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Additional Information

An experimental study of the effects of fuel properties on reactive spray evolution using Primary Reference Fuels

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Abstract

An experimental study on the ignition and combustion of Diesel-type sprays using *n*-heptane, *iso*-octane and four intermediate blends is presented. The choice of components was done in order to represent the transition from conventional diesel fuel (*n*-heptane) to a gasoline-like one (*iso*-octane) in terms of ignition behaviour. The experiments have been carried out in a high pressure high temperature vessel using specifications from the Engine Combustion Network (ECN). Parametric variations of oxygen concentration and air temperature have been performed for each fuel. In order to investigate the spray development, schlieren imaging for the quantification of spray penetration and ignition delay, OH* chemiluminescence imaging for the lift-off length, and broadband radiation imaging for the soot intensity and flame length have been applied. The results show the large effect of mixture reactivity on the ignition times and lift-off length values. Regarding the effect

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of the octane number of the blends on the ignition delay times, a linear effect has been found in the lower half of the blend range, while an exponential trend is evident in the top one. On the other hand, a scaling law for the stabilized flame length based upon momentum-controlled assumptions has shown that results are comparable to those obtained in the literature. Finally, the applicability of the results obtained on the performance and efficiency in real engines is discussed.

Keywords: Primary Reference Fuel, Diesel Spray, Ignition, Combustion, Lift-off Length

1. Introduction

The role of fuel properties on diesel engine performance and emission has been an active field of research for a long time. In recent years, more detailed studies in combustion vessels have helped understanding the fundamental processes dealing with fuel effects on spray development and combustion. Different fuel types are within research focus, such as bio-diesel, synthetic Fischer-Tropsch fuels, oxygenated fuels, diesel-gasoline blends and surrogate fuels, to mention a few. The end goal has been the matching of different combustion strategies and fuel types to improve the engine efficiency and reduce the emission of pollutants. For example, a study with direct diesel injection and port gasoline injection showed that the higher amount of gasoline retarded the combustion phasing. This in turn lowered the heat transferred and allowed for the lowest fuel consumption, which also resulted in low NO_X and PM emissions [1]. Another study replaced entirely the diesel fuel with gasoline and also obtained less specific fuel consumption together with lower

16 smoke levels [2]. Blends of gasoline and ethanol have also been used in diesel
17 engines in order to study the effects on combustion and reduce the amount
18 of diesel injected [3]. Results have shown reduction of soot levels, but at the
19 cost of higher NO_X and compromised combustion stability under some con-
20 ditions. Furthermore, a similar study with blends and changes in the contour
21 conditions also presented improvements in the combustion efficiency [4].

22 Among the most used fuels used for the evaluation of diesel-gasoline
23 blends are those known as Primary Reference Fuels (PRFs), which repre-
24 sent both ends of the octane rating scale, namely *n*-heptane ($ON = 0$) and
25 *iso*-octane ($ON = 100$). Such a difference in octane (and thus cetane) num-
26 bers makes them good representatives of diesel and gasoline, respectively,
27 in terms of ignition and combustion. A very recent study [5] presents the
28 ignition mechanism of *n*-heptane and *iso*-octane under various conditions,
29 showing the expected increase of autoignition delay times when moving from
30 *n*-heptane to *iso*-octane. Such results are also verified by experimental inves-
31 tigation [6], as the ignition delay of four different PRF blends was shown to
32 increase as the composition of *iso*-octane augmented in the blends. Further-
33 more, engine tests also report an increase in the ignition delay times as the
34 octane number of the fuel is larger [7, 8, 9]. Another work done with PRFs,
35 diesel and gasoline, investigated the combustion recession after the end of
36 injection [10]. The results showed that the fuels with highest cetane num-
37 bers presented the least lifted flames and the shortest combustion recession
38 times. Analogously, the lift-off length and ignition delay time relationship
39 was also studied under a wider range of conditions using conventional diesel
40 and a PRF blend of similar properties [11]. Although the trend was not very

41 clear, there was an interaction implying that the condition with longest lift-off
42 length also presented the longest ignition delay times.

43 The present work reports a fundamental investigation on the ignition
44 and combustion behaviour of fuel sprays under Spray A conditions [12], with
45 a detailed focus on fuel properties. For that purpose, binary blends of *n*-
46 heptane and *iso*-octane, which are Primary Reference Fuels (PRFs), have
47 been tested. In terms of ignition behaviour, such blends should be represen-
48 tative of a detailed transition from a conventional diesel fuel (*n*-heptane) to
49 a gasoline-like one (*iso*-octane). The main objective of this work is the ex-
50 perimental characterization of spray mixing, ignition and sooting processes.
51 For each fuel blend, the test plan includes parametric variations of ambient
52 temperature and oxygen concentration, which have the largest effect on spray
53 ignition behaviour. Experiments have been conducted in a constant pressure
54 vessel, where high ambient pressure and temperature conditions typical of
55 Diesel engines can be reproduced. For each condition, high speed schlieren
56 and broadband luminosity imaging have been used to compare ignition, com-
57 bustion and sooting behaviour of all fuel blends; OH* radical imaging has
58 also been performed to measure lift-off length. The present contribution is
59 structured as follows. After this introduction, both the experimental setup
60 and the optical techniques employed will be presented. Test conditions will
61 be summarized, and results of fuel effects will be analysed. Finally, the main
62 conclusions from this study are drawn.

63 **2. Experimental setup**

64 *2.1. High Temperature and High Pressure vessel*

65 Tests have been performed in a high temperature and high pressure test
66 chamber where the thermodynamic conditions obtained in a Diesel engine at
67 the time of injection can be obtained with a maximum ambient temperature
68 of 1000K and a maximum pressure of 15MPa. Compared to similar facilities
69 [13], it is possible to obtain nearly quiescent and steady thermodynamic
70 conditions in the test chamber. More details can be found in [14].

71 *2.2. Optical setup*

72 Different optical techniques have been employed in these experiments.
73 Schlieren imaging has been used to measure spray penetration and autoigni-
74 tion delay, broadband luminosity imaging has been used to assess sooting
75 intensity, and OH* chemiluminescence imaging has been used to measure
76 flame lift-off length. Figure 1 presents a schematic of the optical arrange-
77 ment.

78 *2.2.1. Schlieren imaging*

79 The spray evolution inside the combustion chamber has been recorded
80 by schlieren imaging [15]. This technique is sensitive to the first spatial
81 derivative of density within the combustion chamber, which makes it use-
82 ful to detect spray boundaries and thus evaluate macroscopic spray scales,
83 whether vaporizing or non-vaporizing, inert or reactive. This technique shows
84 the boundary between vaporized liquid and background gas because of the
85 refractive index differences that exist between them, additionally, density
86 gradients are also created in the chamber as the vaporized liquid cools the

87 ambient gas [16, 17]; such refractive index gradients are also present during
88 combustion, as the high temperature creates low density regions. Therefore,
89 this method is valid for inert and reactive conditions. For this technique, the
90 spray has to be illuminated from one side by a collimated beam. The shadow
91 produced by the spray is then gathered with a lens and at its focal length
92 a diaphragm is positioned to produce the schlieren effect by eliminating the
93 diverted light beams. The recorded image is then captured by a high speed
94 camera in order to obtain a time resolved evolution of the spray.

95 An example of an schlieren image can be seen in Figure 2. The routine
96 used for the processing was developed by Sandia National Laboratories as
97 part of the ECN group and is available on-line [18]. The code is based on
98 the successive calculation of two standard deviation images to remove the
99 schlieren effect of the hot ambient gases and to detect the spray boundary.
100 For every instant (I_t), the processing routine subtracts the two preceding
101 images (I_{t-1} & I_{t-2}), then a two-step derivative process highlights the zones
102 where the pixels have changed due to either spray or background gas move-
103 ment, then the image is segmented [19, 20, 21]. Once the boundaries have
104 been defined, the spray penetration is calculated by the procedure shown
105 in [17]. Additionally, the ignition delay based upon schlieren images has
106 also been calculated using the method described in [12, 16, 22], which relies
107 on the change in refractive index of the mixture and the shortening of the
108 penetration .

109 A schematic of the optical arrangement is shown in Figure 1. The spray
110 has been illuminated from the left window and the light has been captured by
111 a CMOS camera from the opposite side. The light from a Xenon lamp passed

112 through a 1mm diameter pinhole that simulates a single-point light source.
113 The light was reflected on a 150mm parabolic mirror to obtain collimated
114 light. After passing through the spray, the light has been collected by a
115 biconvex lens and at its focal point a 4mm diaphragm has been positioned to
116 produce the schlieren effect. A BG39 bandpass filter (360-580nm) was used
117 to minimize soot radiation effects. A 10-bit Photron SA-5 CMOS high-speed
118 camera equipped with a Nikon 50mm f=1:8 lens were used, image acquisition
119 frequency was 42000FPS with exposure time of $4.18\mu s$ and a pixel/mm ratio
120 of 5.26 leading to a field of view of 97mm.

121 *2.2.2. Broadband radiation imaging*

122 The soot distribution and intensity inside the combustion chamber have
123 been recorded by direct imaging. This technique records the flame broad-
124 band radiation, which corresponds to the soot thermal radiation during the
125 diffusion combustion phase.

