transfer: A Practical Approach*. Mc Graw-Hill 2003:785–841.
- [144] Kramers H. Heat Transfer from Spheres to Flowing Media. *Physica* 1946;12:61–80. doi:10.1016/S0031-8914(46)80024-7.
- [145] Polling BE, Prausnitz JM, O’Connell JP. *The Properties of Gases and Liquids*. 2001.
- [146] Watson KM. Prediction of Critical Temperatures and Heats of Vaporization. *Ind Eng Chem* 1931;23:360–4. doi:10.1021/ie50256a006.

Ob NILAPHAI

Procédés de Vaporisation et Combustion des Alcools et de l'Acétone-Butanol-Ethanol (ABE) Mélangés au n-dodécane dans des Conditions de Haute-Pression et Haute-Température: Application au Moteur à allumage par compression

Résumé :

La préoccupation de plus en plus importante ces dernières décennies, liée à l'épuisement des ressources pétrolières et au réchauffement climatique par les gaz à effet de serre a accentué l'intérêt du butanol comme carburant alternatif dans le secteur des transports grâce à ses propriétés adaptées pour le moteur à allumage par compression. Cependant, le faible rendement des procédés de production et de séparation empêche encore sa commercialisation en tant que carburant. C'est pourquoi le mélange de fermentation intermédiaire de la production de butanol, Acétone-Butanol-Ethanol (ABE), est de plus en plus considéré comme un carburant alternatif potentiel en raison de ses propriétés similaires au butanol et de ses avantages quant à son coût énergétique pour sa fabrication.

Dans ce cadre, ce travail a pour objectif d'étudier l'impact des propriétés de différents mélanges d'ABE et n-dodécane en comparaison avec des mélanges d'alcools (éthanol et butanol) sur le processus de pulvérisation et de combustion et ce, pour différentes proportions en volume allant de 20% à 50%. Pour cela, une nouvelle chambre de combustion appelée "New One Shot Engine", a été réalisée et utilisée car les conditions haute pression et haute température de "Spray-A" (60 bars, 800-900 K et 22,8 kg/m³) définies par le réseau Engine Combustion network (ECN) peuvent être atteintes. Autant les phases liquides et vapeur que de combustion ont été caractérisées grâce à l'utilisation des plusieurs techniques optiques (extinction, Schlieren, chimiluminescence d'OH*) dans des conditions non réactives (Azote pur) et réactives (avec 15% d'oxygène). Ces résultats expérimentaux ont non seulement permis d'étudier l'impact en oxygène moléculaire et de fournir une nouvelle base de données fiables, mais aussi d'affirmer la possibilité d'utiliser jusqu'à 20% d'ABE en volume dans des moteurs à allumage par compression, grâce à ses caractéristiques de pulvérisation et de combustion similaires au carburant Diesel conventionnel.

Mots clés: Mélange Acétone-Butanol-Ethanol, Mélange d'alcool, Caractéristiques du spray, longueur de lift-off, délai d'auto-inflammation, Conditions haute température et haute pression

Vaporization and Combustion Processes of Alcohols and Acetone-Butanol-Ethanol (ABE) blended in n-Dodecane for High Pressure-High Temperature Conditions: Application to Compression Ignition Engine

Abstract :

The growing concern in recent decades, linked to the depletion of oil resources and global warming by greenhouse gases has increased the interest of butanol as an alternative fuel in the transport sector. However, the low yield of production and separation processes still prevents its commercialization as a fuel. Therefore, the intermediate fermentation mixture of butanol production, Acetone-Butanol-Ethanol (ABE), is increasingly considered as a potential alternative fuel because of its similar properties to butanol and its advantages in terms of the energy and cost in the separation process.

The context of this work aims to study the impact of fuel properties on the spray and combustion processes of ABE mixture and alcohol fuels, blended with the diesel surrogate fuel, n-dodecane, in different volume ratio from 20% to 50%. A new combustion chamber called "New One Shot Engine," was designed and developed to reach the high-pressure and high-temperature conditions of "Spray-A" (60 bar, 800-900 K and 22.8 kg/m³) defined by the Engine Combustion Network (ECN). The macroscopic spray and combustion parameters were characterized by using the several optical techniques (extinction, Schlieren, chemiluminescence of OH*) under non-reactive (pure Nitrogen) and reactive (15% of oxygen) conditions. These experimental results not only made it possible to study the molecular oxygen impact and provide a new accurate database, but also to affirm the possibility of using ABE up to 20% by volume in compression-ignition engines, as its spray and combustion characteristics similar to conventional diesel fuel.

Keywords : Acetone-Butanol-Ethanol mixture, Alcohol blend, Spray characteristics, Lift-off length, Auto-ignition delay, High-pressure and high-temperature conditions.



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