126 Figure 3 shows a sample image of broadband radiation. An average back-
127 ground image is calculated for each repetition and based on that image and a
128 two constant thresholds, a mask is generated to define the region of interest.
129 It is important to clarify that given the strong difference between the inten-
130 sity levels in the soot onset area (in the vicinity of the lift-off) and further
131 downstream, two threshold values (a lower one for the onset and a higher one
132 for the tip) were selected in order to accurately detect the contour. Then, the
133 area of the flame and cumulative digital intensity are computed, and based
134 on those two values the specific intensity is obtained. Also, and in a similar
135 way to the spray penetration, the soot onset length and soot penetration
136 (or flame length) are obtained as the distance from the nozzle to the points

137 closest and furthest away from the injector, respectively. After all cases have
138 been processed, the normalized intensity and specific intensity are calculated
139 taking into account the camera settings of exposure time and aperture. It is
140 worth noting that the soot onset length is not a replacement of the lift-off
141 length calculated by means of OH* chemiluminescence, because significant
142 amounts of soot do not form until downstream from the lift-off location [23].

143 A schematic of the optical arrangement is shown in Figure 1 as well. A
144 50/50 beam splitter has been positioned in between the parabolic mirror and
145 the left window with a 45° angle so the camera axis could be parallel to the
146 spray axis but the reflected image perpendicular to it. A 10-bit Phantom
147 V12 CMOS high-speed camera equipped with a Zeiss 100mm f=2 lens were
148 used, image acquisition frequency was 42000FPS with exposure times ranging
149 from 0.4 to 23.29 μ s and a pixel/mm ratio of 7.23 leading to a field of view
150 of 105mm.

151 2.2.3. OH* Chemiluminescence imaging

152 The lift-off length (LoL) was recorded by OH* chemiluminescence imag-
153 ing. This technique records radiation at 310nm, which is controlled by the
154 OH* radical, and thus of the lift-off length for diesel sprays [23]. The OH*
155 radical is a marker of the high temperature combustion [24], for example
156 the one occurring at the lift-off length. Additionally, the band at 310nm is
157 the strongest one, and therefore the best for determining the lift-off length
158 [23, 24]. Although soot radiation could also be contributing to the recorded
159 signal in the images, previous studies in the literature [23] also indicate that
160 there should exist a spatial separation in both contributions. Therefore, while
161 the downstream radiation will most probably be dominated by soot, the most

162 upstream one is assumed to be essentially related to OH* chemiluminescence.

163 Figure 4 shows an image of OH* radiation. These images are similar in
164 appearance to the broadband ones, but with different spectral information.
165 Additionally, these images have been taken with a long exposure, from the
166 start of combustion until the end of injection ($\approx 3000\mu s$); as opposed to the
167 broadband radiation where the exposure times were much shorter ($\approx 20\mu s$).
168 The field of view in this case is located closer to the injector, in order to be
169 able to measure the lift-off length with an adequate resolution. The process-
170 ing algorithm for OH* images is similar, but lift-off length is calculated as
171 the closest zone to the nozzle where flame can be found [23]. The algorithm
172 divides the image in two parts (upper and lower in Figure 4), based on the
173 injector axis, because the time averaged images show two bright bands of
174 light corresponding to the OH* chemiluminescence from the diffusion flame.
175 Nevertheless, these bands do not imply that the combustion extends further
176 on the edges of the spray, but instead, they correspond to line-of-sight aver-
177 aging of the light from the flame [25, 26]. Carrying on with the processing,
178 the values per row and side are added up so two curves Digital Level vs
179 Axial Distance can be obtained. Finally, the lift-off is calculated as the aver-
180 age level between valley and first peak of each curve, as this gives the mean
181 location of the turbulently fluctuating lift-off length [23].

182 A schematic of the optical arrangement is also shown in Figure 1. Due to
183 the lack of available optical accesses, the camera has been placed next to the
184 parabolic mirror and at a small angle in order to image the spray properly.
185 A 16-bit Andor iStar ICCD intensified camera equipped with a 100mm focal
186 length f=2 UV objective (by Bernhard Halle Nachfolger GmbH) and a 310nm

187 interference filter (FWHM = 10nm) was used to eliminate any additional
188 radiation such as the soot luminosity. Because of the quasi-steady nature
189 of the diffusion flame only one image was recorded per injection event, with
190 an exposure time of 3ms starting 2ms after SoI and pixel/mm ratio of 5.85
191 leading to a field of view of 78mm.

192 **3. Test conditions**

193 Keeping in mind the objective of the present work, six different blends
194 of *n*-heptane and *iso*-octane in increments of 20% have been used, including
195 the pure components. The nomenclature of each blend is PRF#, where the
196 # stands for the percentage in volume of *iso*-octane in the blend, being the
197 rest *n*-heptane.

198 The so-called Spray A injector has been used; this is a standard within
199 the Engine Combustion Network (ECN) group, which is an international
200 collaboration among different research laboratories in the world [12]. The
201 injector has a single-hole nozzle with a nominal diameter of 90 μ m (Serial
202 No. 210675). Reference injection pressure, chamber density, temperature
203 and oxygen mole fraction for Spray A are 150MPa, 22.8kg/m³, 900K and
204 15%, respectively. The only difference of the present study compared to the
205 standard Spray A is the use of *n*-heptane/*iso*-octane blends, instead of the
206 standard *n*-dodecane. As previously described, the reactive spray has been
207 characterized in terms of spray tip penetration, lift-off length and soot radi-
208 ation. Parametric variations of temperature and oxygen concentration have
209 been performed as shown in Table 1. Additionally, for some experimental
210 conditions (Table 2) the study was also carried out in an inert atmosphere,

211 i.e. with no oxygen in the ambient with the main purpose of having a refer-
212 ence for the comparison of spray tip evolution.

213 Figure 5 shows a sample of the scattering among repetitions based on
214 the inert spray penetration, for each operation condition 15 repetitions were
215 performed. It shows that all the values are within two standard deviations
216 (blue lines), which should enclose approximately 95% of the values according
217 to the two-sigma (2σ) rule of the Normal distribution. Since the tests have
218 proven to be repetitive, the results shown throughout the rest of the section
219 will only present the average values of all the repetitions (red line). For time-
220 averaged values such as lift-off lengths and ignition delay times, the error bars
221 presented will also correspond to two standard deviations (95%).

222 4. Results

223 4.1. Analysis of the baseline case

224 Figure 6 shows a sequence of half-images that describes the evolution
225 of the vapour penetration throughout the whole injection event for the inert
226 and reactive sprays. For this example Spray A nominal conditions and PRF0
227 fuel have been selected.

228 From the start of injection (SoI), the spray penetrates as a clearly defined
229 shadow under inert and reactive conditions. At around $500\mu\text{s}$ after SoI, the
230 tip of the reactive spray starts becoming transparent, this is due to the low
231 temperature pre-reactions (also known as “cool flames”) that precede the
232 start of high temperature heat release. Such reactions result in the spray
233 having similar refraction index as the surrounding air, and therefore becom-
234 ing transparent [16, 27]. At $750\mu\text{s}$ after SoI, the spray tip of the reactive

235 spray becomes visible again, even though some parts are still transparent;
236 also a widening of the spray tip is evident, this indicates that the ignition
237 has begun as the premixed combustion of the air-fuel mixture has caused a
238 sudden increase in the spray volume due to the lower density of the products
239 from the high temperature reactions taking place. After $1000\mu s$, the whole
240 reactive spray shadow is visible again.

241 The reactive spray is narrow in the non-reacting region, closer to the noz-
242 zle and up to the lift-off length; after this point its width increases abruptly
243 due to combustion, which expands the original flow as explained in the previ-
244 ous paragraph. This difference can clearly be seen by comparing the shapes of
245 the inert and reactive sprays after the ignition has taken place and the spray
246 is fully visible again ($1500\mu s$). The inert spray maintains a constant angle
247 and a steadily increasing radius all the way to the transient tip, while the re-
248 active one is very similar to the inert up to the lift-off length (which is 23mm
249 for the present operating conditions), then the radius increases suddenly and
250 the heat release region extends up to the spray tip. The combustion also
251 causes the tip of the reactive spray to accelerate and penetrate at a faster
252 rate than its inert counterpart, which can be observed on the images from
253 $1500\mu s$ onwards. This means that the subsequent spray evolution is also
254 governed by the combustion process. The reactive spray structure remains
255 similar until the end of injection, with the spray tip penetrating steadily with
256 time.

257 Figure 7 shows the broadband radiation images corresponding to the same
258 spray evolution sequence, broadband luminosity is an indicator of the pres-
259 ence of soot in a reactive spray. At around $1000\mu s$ after SoI combustion

260 has already started, as explained in the previous paragraph. However, soot
261 is not visible yet up to this time, either due to the low flame temperature
262 or because not enough soot is formed yet. After $1500\mu s$ from the SoI, soot
263 starts to become visible at the tip of the spray; and as the spray keeps on
264 penetrating further, the sooting region also grows axially. Nevertheless, the
265 soot region widths are narrower than those of the spray due to the fact that
266 schlieren marks the whole spray region, while soot radiation mainly occurs
267 within the stoichiometric diffusion flame front [25].

268 Figure 8 (top) shows the average spray tip penetration for inert and re-
269 active conditions and the flame length and soot onset length measured from
270 image sequences such as the ones shown in Figures 2 and 3. From Figure 8
271 (top), it can be seen that the measured inert and reactive penetrations are
272 close to one another until autoignition. Looking back at the $500\mu s$ image
273 in Figure 6, corresponding to the cool flame period, one can already discern
274 some differences, which become evident after the high-temperature start of
275 combustion at $666\mu s$. After this point, the reactive spray enters the accel-
276 eration phase and its penetration separates from the the inert case. This
277 can be appreciated in Figure 8 (bottom), where the ratio between the react-
278 ing and inert penetration gas been plotted. This variable has a peak at the
279 SoC, it decreases slightly and then starts increasing steadily until it reaches
280 a maximum value and stabilizes under the given conditions. Although for
281 this nominal case the stabilized maximum is found close to the end of the
282 observation window, the parametric variations of ambient temperature and
283 oxygen in the following sections will show a similar behaviour, with a first
284 well defined acceleration followed by a second more stable period. This means

285 that after the acceleration period of the reactive spray has ended, the ratio
286 between reactive/inert velocities is approximately constant and no longer
287 increasing [28].

288 As explained earlier, the sooting region of the spray tends to reach a
289 steady value after a certain time. This can be seen in Figure 8 (top), where
290 the soot onset length (SOL) reaches a constant value fairly quickly while the
291 flame length (FL) keeps on penetrating along with the vapour until it starts
292 deviating to come to a steady length which under this nominal condition
293 occurs close to $4000\mu s$. Although this is close to the end of the observation
294 window, the subsequent study of this FL under oxygen concentration vari-
295 ation (Figure 16) will confirm that also for the present nominal condition
296 stabilization occurs.

297 The OH^* lift-off length (LoL) is also shown in Figure 8 (top), but unlike
298 the other parameters shown, this value is not time resolved as explained in
299 Section 2. A remark worth to be made is the difference between the LoL and
300 SOL, while both parameters measure the position of the flame, their spectral
301 information is different. The broadband luminosity comes from the radiation
302 of the soot, as opposed to the chemiluminescence of the OH^* radical. This
303 latter value is the best indicative that combustion is taking place within a
304 spray and is always present. The soot, on the other hand, depends strongly
305 on the conditions and fuel used, and may not be present even if the spray is
306 burning.

307 Summarizing, the reactive spray evolution can be broken down into four
308 well defined stages. First, there is no combustion and its behaviour is like
309 an inert spray ($0-250\mu s$). Second, pre-reactions start taking place, the spray

310 becomes transparent due to the changes in density, broadband radiation is
311 not visible due to low temperatures or not enough soot formed (250-500 μ s).
312 Third, (500-2500 μ s) high temperature ignition happens. In a first moment,
313 the spray expands radially but not axially, but this is followed by the accel-
314 eration of the spray tip velocity compared to the inert case. Soot becomes
315 visible, if conditions are adequate, SOL starts rising and so does the flame
316 front. Fourth and last, the acceleration phase of the reacting case compared
317 to the inert one ends, and the spray reaches a quasi-steady period where, its
318 tip speed is similar to its inert counterpart (2500-4000 μ s). This four stages
319 are consistent with observations of the authors in previous studies [28].

320 *4.2. Spray tip penetration*

321 Air temperature has no effect at all on the non-reacting part of the spray
322 under reactive conditions, the density has kept at a constant value by ad-
323 justing the ambient pressure. This can be seen in Figure 9 (top) where all
324 penetration curves overlap the inert one up to 600 μ s approximately. At this
325 point all reactive curves separate from the inert reference due to the pre-
326 reactions occurring at the spray front, this is shown more clearly in Figure 9
327 (bottom) where the ratio between reactive and inert penetrations is depicted.
328 Once the ignition has taken place, the reactive spray will continue deviating
329 from the inert case at a higher rate during the acceleration phase; but when
330 it reaches the quasi-steady phase, the acceleration will cease and the ratio
331 between Reactive/Inert penetration will remain constant. It can be seen that
332 the higher the temperature of the air, the sooner the acceleration period will
333 begin and, therefore, the stabilization period will be reached earlier as the
334 combustion is faster. As mentioned earlier, the temperature does not have

335 an effect on the non-reacting region, but will affect the ignition delay time
336 and hence the point at which the acceleration of the tip commences. Con-
337 currently, Figure 9 (top) shows that the higher air temperature causes the
338 lift-off length to become shorter for the same injection pressure.

339 The oxygen concentration has an effect on the start of combustion of
340 a spray and it doesn't affect the mixing or evaporation of the non-reactive
341 phase. Figure 10 shows the comparison of the penetrations under the para-
342 metric variation of oxygen. It can be seen that not only the reactivity of the
343 air causes the curves to depart at different positions, but the more pronounced
344 slopes as the oxygen fraction increases is an indicator of a combustion hap-
345 pening more aggressively. Estimations of adiabatic flame temperature for a
346 stoichiometric mixture, initially at the adiabatic mixing conditions, indicate
347 that it changes from around 2337 K for the lowest oxygen case to 2524 K and
348 2681 K for the medium and highest cases. This approximate 350 K tem-
349 perature variation with oxygen is much stronger than that observed when
350 changing the ambient air temperature, 2256 , 2337 and 2405 K for the 800 ,
351 900 and 1000 K cases shown in Figure 9. Therefore it can be hypothesized
352 that the corresponding acceleration of the reacting vs. the inert case is de-
353 pendent on the combustion-induced temperature variation, which will create
354 a corresponding density drop. Finally, Figure 10 (top), also shows the lift-off
355 length to be shorter as the oxygen increases, this proves that the increased
356 reactivity of the mixture is shifting the reactive region of the spray closer to
357 the nozzle.

358 The fuel effect on the reactive penetration is very similar to that of the
359 oxygen, because it will modify the reactivity of the mixture. The fuel has

360 very little effect on the inert spray [29, 30]; on the other hand, the reactive
361 penetration shows a strong dependency on the fuel due to different ignition
362 delay times. Figure 11 (top) shows the penetration of the baseline case for
363 all fuels and the inert penetration of PRF0 as a reference point. It can
364 be seen that as the percentage of *iso*-octane increases (higher PRF), the
365 penetration starts deviating from the inert case at a later time and with a
366 less pronounced slope, and for some cases it doesn't seem to separate at all.
367 This last phenomenon could be due to two factors, either the ignition takes
368 place much later than the time window studied, or because it doesn't occur
369 at all. This also explains why the stabilized penetrations for all fuels do
370 not converge on the same values. Figure 11 (bottom) shows the penetration
371 ratios for all PRFs. In a similar trend to that of the oxygen, being that a
372 more reactive mixture will cause the curve to deviate earlier and faster, not
373 all curves start deviating, meaning that the ignition has not been achieved
374 yet. Moreover, the blends that burn do not seem to reach the same steady
375 value. Finally, the effect of the fuel on the lift-off length can be appreciated
376 in Figure 11 (top), where the lower the percentage of *n*-heptane (lower PRF)
377 the longer the lift-off length is. This is analogue with increasing the air
378 temperature or the oxygen concentration, which results in a more reactive
379 mixture and hence a shorter lift-off length.

380 The previous results also help at the understanding of lift-off stabiliza-
381 tion mechanism. Although originally thought as based upon a flame front
382 velocity balance, extensive evidences starting from [31] indicate that lift-off
383 stabilizes based upon the autoignition of fuel elements being injected. In this
384 particular case, the fuel composition has been swept from *n*-heptane to *iso*-

385 octane, both of which have very similar laminar flame speeds [32] but highly
386 different autoignition properties. From a point of view of flame stabilization
387 by velocity equilibrium, both fuels should produce the same lift-off length.
388 However, experimental results presented here confirm that both lift-off and
389 autoignition delay change with operating conditions in a highly similar fash-
390 ion, which indicates the leading role of autoignition on lift-off stabilization.

391 *4.3. Ignition delay*

392 During the study of the penetration it was observed that some parameters
393 had a stronger effect on the ignition delay. This was seen where the Reac-
394 tive/Inert penetration ratio started deviating from unity. In this subsection,
395 the analysis of the ignition delay time under the parametric variations (Table
396 1) is presented.

397 The oxygen concentration appears to have an effect on the start of com-
398 bustion. This is because while the same amount of air is being entrained,
399 more oxygen is available, leading to a more reactive air-fuel mixture, so the
400 ignition can happen sooner [33]. Figure 12 shows the effect of varying the
401 oxygen concentration for each blend tested. Altering the fuel reactivity and
402 the oxygen concentration at the same time has a combined effect, where the
403 higher PRF (more *iso*-octane) causes the differences in ignition delay to be
404 greater among oxygen concentrations. As mentioned previously, this com-
405 bined effect is related to the reactivity of the air-fuel mixture and it seems
406 to have a non-linear trend.

407 Air temperature has the strongest effect on the ignition delay than any
408 of the other parameters. Figure 13 shows that the difference among 950K
409 and 900K is smaller (around $200\mu\text{s}$ for PRF20) compared to the effect of

410 reducing the temperature from 900K to 800K (approx. $1000\mu\text{s}$ for PRF0).
411 The explanation for this non-linear effect is that at low temperatures the rate
412 of chemical reaction is slow enough to ignore the time required to form the
413 ignitable mixture, while at high temperatures the ignition delay chemistry
414 progresses very fast, and delay is mainly dominated by physical processes
415 [34]. Missing points for the low temperature cases for PRF60 to PRF100,
416 as well as the intermediate temperature for PRF100 are due to combustion
417 not occurring within the investigated conditions. Additionally, it can be seen
418 that the difference in ignition delay between 15% and 18% of oxygen is similar
419 to changing the temperature from 900K to 950K for PRF20.

420 4.4. *Flame lift-off length*

421 As was also seen during the analysis of the penetration, the boundary
422 conditions not only affected the time at which the reactive curve started
423 deviating from the inert one (ignition delay time), but also on the flame
424 lift-off length, which will be analyzed in the present section.

425 The lift-off length seems to be dramatically affected by changes in the
426 air temperature. This is very clear to see in Figure 14, where the lower the
427 temperature the longer the lift-off length is going to be [23, 33, 35, 36, 31], but
428 more important is that the effect is non-linear. A statistical regression fitting
429 of the results shown in Figure 14 indicates that the temperature dependence
430 of the lift-off length occurs with an exponent of -4.27 , -4.57 , -4.84 and
431 -5.28 for PRF0 to PRF60, which indicates that the higher the fuel reactivity,
432 the more important the temperature dependence is. The fitted lines are also
433 presented in Figure 14 as dashed lines along with the expressions. Compared
434 to a reference work in [31], with a temperature dependence of -3.74 , the

435 temperature sensitivity is higher for all cases in the present study. However,
436 the present results are coherent with previous results obtained in the same
437 experimental facility (-5.0 to -5.4 as reported in [21]).

438 The oxygen concentration causes a similar effect to that of the air tem-
439 perature. Figure 15 shows that the higher the oxygen concentration, the
440 shorter the lift-off length is due to the higher reactivity of the mixture caus-
441 ing the spray to burn earlier (shorter ignition delay) and since the velocity
442 of the spray is not altered (same injection pressure), this happens closer to
443 the injector [23, 35].

444 Figures 14 and 15 also shows the effect of the fuel composition, and it can
445 be seen that it has a strong effect on the lift-off length. Like it was mentioned
446 earlier, the percentage of *iso*-octane on the blend reduces the reactivity of the
447 mixture tremendously, especially when the percentage is over 50. Moreover,
448 the results shown only present values up to PRF80, due to the fact that
449 the camera setup recorded the OH* chemiluminescence in a fixed temporal
450 window, and greater stabilization times of the lift-off length were not able
451 to be registered. Additionally, some conditions were not favourable for the
452 ignition of PRF100 such as 800K and 900K at 15% oxygen. In a similar
453 way as the effect on the ignition delay, the effects between 15% and 18% of
454 oxygen are similar to changing the temperature from 900K to 950K.

455 4.5. *Stabilized flame length*

456 The length of the flame was measured by means of broadband radiation,
457 but stabilized values are not achieved for all operating conditions due to
458 either spatial or temporal limitations in the acquisition setup.

459 Radiation onset occurs after ignition delay. If resulting radiation is strong

460 enough to be detected, measured flame penetration is similar to that of the
 461 reacting spray tip penetration. Figure 16 shows the evolution of the flame
 462 penetration under the oxygen concentration variation. For all three cases it
 463 can be seen that the flame penetrates faster than the corresponding spray tip
 464 of the non-reacting references. Also, and according to what was seen in the
 465 study of the spray penetration, the deviation of the flame penetration occurs
 466 earlier and more aggressively as the oxygen concentration increases. Finally,
 467 the higher concentration of oxygen also causes the flame to stabilize closer
 468 to the nozzle. The reason for this behaviour is that the more reactive the
 469 air-fuel mixture the closer the stoichiometric surface will be to the injector,
 470 resulting in a shorter stabilized flame length.

471 Stabilized flame length measurements under Diesel engine conditions are
 472 rarely available in the literature, mainly due to the length, which is usually
 473 larger than most optical accesses, and the time needed for stabilization, which
 474 is quite long in terms of engine scales. Comparable results to the ones shown
 475 here are those reported in [37], which use long-exposure OH* chemilumines-
 476 cence images to quantify the stabilized FL for different nozzle diameters. To
 477 compare the present results with those measurements, the obtained FL val-
 478 ues have been normalized for the different experimental conditions according
 479 to the following scaling law based on a momentum-controlled diffusion flame
 480 description:

$$FL_{norm} = FL \cdot \frac{z_{st}}{d_0 \cdot \sqrt{\frac{\rho_f}{\rho_a}} \cdot \sqrt{\frac{\rho_a}{\rho_{st,r}}}} \quad (1)$$

481 where $d_{eq} = d_0 \cdot \sqrt{\frac{\rho_f}{\rho_a}}$ is the equivalent diameter, which was already used

482 for the normalization under inert conditions, z_{st} is the stoichiometric mixture
483 fraction, and $\sqrt{\frac{\rho_a}{\rho_{st,r}}}$ is a term that accounts for entrainment reduction due
484 to the combustion-induced density decrease, where $\rho_{st,r}$ is the stoichiometric
485 mixture density under reacting conditions. This term has been demonstrated
486 to justify entrainment decrease under atmospheric pressure gas flames [38].
487 Figure 17 presents the results of the normalized flame length (FL_{norm}), which
488 shows the values to be in the range of 4-6 for most operating conditions, in
489 agreement with those from [37]. Therefore, it confirms that the stabilization
490 of the diffusion flame is controlled by mixing arguments, and not by fuel
491 reactivity.

492 5. Conclusions

493 The conclusions drawn from this investigation are as follows:

- 494 • The ambient temperature and oxygen concentration have very similar
495 effects. They have no apparent effect on spray penetration during the
496 inert spray evolution, but they do have an effect on the reacting spray
497 evolution. As temperature rises or oxygen concentration increases, the
498 reactivity of the mixture increases dramatically, so the fuel will start to
499 burn earlier and closer to the nozzle, resulting in shorter ignition delay
500 times and lift-off lengths. Where they have different effects is on the
501 stabilized flame lengths, as a higher oxygen concentration will results
502 in shorter lengths while the temperature does not have an effect on
503 the stabilized flame. Finally, even though they have no effect on the
504 inert vapour penetration, the shorter ignition delay times will cause the

505 start of the acceleration phase to start sooner and its slope to be more
506 pronounced, therefore resulting in longer penetrations.

507 • Increasing the amount of *iso*-octane in the mixture has a completely
508 opposite effect on the combustion behaviour in comparison to increas-
509 ing oxygen content or temperature in the air. As *iso*-octane is less
510 reactive than *n*-heptane, increasing its concentration will only cause
511 the mixture to start to burn later and further away from the injector
512 tip. Even though *iso*-octane has a slightly higher sooting tendency
513 than *n*-heptane, the increase in lift-off causes much leaner mixtures,
514 resulting in lower soot formation and a concurrent decrease in broad-
515 band radiation intensity. Two trends are defined regarding the octane
516 number of the blend. On one hand, for the lower half of the octane
517 scale (PRF0-20-40) the reactivity of the mixture (lift-off lengths and
518 ignition delay times) decreases linearly with the fuel proportion, while
519 on the the upper half (PRF60-80-100) a non linear trend can be seen.

520 A scaling law for the stabilized flame length based on momentum-controlled
521 considerations has been validated for those conditions where such stabiliza-
522 tion occurs. This scaling law agrees with similar results in the literature.

523 Finally, a small projection on the applicability of the present results for
524 engine performance will be made. For that purpose, ignition delay and lift-
525 off results (Figures 12 and 15) for PRF0 with 15% of oxygen and PRF40
526 with 21% of oxygen will be revisited. They could be taken as representa-
527 tive of a Diesel engine running with pure Diesel and an EGR level of 30%
528 for a high load case, or with a Diesel-gasoline blend and no EGR. One can
529 see that both cases have an ignition delay time of $600\mu\text{s}$ and approximately

530 the same lift-off length, 23mm and 22mm. This would mean a similar com-
531 bustion timing for both fuels, which is always interesting in terms of engine
532 calibration. Furthermore, due to the higher oxygen amount in ambient air,
533 the equivalence ratio at the lift-off for the gasoline (PRF40) would be much
534 leaner, which should result in lower soot formation within the flame, and
535 therefore lower exhaust particulates. The aforementioned comparisons agree
536 with general trends presented in recent studies using primary reference fuels
537 and similar strategies to reduce emissions while maintaining engine perfor-
538 mance [2, 7, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]. Nevertheless, further
539 research on this topic is needed, to confirm the previous conclusion.

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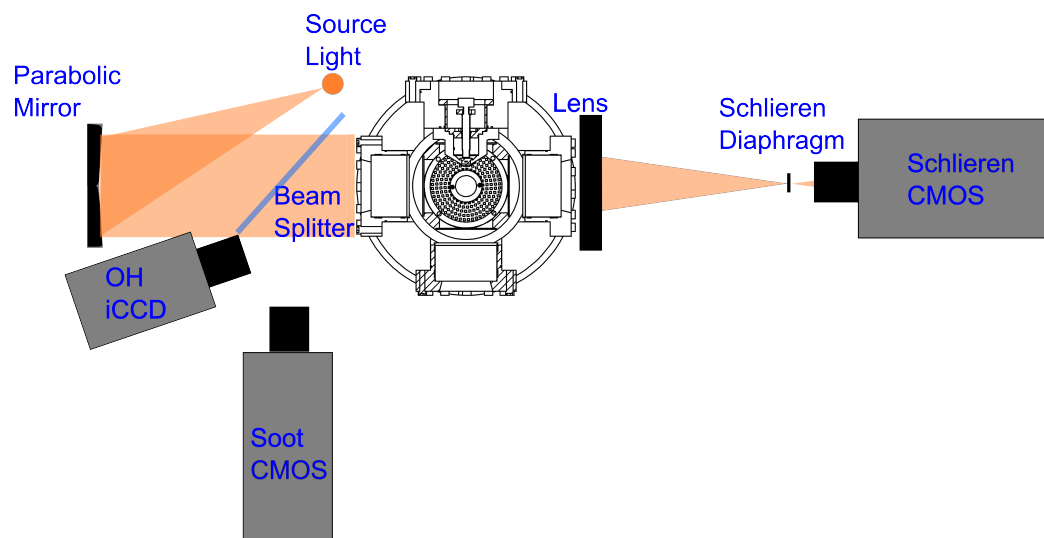


Figure 1: Schematic of the experimental setup for the study of the reactive spray

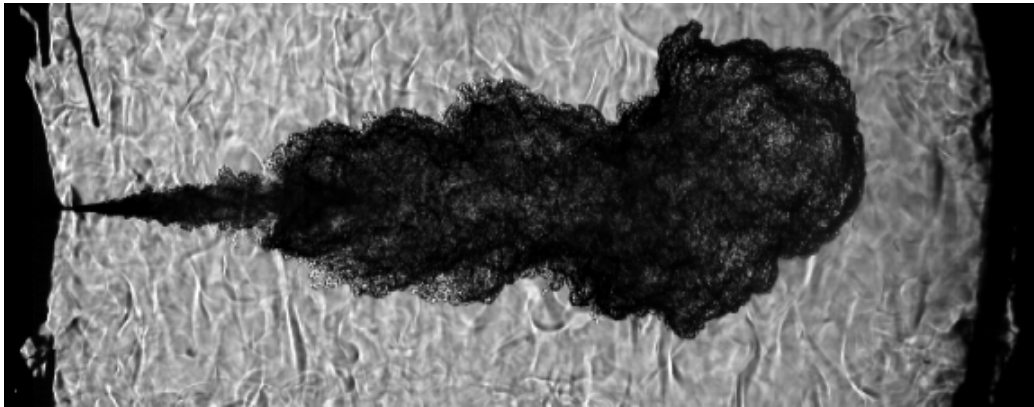


Figure 2: Sample image of the schlieren technique at $3000\mu s$ after SoI



Figure 3: Sample of the broadband radiation imaging at $3000\mu s$ after SoI

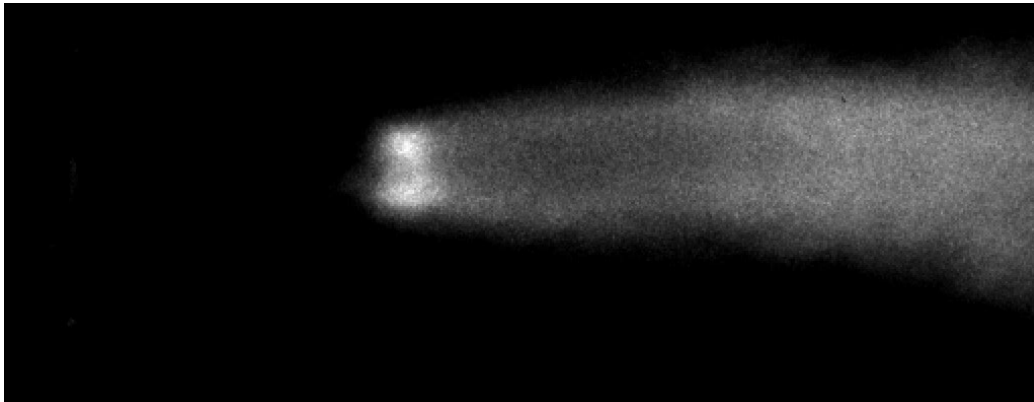


Figure 4: Sample image of the OH* chemiluminescence technique from $2000\mu s$ to $5000\mu s$ after SoI

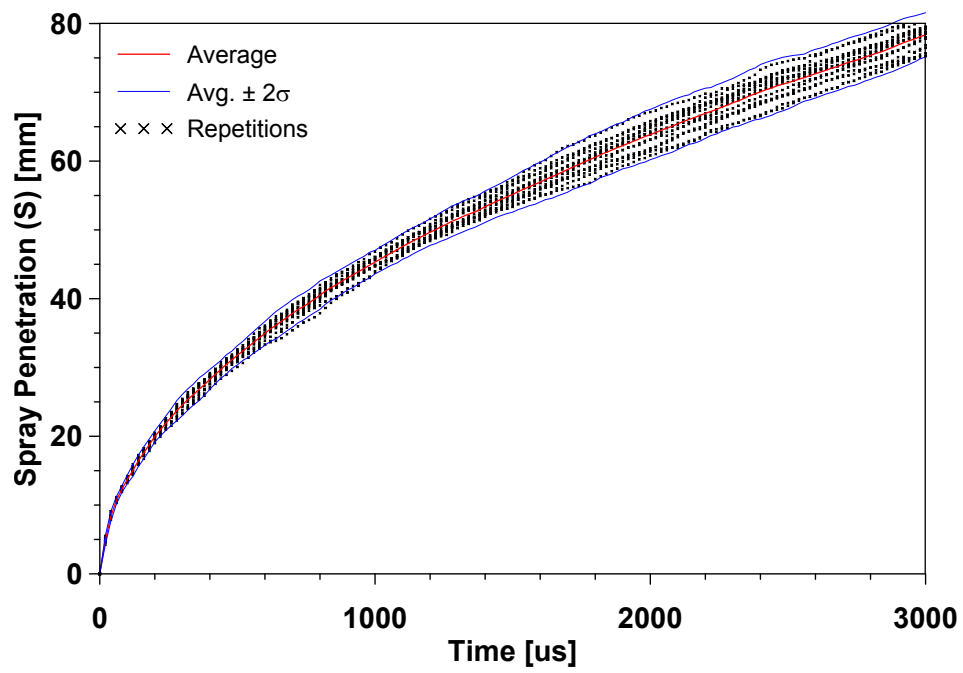


Figure 5: Spray penetration scattering of all 15 repetitions and average value, for PRF0 at 900K, 15%O₂ and 150MPa, time after SoI.

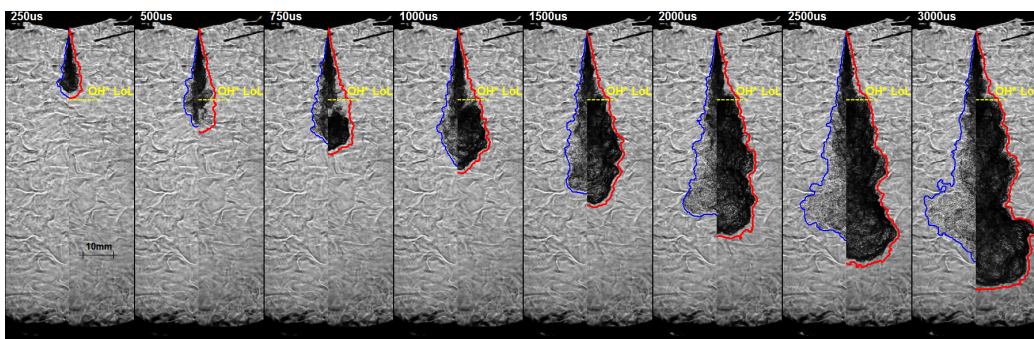


Figure 6: Evolution of inert (blue) and reactive (red) spray penetration for PRF0 at 900K, 15%O₂ and 150MPa, time after SoI.

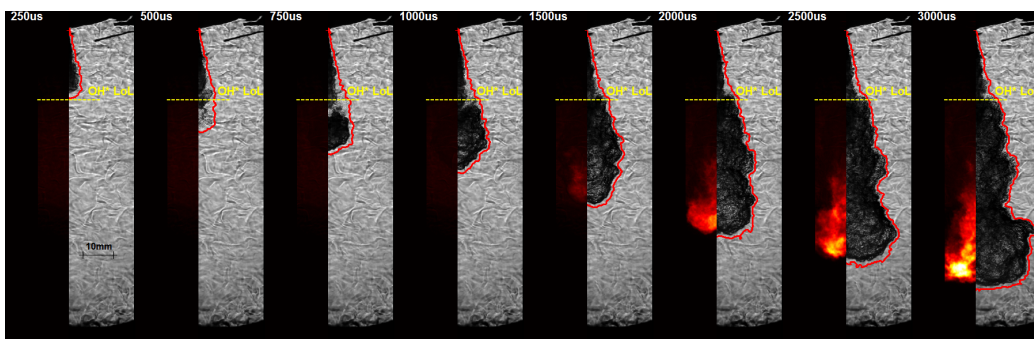


Figure 7: Evolution of soot luminosity and spray penetration simultaneous images for PRF0 at 900K, 15%O₂ and 150MPa, time after SoI.

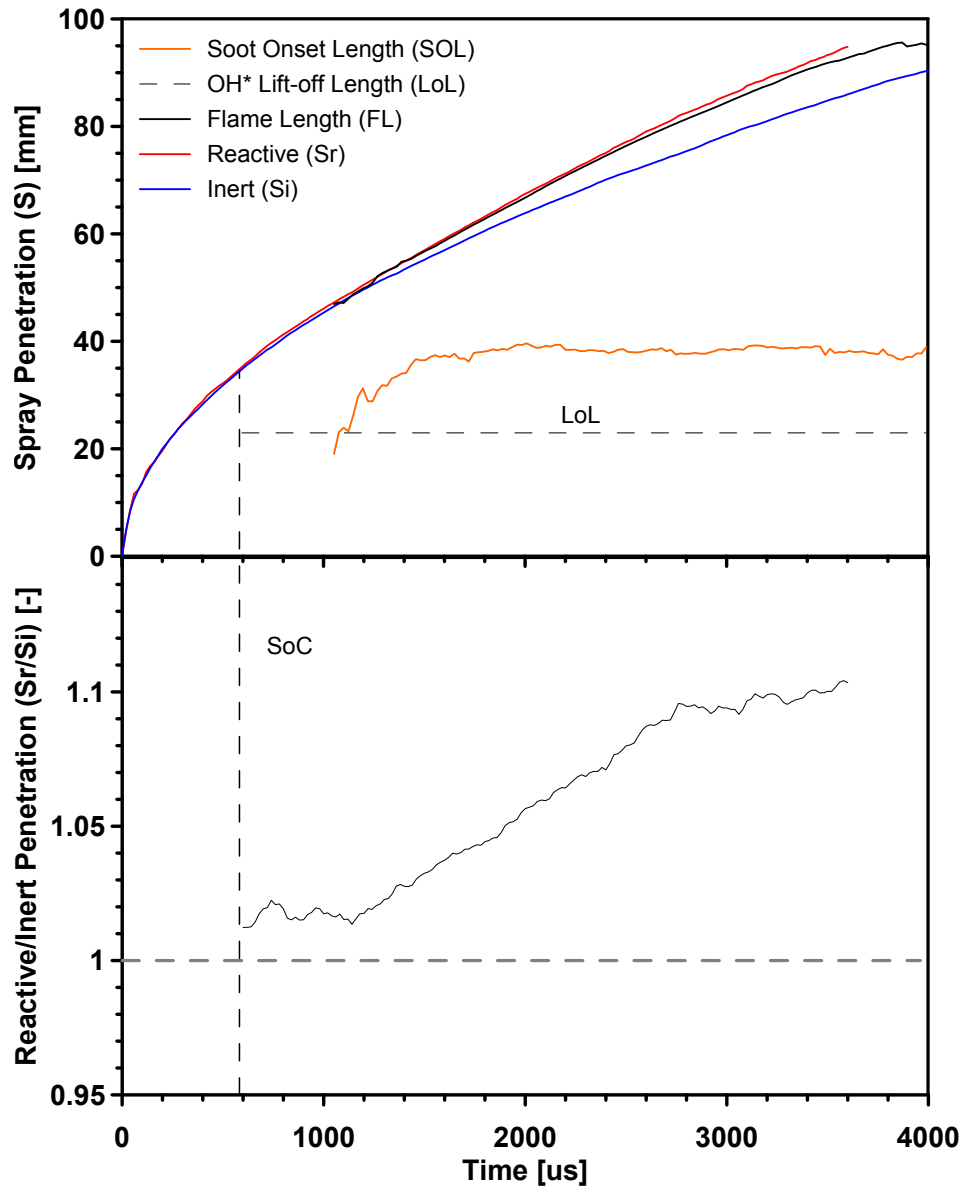


Figure 8: Time resolved evolution of the inert and reactive penetrations, along with flame length, soot onset length and lift-off length (top) and Reactive-Inert spray penetration ratio (bottom) for PRF0 at 900K, 15%O₂ and 150MPa, time after SoI.

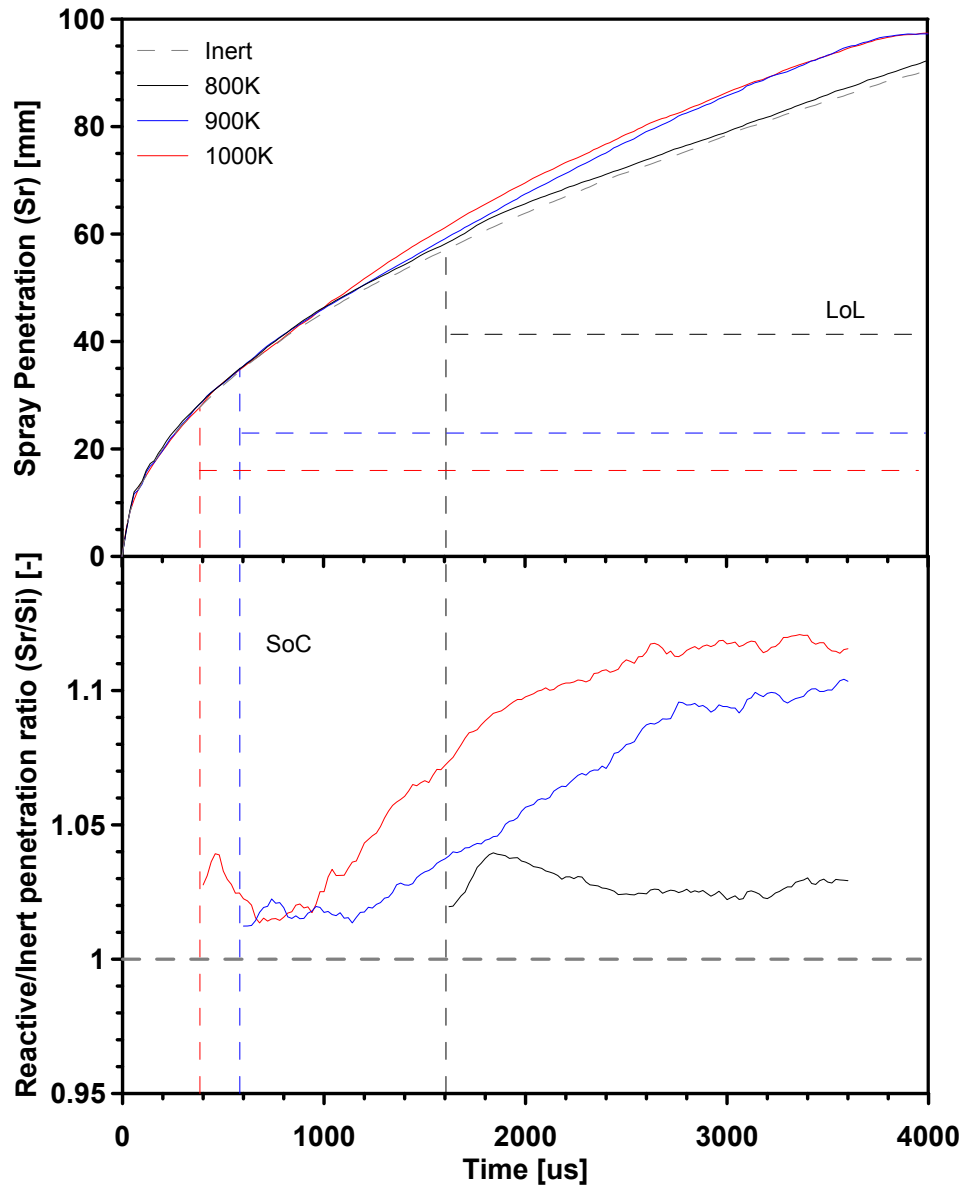


Figure 9: Reactive spray penetration (top) and Reactive/Inert spray penetration ratio (bottom) comparison for PRF0 under air temperature variation at 15%O₂, time after SoI.

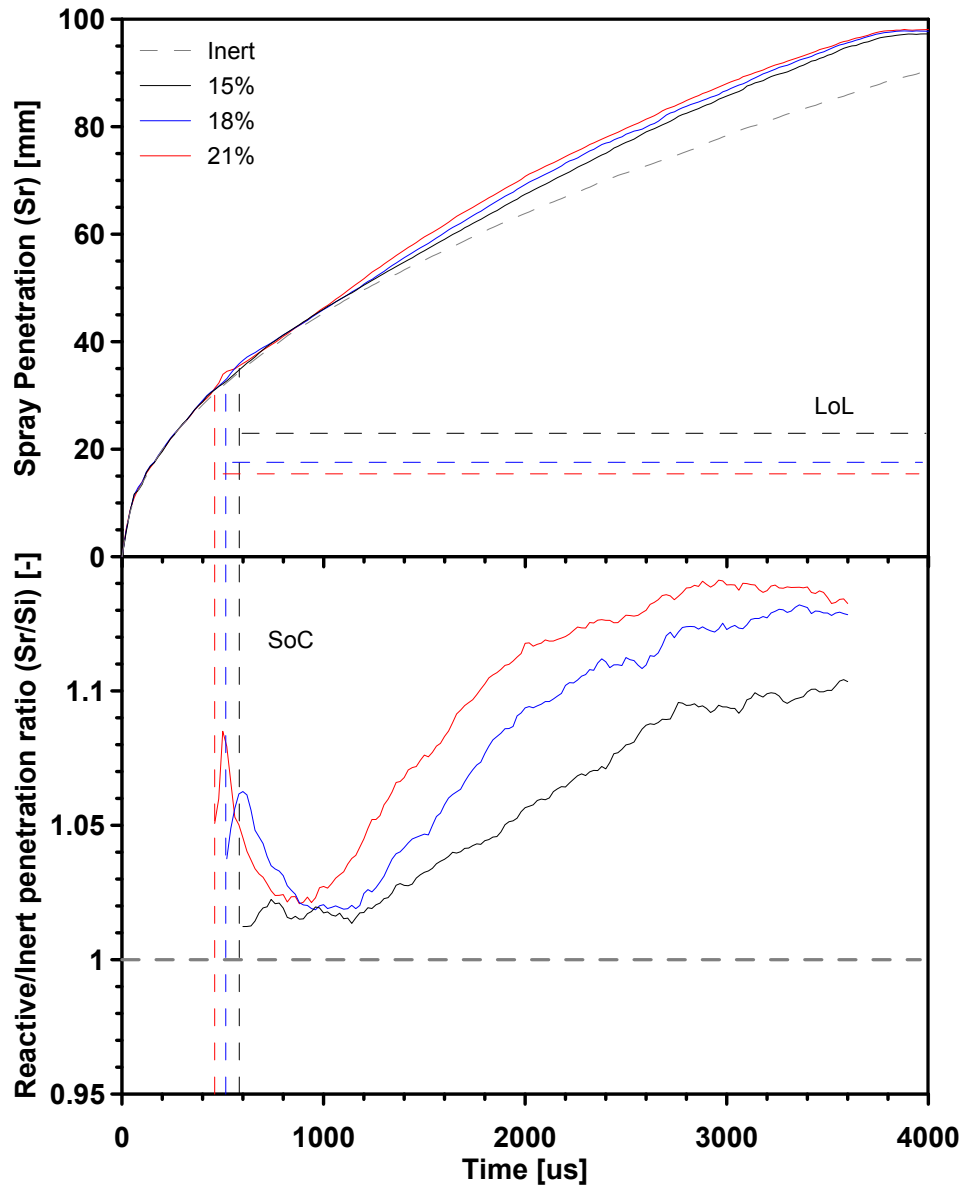


Figure 10: Reactive spray penetration (top) and Reactive/Inert spray penetration ratio (bottom) comparison for PRF0 under oxygen concentration variation at 900K, time after SoI.

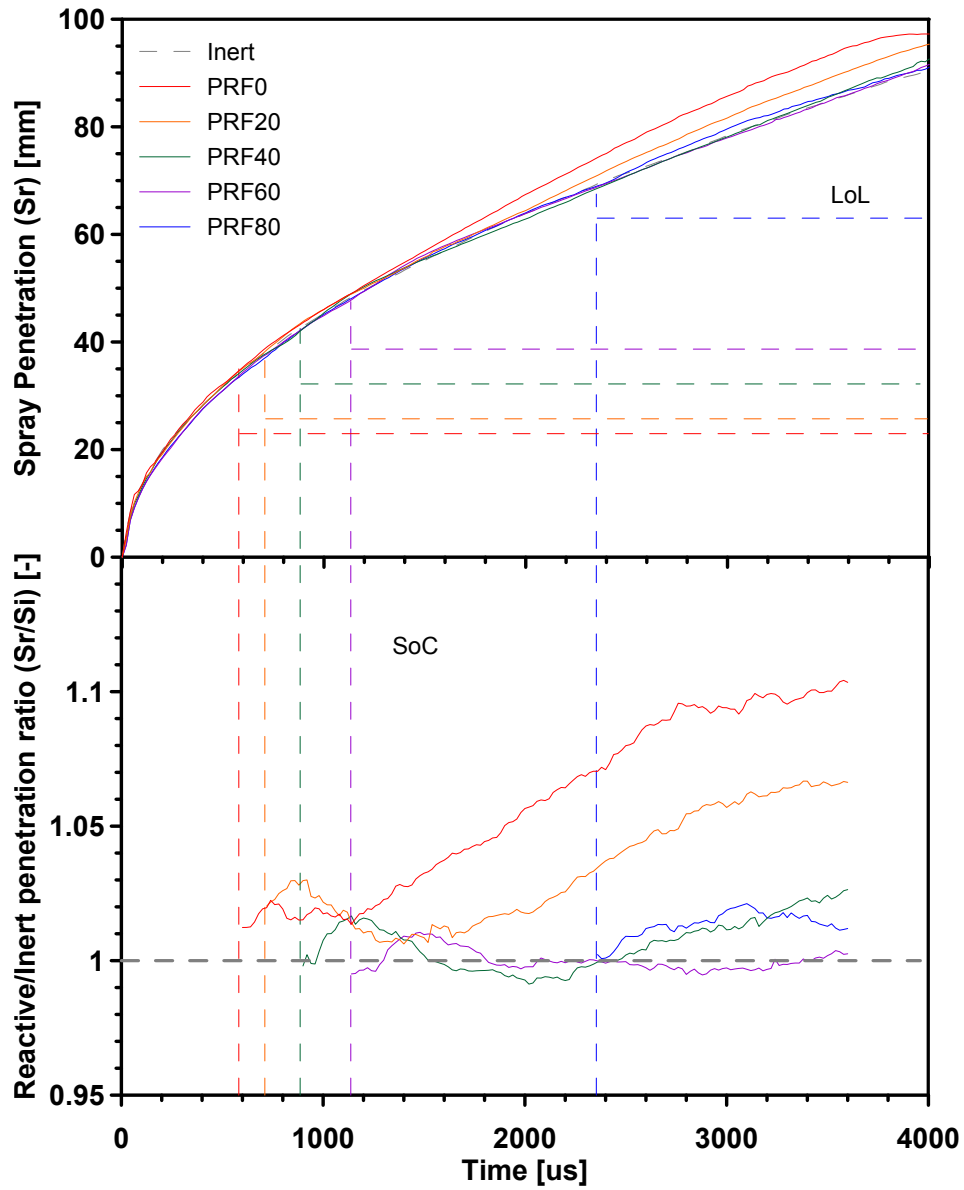


Figure 11: Reactive spray penetration (top) and Reactive/Inert spray penetration ratio (bottom) comparison for PRF0 to PRF100, at 900K and 15%O₂, time after SoI.

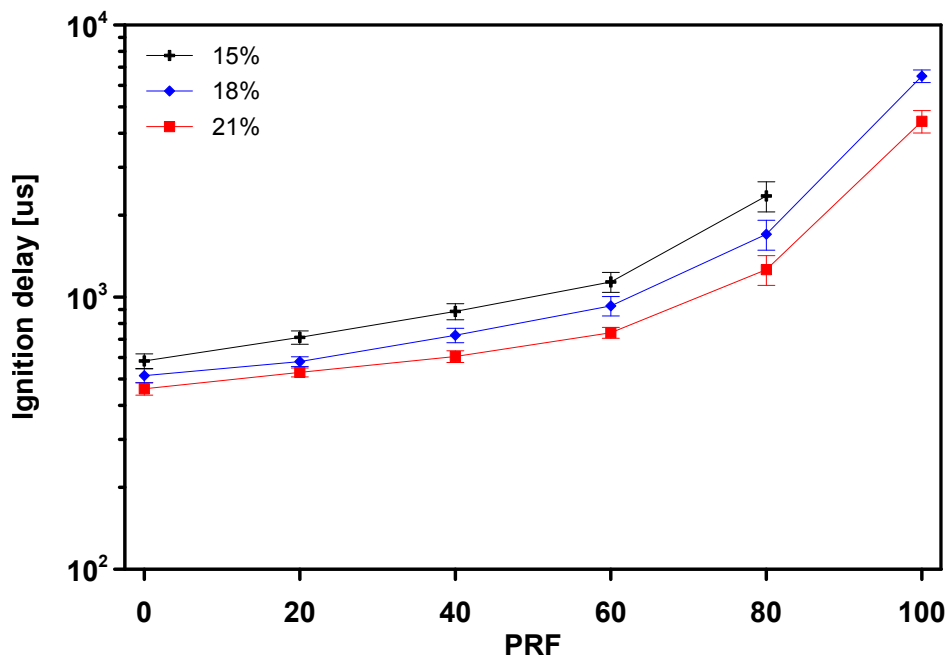


Figure 12: Ignition delay comparison under oxygen concentration variation, time after SoI

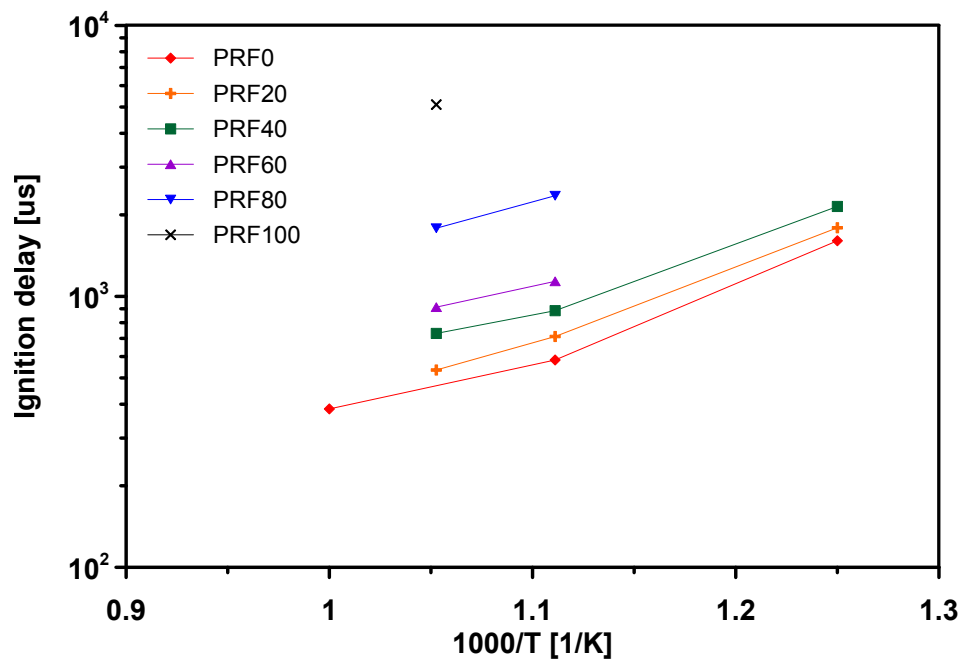


Figure 13: Ignition delay comparison under air temperature variation, time after SoI.Oxygen concentration 15%

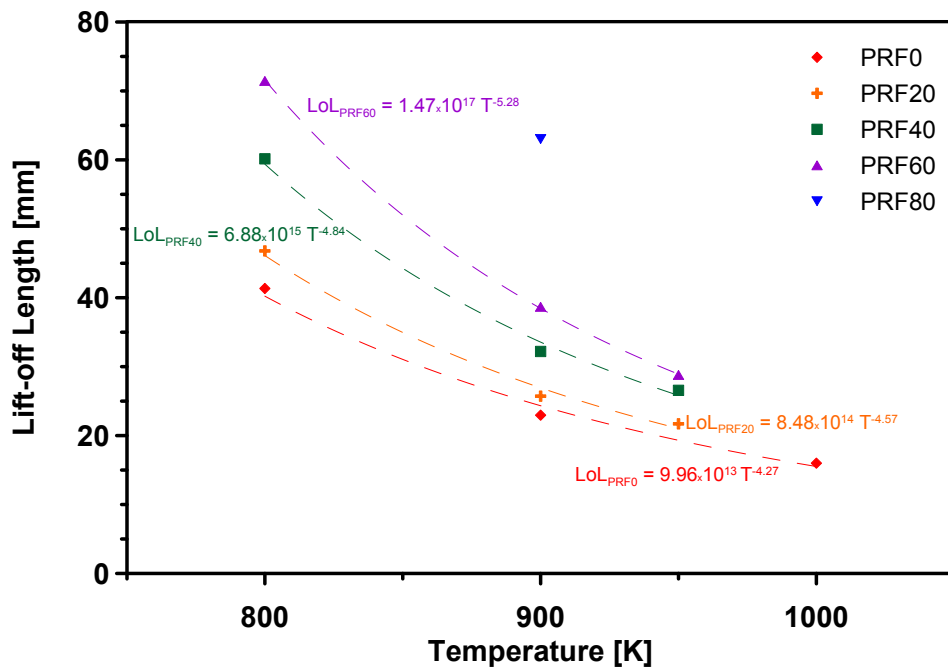


Figure 14: Lift-off length comparison under air temperature variation.

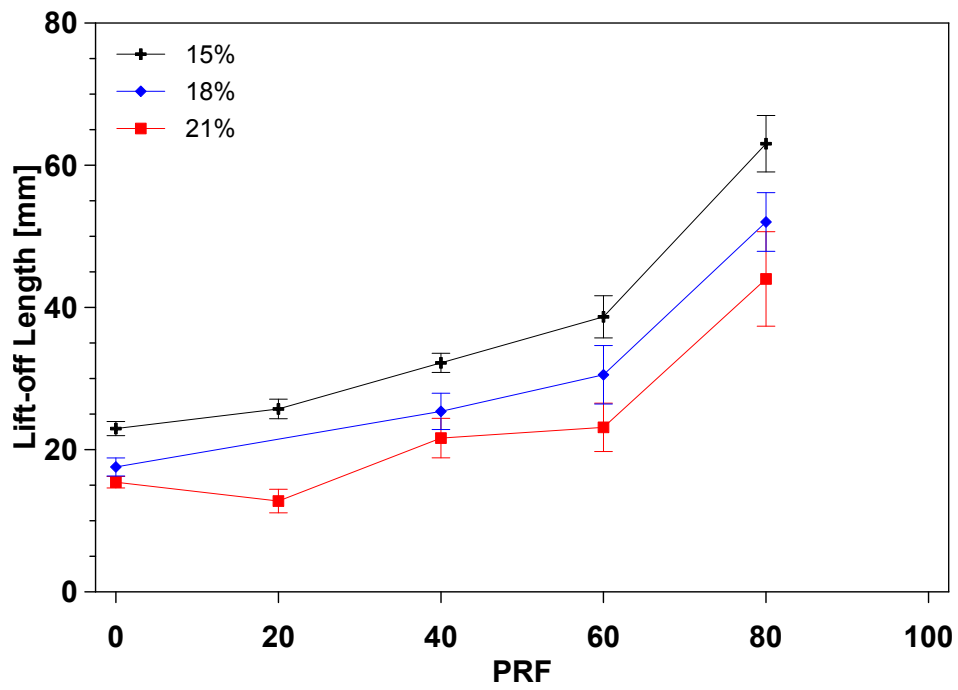


Figure 15: Lift-off length comparison under oxygen concentration variation.

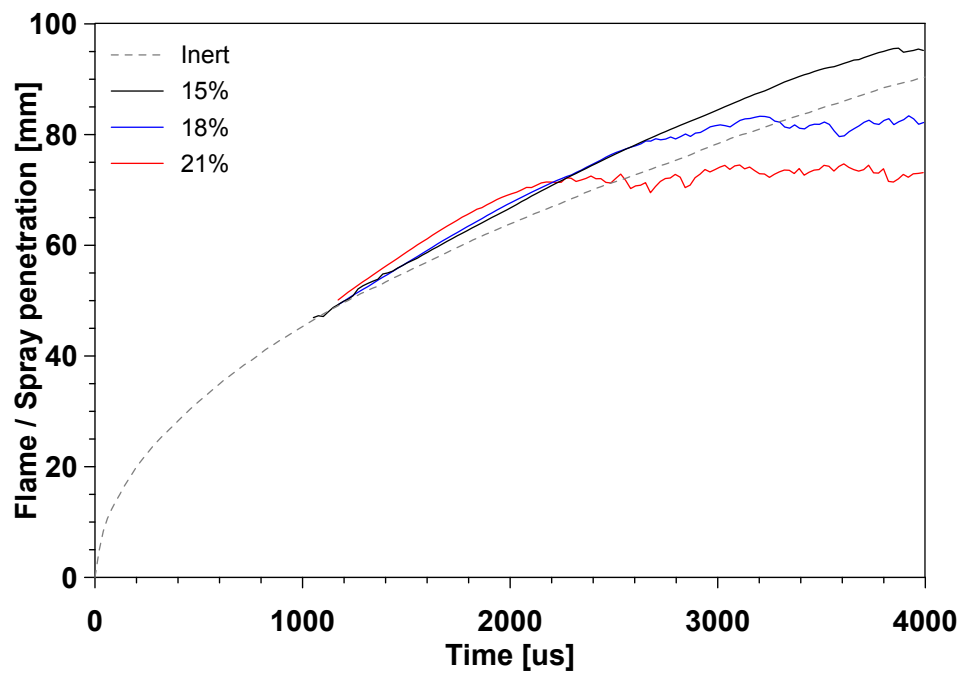


Figure 16: Flame length comparison for PRF0 under oxygen concentration variation at 900K with inert spray penetration, time after SoI.

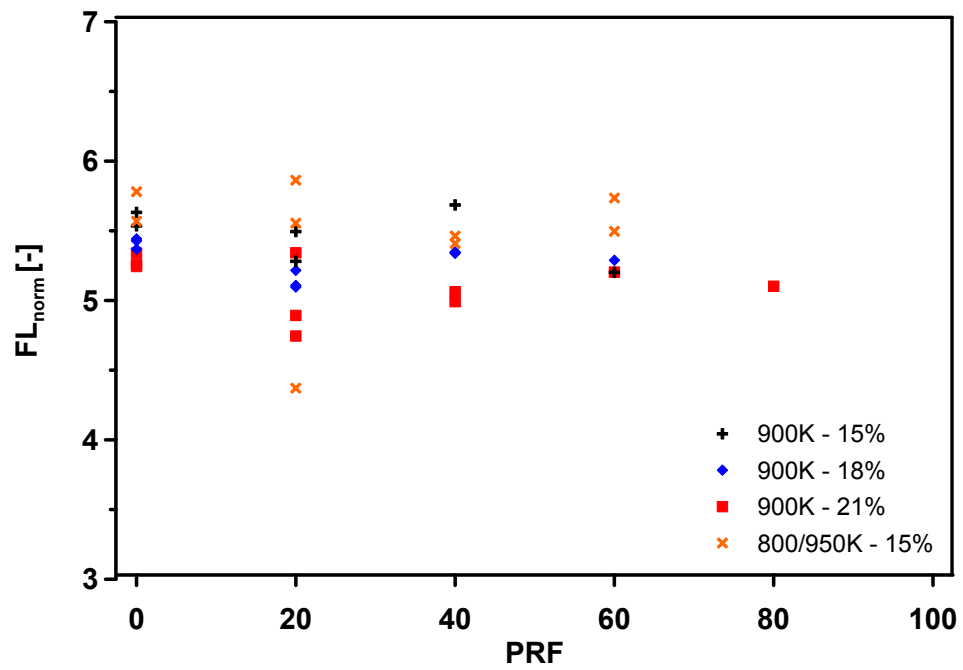


Figure 17: Normalized flame length (FL_{norm}) versus fuel composition at ambient temperature and oxygen concentration variations.

Table 1: Test matrix for parametric variation under reactive atmosphere. “A” indicates Spray-A standard conditions. All points performed at 150MPa of injection pressure and 22.8kg/m^3 of ambient density. *For PRF0, high temperature tests were performed at 1000K.

$O_2 \backslash T$	800K	900K	950K*
15%	X	A	X
18%		X	
21%		X	

Table 2: Test matrix for inert conditions. “A” indicates Spray-A standard conditions. All points performed at 150MPa of injection pressure and 0% of oxygen concentration.

$\rho \backslash T$	700K	800K	900K
$15.2kg/m^3$		X	
$22.8kg/m^3$	X	X	A
$45.6kg/m^3$		X	